# Quantum Physics

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# Contents

## Acknowledgements

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# 1    Introduction

Ancient Greek philosophers used to speculate (as early as 500 BC) on whether matter could be divided at infinitum or whether every material has a smallest part that still shares its properties, the atom (or more generally, the molecule). It took until the late 19-th century to answer this question affirmatively and decisively, mostly via chemistry, statistical mechanics and finally Brownian motion. Feynman was once asked the following question by a reporter: if we wanted to send a single message to extra-terrestrial life, showing the achievements of mankind on earth, what would it be ? His reply was *"matter is composed of atoms"*.

While a century ago, it was conclusively established that all matter is composed of atoms, it remained an open question as to what atoms themselves looked like, and if they themselves were composites of smaller parts, but whose nature is no longer the same as the atom itself. Of course, we now know that atoms are composed of a nucleus and electrons, and that the nucleus in turn is built from protons and neutrons, themselves built out of quarks and gluons.

Constructing a viable model for the electronic structure of atoms is what originally and primarily drove the development of quantum mechanics. *The existence and stability of atoms is a purely quantum mechanical effect.* Without the Pauli exclusion principle and the shell structure of electrons, we would loose the chemical and physical properties that distinguish different elements in the Mendeleev table, and there would be no chemistry as we know it. Similarly, the molecular and collective properties of conductors and insulators of heat and electricity have quantum origins, as do the semi-conductors used in building transistors and integrated circuits. Atomic and molecular spectral lines, observed from distant stars and nebulae, have allowed astronomers to conclude that the visible matter in the universe at large is the same as that found on earth. The systematic displacements of these lines inform us on the velocities and the distances of these objects. In summary, quantum physics and quantum phenomena are pervasive in modern science and technology.

## 1.1    Brief History

Physics known at the end of the 19-th century falls into three fields,

- classical mechanics (Newton, Euler, Lagrange, Hamilton, Leverrier, ...)
- electro-magnetism (Coulomb, Faraday, Ampère, Gauss, Maxwell, Lorentz, ...)
- statistical mechanics and thermodynamics (Joule, Carnot, Boltzmann, ...)

Around that time, Lord Kelvin apparently stated that physics just had a few loose ends to tie up, and that physics would be complete by 1900. Nothing

about by *special relativity*, which was invented to resolve a conflict between electro-magnetism and mechanics, and in doing so profoundly altered our concepts of space and time.

The most radical revolution, however, was quantum mechanics. The key experiments that were crucial in the development of quantum theory may be summarized as follows,

- discrete emission and absorption spectra of simple atoms (Balmer, ...);
- existence of radioactivity (Becquerel 1896);
- frequency dependence of back body radiation (Planck 1900);
- photo-electric effect (Einstein 1905);
- existence of a hard core (i.e. the nucleus) inside atoms (Rutherford 1909);
- incompatibility of the *planetary atom* with classical electrodynamics (Bohr 1913);
- discovery of strong and weak forces (Rutherford 1920);
- electrons diffract just as light does (de Broglie 1923);
- need for a Pauli exclusion principle in the Bohr model of atoms (Pauli 1925);
- Goudsmit and Uhlenbeck discover *spin* (1925).

This wealth of novel experimental facts and their apparent contradiction with (classical mechanics and electromagnetic) theory led to the formal development of quantum mechanics,

- 1925 : Heisenberg introduces *matrix mechanics*, and quantized the harmonic oscillator;
- 1926 : Schrödinger invents *wave mechanics* (inspired by de Broglie's particle/wave duality), and shows the equivalence of matrix and wave mechanics;
- 1927 : Dirac gives what is to be the present day formulation of quantum mechanics.

Subsequent developments include primarily the development of *quantum field theory*, a theory which unifies quantum mechanics and special relativity. Its foundations were laid in 1928 by Dirac, Heisenberg and Pauli, but its elaboration continues actively still today. It is important to realize though that there has been no serious need since 1927 to alter the fundamental principles of quantum mechanics, either for experimental or theoretical reasons.

For extensive accounts of the history and conceptual development of quantum mechanics, the reader is referred to the books by Jammer and by Pais.

## 1.2   Constants of Nature

There are three fundamental dimensionful constants in Nature: the speed of light $c$, Planck's constant $\hbar = h/2\pi$, and Newton's constant of gravity $G_N$. Their values are given by

$$
\begin{aligned}
c &= 2.99792 \times 10^8 \ m/s \\
\hbar &= 1.05457 \times 10^{-34} \ Js \\
G_N &= 6.6732 \times 10^{-11} \ Jm/(kg)^2
\end{aligned}
$$

Instead of Joules $(J)$, one often uses electron-volts $(eV)$ to express energy; the two are related by $1\ eV = 1.60219 \times 10^{-19}\ J$. All other dimensionful constants are either artifacts of the units used (such as the Boltzmann constant $k_B$, which converts temperature to energy by $k_B T$) or composites (such as Stefan-Boltzmann's constant $\sigma = \pi^2 k_B^4/60 c^2 \hbar^3$).

Using $c$ to convert a frequency $\nu$ into a wavelength $\lambda$ by $\lambda = c/\nu$ and vice-versa, and $\hbar$ to convert frequency into energy $E$ by $E = h\nu$ and vice-versa, all length scales, times and energies may be converted into one another. Finally, with the help of Einstein's relation $E = mc^2$, we may also convert a rest mass $m$ into an energy $E$. It is therefore common practice to describe masses, times and length-scales all in $eV$.

The role of Newton's gravitational constant $G_N$ is actually to set an absolute scale (the so-called Planck scale) of energy $E_P$, (and thus of mass, length, and time), whose value is $E_P = (\hbar c/G_N)^{1/2} = 1.22 \times 10^{19}\ GeV$. This energy scale is very much larger than the highest energies reachable by particle accelerators today (only about $10^3\ GeV$), and corresponds to and energy where quantum effects in gravity become strong. In this course, gravitational effects will always be neglected.

## 1.3  Scales

The orders of magnitude of the length scales of the known world are as follows,

| Object | size in $m$ |
| --- | --- |
| known Universe | $10^{26}$ |
| Milky Way | $10^{21}$ |
| Earth's orbit around Sun | $10^{11}$ |
| Earth | $10^{7}$ |
| human | $1$ |
| grain of salt | $10^{-4}$ |
| wavelength of visible light | $5 \times 10^{-7}$ |
| atom | $10^{-10}$ |
| Lead nucleus | $10^{-14}$ |
| strong interaction scale (mass of the proton) | $10^{-15}$ |
| weak interaction scale (mass of $W^{\pm}/Z$) | $10^{-17}$ |
| Planck length | $10^{-34}$ |

Quantum mechanics is crucial to understand physics at atomic scales and smaller, but may also govern certain larger objects. The macroscopic structure of a neutron star, for example, is quantum mechanical. To date, there appear to be no compelling experimental results that vitiate the validity of quantum mechanics at all length scales.

## 1.4   Reductionism

The success of modern science, including physics, is due to ever advancing experimentation, as well as to the success of the reductionist approach to understanding the Universe. The basic assumption is that the behavior of larger objects may be determined, at least in principle, in terms of the dynamics and interactions of its constituents. Thus, the structure of a molecule can be understood in terms of the dynamics of the atoms out of which it is built. The structure of the atoms and the strength of their mutual interactions can, in principle, be calculated from the quantum electro-dynamics of electrons and nuclei. The structure of the nuclei is governed by the strong and electro-magnetic forces between their proton and neutron constituents, whose own structure may be understood in terms of quarks and gluons.

Does this mean that we need to control the dynamics of quarks and gluons in order to understand semi-conductors, for example ? Remarkably, the answer is no, at least in most circumstances. *The reason is that physics at two widely different length scales (or equivalently energy scales) tends to decouple from one another.* For most of chemistry, you do not need to know the detailed nuclear structure of the atoms in the molecules, and it is enough to know their mass, charge and spin. Occasionally though, such as with radioactive nuclei, the nuclear structure and its modifications under radioactivity do have chemical consequences.

In summary, we shall be able to go a long way in describing Nature if we can understand well various dramatically simplified approximations to a problem. Such simplified cases give *models* for physical behavior. A good model will capture the essence of the physical phenomenon while relaying to the background less important and/or more complicated aspects. In this course, we shall use such simplified models throughout.

# 2 Two-state quantum systems

The configuration of a quantum system is described in terms of a *quantum state*. The bound states of the electron in a Hydrogen atom, organized in various shells, all correspond to different quantum states which an electron can occupy, for example. Here, we shall start the description of quantum states by specializing to the simplest non-trivial systems which have only 2 quantum states. All the fundamental principles of quantum mechanics and of quantum measurement can be dealt with simply and concisely, on the basis of this simple example.

We shall look at two different systems: the polarization of light, and the spin 1/2 degree of freedom of the electron. Assuming the wave vector $\mathbf{k}$ of light to be fixed, the photon can be in precisely two polarization states; similarly, with the electron momentum $\mathbf{p}$ fixed, the electron has only the spin 1/2 degree of freedom left. As we shall see below, each system will have just two states.

## 2.1 Polarization of light

Consider light propagating along the $z$ direction, with wave number $k = |\mathbf{k}|$ and frequency $\omega = ck$. *Classically*, light is an electro-magnetic wave, whose electric and magnetic fields are transverse to $\mathbf{k}$, and thus lie in the $xy$ plane. A *polarizer* is a planar material that, when inserted into a beam[1] and orthogonally to it, transmits only light whose electric field is along the direction of the polarizer. Light whose polarization direction is perpendicular to the polarization direction is absorbed by the polarizer and converted into heat.

We shall denote this polarization direction by the angle $\theta$ with the $x$ axis. The electric field $\mathbf{E} = (E_x, E_y, 0)$ of this wave is linearly polarized, and has

$$
\begin{aligned}
E_x &= E_0 \cos\theta \, \cos(\omega t - kz) \\
E_y &= E_0 \sin\theta \, \cos(\omega t - kz)
\end{aligned}
\tag{2.1}
$$

An *analyzer* is a second polarizer, but whose polarization direction is $\alpha$, depicted in figure 1. The electric field of the light emerging from the analyzer is the result of projecting the electric field that emerges from the polarizer onto the polarization direction $\alpha$ of the analyzer,

$$
\begin{aligned}
E_x &= E_0 \cos\alpha \, \cos(\theta - \alpha) \, \cos(\omega t - kz) \\
E_y &= E_0 \sin\alpha \, \cos(\theta - \alpha) \, \cos(\omega t - kz)
\end{aligned}
\tag{2.2}
$$

If the light intensity emerging from the polarizer was $N$, then the light intensity emerging from the analyzer will be $N\cos^2(\theta - a)$.

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[1] Light in a beam is strictly speaking a wave packet, whose wave vector has a small dispersion around $\mathbf{k}$.

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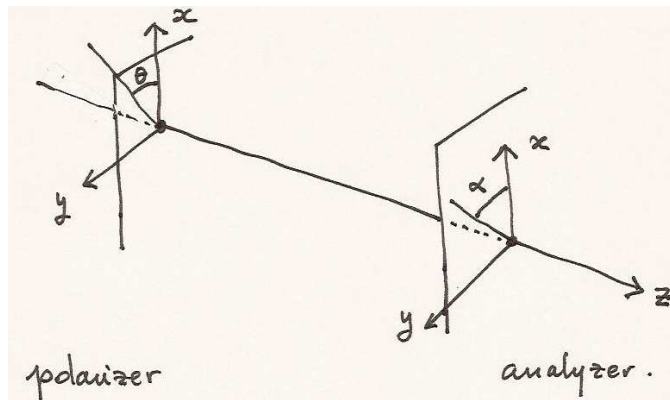
Figure 1: Polarizer and analyzer set-up

A more elaborate tool is a *birefringent plate*, which may again be inserted into the beam and orthogonally to it, and which now transmits light which is polarized parallel to the optical axis along one path, but transmits light polarized perpendicularly to the optical axis along a different path.
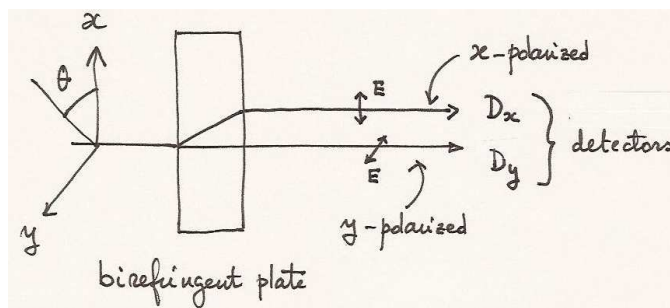


Figure 2: Polarizer and birefringent plate set-up

Light emerging from the polarizer with polarization angle $\theta$ and intensity $N$, will be split by the birefringent plate into two beams: one polarized along the $x$-direction, the other along the $y$-direction. The intensities of these beams may be measured by two detectors $D_x$ and $D_y$, and are found to be,

$$
\begin{aligned}
N_x &= N \cos^2 \theta \\
N_y &= N \sin^2 \theta
\end{aligned}
\tag{2.3}
$$

Here, we are assuming an idealized birefringent plate, for which no light intensity is lost during transmission, so that $N = N_x + N_y$. Note that a birefringent plate may be converted into a polarizer by dumping one of its exit beams.

## 2.2   Polarization of photons

The entire discussion of the preceding subsection has concentrated on the behavior of classical waves. Einstein's explanation of the photo-electric effect (1905) demonstrates that light is actually composed of individual quanta (*photons*), whose behavior is that of particles. If the light intensity is sufficiently reduced, it actually becomes possible to study individual photons, and to access the quantum behavior of the polarization degree of freedom of photons.[2]   The intensity of a beam, such as $N$, is then given by the number of photons (per second). A *measurement* will consist simply in counting the number of photons in a given beam, and thereby yielding the intensity of that beam.

We now list the key experimental observations which point to the key ingredients of quantum behavior.

**(1)** From observing individual photons, it is found that the detectors for $x$-polarization and for $y$-polarization are never triggered simultaneously. Thus, we must conclude that the entire photon emerging from the birefringent plate either has $x$-polarization or $y$-polarization.

**(2)** It is *impossible* to predict whether a photon incident on the birefringent plate will trigger detector $D_x$ or detector $D_y$ (unless $\theta = 0, \pi$, as we shall see later). Instead, a photon will reach detector $D_x$ and $D_y$ with certain probabilities $p_x$ and $p_y$. In the limit where the number of photons $N$ becomes very large, the probabilities are given by

$$
\begin{aligned}
p_x &= \lim_{N \to \infty} (N_x/N) = \cos^2 \theta \\
p_y &= \lim_{N \to \infty} (N_y/N) = \sin^2 \theta
\end{aligned}
\tag{2.4}
$$

The relation $N = N_x + N_y$, obtained previously for an ideal birefringent plate, translates then to the conservation of probability $p_x + p_y = 1$.

**(3)** The rule according to which probabilities combine may be inferred from an experiment in which the beam of photons is first split and then recombined using two birefringent plates, depicted in Fig. 3.

We assume that the intensity of the light beam emerging from the polarizer is $N$. The first birefringent plate splits the beams into $x$ and $y$ polarizations, which are recombined by the second birefringent plate (whose optical axis is opposite to the one of the first plate), thus reproducing the original beam. From this consideration, it is clear that the intensity

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[2]With present day technology of photo-multipliers and CCD (charge coupling devices), it is possible to detect individual photons, one by one. Actually, even the human retina is capable of detecting single photons, though very few of the photons that reach the retina will actually stimulate a molecule of visual pigment (rhodopsin), producing a perception.
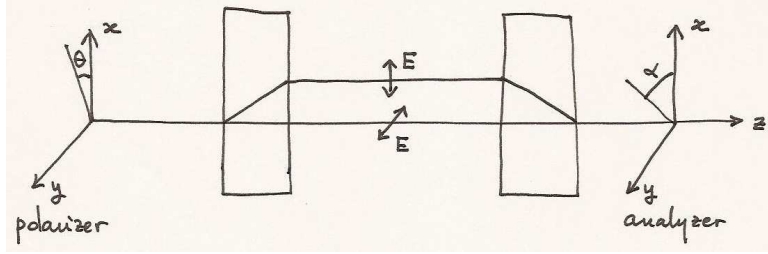
Figure 3: Experiment with two birefringent plates

found after the analyzer will be $N \cos^2(\theta - \alpha)$. Translated into probabilities, the original beam has probability 1, and the analyzer will find polarization angle $\alpha$ with probability

$$p_{\text{tot}} = \cos^2(\theta - \alpha) \tag{2.5}$$

But a different way in which to evaluate this same probability is to combine the probabilities as the light traverses the two birefringent plates.

If probabilities combined according to classical rules, we would find the following sequence. After the first, but before the second birefringent plate, the probability that the photon has polarizations $x$ or $y$ is given by (2.4). After the second plate, the probabilities that the $x$ and $y$ polarized beam yield polarization angle $\alpha$ in the analyzer is

$$\begin{aligned}
p'_x &= \cos^2 \alpha \\
p'_y &= \sin^2 \alpha
\end{aligned} \tag{2.6}$$

According to the classical rules, the combined probability would be

$$p'_{\text{tot}} = p_x p'_x + p_y p'_y = \cos^2 \theta \cos^2 \alpha + \sin^2 \theta \sin^2 \alpha \tag{2.7}$$

which is in disagreement with $p_{\text{tot}} = \cos^2(\theta - \alpha)$ for general $\theta$ and $\alpha$. In fact, we have $p_{\text{tot}} - p'_{\text{tot}} = 2 \cos \theta \sin \theta \cos \alpha \sin \alpha$. This is an interference term: it arises from the fact that when the two beams from birefringent plate 1 recombine, they interfere, just as the electric fields of electro-magnetic waves did. Although photons behave like particles in that they form discrete quanta, their probabilities combine like waves. This is an aspect of the particle/wave duality of quantum mechanics.

**(4)** The correct rule for the combination of probabilities is given in terms of the *probability amplitudes* $a_x, a_y, a'_x, a'_y$, related to the previously defined probabilities by

$$\begin{aligned}
p_x &= |a_x|^2 & p'_x &= |a'_x|^2 \\
p_y &= |a_y|^2 & p'_y &= |a'_y|^2
\end{aligned} \tag{2.8}$$

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In our context, these are given by $a_x = \cos\theta$, $a_y = \sin\theta$, and $a'_x = \cos\alpha$, $a'_y = \sin\alpha$. The total amplitude results from linearly combining these partial amplitudes,

$$
\begin{aligned}
a_{\text{tot}} &= a_x a'_x + a_y a'_y \\
&= \cos\theta \cos\alpha + \sin\theta \sin\alpha \\
&= \cos(\theta - \alpha)
\end{aligned}
\tag{2.9}
$$

Thus, the probability amplitudes satisfy a *linear superposition principle*.

The total probability $p_{\text{tot}}$ is given in terms of the probability amplitude $a_{\text{tot}}$ by,

$$
p_{\text{tot}} = |a_{\text{tot}}|^2 = \cos^2(\theta - \alpha)
\tag{2.10}
$$

which is now in agreement with the result from electro-magnetic wave theory.

## 2.3 General parametrization of the polarization of light

The polarization of light and photons described above is not the most general one. The most general polarization (at fixed wave vector $\mathbf{k}$) has the electric field given by

$$
\begin{aligned}
E_x &= E_0 \cos\theta \cos(\omega t - kz - \delta_x) = E_0 \text{Re}(a_x e^{-i\omega t + ikz}) \\
E_y &= E_0 \sin\theta \cos(\omega t - kz - \delta_y) = E_0 \text{Re}(a_y e^{-i\omega t + ikz})
\end{aligned}
\tag{2.11}
$$

By time-translation and periodicity, it is clear that only the difference in phases $\delta_x - \delta_y$ modulo $2\pi$ is physically significant. When $\theta = \pm\pi/4$, and $\delta_x - \delta_y = \pm\pi/2$, this is circular polarization, while for general values, it is elliptical, and we have

$$
\begin{aligned}
a_x &= \cos\theta \; e^{i\delta_x} \\
a_y &= \sin\theta \; e^{i\delta_y}
\end{aligned}
\tag{2.12}
$$

The complex two-component vector $(a_x, a_y)$ obeys $|a_x|^2 + |a_y|^2 = 1$ and its phase is physically immaterial, thus leaving two real parameters.

## 2.4 Mathematical formulation of the photon system

The combination of the polarizer and birefringent plate demonstrates that photons with polarization angle $\theta$ decompose into $x$- and $y$-polarization for all $\theta$, the only difference being the relative intensity of these components. The photon states with $x$- and $y$-polarizations will be represented mathematically by two vectors $|x\rangle$ and $|y\rangle$ in a two-dimensional complex vector space $\mathcal{H}$. In the system of a polarizer and analyzer, the state $|x\rangle$ corresponds to the

polarization angle $\theta = \alpha = 0$, while the state $|y\rangle$ corresponds to $\theta = \alpha = \pi/2$. From this correspondence, we deduce the probabilities, and probability amplitudes,

$$p\left(|x\rangle \rightarrow |x\rangle\right) = p\left(|y\rangle \rightarrow |y\rangle\right) = 1 \quad \Rightarrow \quad \langle x|x\rangle = \langle y|y\rangle = 1$$
$$p\left(|x\rangle \rightarrow |y\rangle\right) = p\left(|y\rangle \rightarrow |x\rangle\right) = 0 \quad \Rightarrow \quad \langle x|y\rangle = \langle y|x\rangle = 0 \tag{2.13}$$

Here $\langle \ | \ \rangle$ denotes the Hermitian inner product in the two-dimensional complex vector space $\mathcal{H}$ (we shall define this Dirac notation more carefully soon). Thus, the states $|x\rangle$ and $|y\rangle$ form an orthonormal basis for $\mathcal{H}$.

The polarizer-birefringent plate experiment, and the linear superposition principle, show that a photon with arbitrary polarization angle $\theta$ corresponds to a state in $\mathcal{H}$ which is a linear combination of the states $|x\rangle$ and $|y\rangle$,

$$|\theta\rangle = a_x|x\rangle + a_y|y\rangle \tag{2.14}$$

for complex coefficients $a_x$ and $a_y$. As we have seen earlier, conservation of probability requires the relation $|a_x|^2 + |a_y|^2 = 1$. Actually, the coefficients $a_x$ and $a_y$ are nothing but the probability amplitudes to find the photon $|\theta\rangle$ in either state $|x\rangle$ or state $|y\rangle$, $a_x = \langle x|\theta\rangle$ and $a_y = \langle y|\theta\rangle$. Conservation of probability thus leads to

$$|\langle x|\theta\rangle|^2 + |\langle y|\theta\rangle|^2 = 1 \tag{2.15}$$

so that the state $|\theta\rangle$ has also unit norm, $\langle\theta|\theta\rangle = 1$. It follows that we have a formula for $\langle\theta|$, for any values of $a_x$ and $a_y$, given by

$$\langle\theta| = a_x^*\langle x| + a_y^*\langle y| \tag{2.16}$$

where $*$ denotes complex conjugation.

We are now in a position to give the mathematical formulation for all the polarizer-analyzer-birefringent plate experiments described earlier. The polarizer and analyzer prepare a photon in a definite state, given respectively by the state vectors

$$\begin{aligned} |\theta\rangle &= \cos\theta \ |x\rangle + \sin\theta \ |y\rangle \\ |\alpha\rangle &= \cos\alpha \ |x\rangle + \sin\alpha \ |y\rangle \end{aligned} \tag{2.17}$$

The probability amplitude to observe the $|\theta\rangle$ photon in the states $|x\rangle$ and $|y\rangle$ after the birefringent plate, and $|\alpha\rangle$ after the analyzer are given respectively by

$$\begin{aligned} a_x &= \langle x|\theta\rangle = \cos\theta \\ a_y &= \langle y|\theta\rangle = \sin\theta \\ a_{\text{tot}} &= \langle\alpha|\theta\rangle = \cos(\theta - \alpha) \end{aligned} \tag{2.18}$$

The instruments of the polarizer, analyzer (which, recall, is just a polarizer) and the bire-fringent plate have mathematical interpretations as *linear operators on* $\mathcal{H}$. Quite literally, the analyzer transforms photons in the state $|\theta\rangle$ to photons in state $|\alpha\rangle$ with probability amplitude $\langle\theta|\alpha\rangle$. Mathematically, this corresponds to a projection of the state $|\theta\rangle$ onto the state $|\alpha\rangle$, and may be represented by the operator,

$$P_\alpha = |\alpha\rangle\langle\alpha| \tag{2.19}$$

This is a projection operator because we have $P_\alpha^2 = P_\alpha$, and applying $P_\alpha$ to $|\theta\rangle$ yields $|\alpha\rangle\langle\alpha|\theta\rangle$. The birefringent plate transforms photons in state $|\theta\rangle$ into two separate beams, one corresponding to $P_x|\theta\rangle$, the other to $P_y|\theta\rangle$. Recombining the two beams with the second birefringent plate, subject to the linear superposition principle of the photon states, yields

$$|\theta\rangle \quad \rightarrow \quad (P_x + P_y)|\theta\rangle \tag{2.20}$$

but in view of $P_x P_y = 0$, the sum of the two projection operators is the unit matrix $I$ in $\mathcal{H}$, namely $P_x + P_y = I$. Indeed, the beam emerging from the system of two birefringent plates is really the same beam that went into that system.

## 2.5    The Stern-Gerlach experiment on electron spin

A number of other two-state quantum systems are often used to bring the key principles of quantum physics to the fore. Feynman discusses the famous two-slit interference experiment on electrons. Here, we shall concentrate on the Stern-Gerlach (SG) experiment in which the two states are those of the spin 1/2 degree of freedom of an electron (carried by a silver atom in the SG experiment). We choose this case because earlier we illustrated the photon behavior of the classical electro-magnetic wave, while in SG, we illustrate the wave behavior of a classical particle. The SG also differs from the photon case in that the electron spin is itself already a purely quantum phenomenon with no classical counterpart.

The physical system of interest is the spin and magnetic moment of the electron. Angular momentum and magnetic moments of course also arise in classical mechanics, but they are both invariably associated with orbital motion. As far as we know, the electron is a point-like particle, with no room for internal orbital angular momentum. It is a purely quantum effect that the electron can nonetheless have non-vanishing angular momentum $\mathbf{S}$, and magnetic moment $\mathbf{m}$. Both quantities are actually related by

$$\mathbf{m} = g\left(\frac{e}{2mc}\right)\mathbf{S} \tag{2.21}$$

Here, $e$ is the unit of electric charge, $m$ is the mass, and $g$ is the so-called $g$-factor, which equals 2.00 for electrons, 5.58 for protons, and $-3.82$ for neutrons.
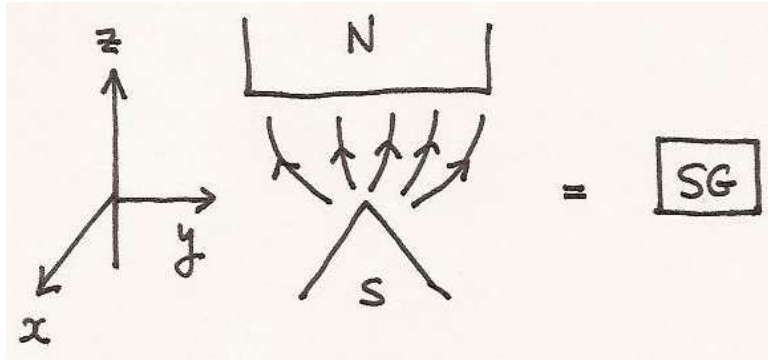
Figure 4: The Stern-Gerlach apparatus

SG deals with measuring $\mathbf{S}$, or equivalently $\mathbf{m}$. To measure $\mathbf{m}$, we place it in a magnetic field $\mathbf{B}$, which produces an energy dependence $E$ and a force $\mathbf{F}$ on the electron, given by

$$E = -\mathbf{m} \cdot \mathbf{B} \qquad \mathbf{F} = \vec{\nabla}\left(\mathbf{m} \cdot \mathbf{B}\right) \tag{2.22}$$

Thus, a magnetic moment placed in an inhomogeneous magnetic field will experience a force, which will lead to bending of the trajectory and is observable. To create an inhomogeneous magnetic field, one uses asymmetrical poles, as in the figure above. Henceforth, the entire SG apparatus will simply be represented by a box, as in the figure. A beam of neutral silver atoms is now sent trough the SG apparatus (along the $x$-axis) and the signal is received on a screen placed perpendicularly to the beam.
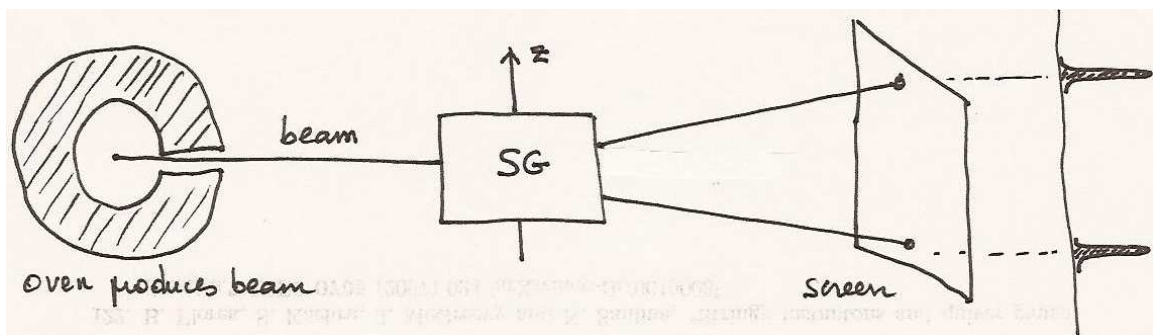


Figure 5: The Stern-Gerlach experimental set-up

The experimental outcomes are as follows,

**(1)** With a strong magnetic field, the signal of the individual atoms emerging from SG is centered sharply on two outcomes, which correspond to opposite values of the magnetic moment. The detectors counting the number of atoms for each outcome are never triggered simultaneously. Thus each silver atom must have $+$ or $-$ value for the spin.

**(2)** The observed values of spin are along the $z$-axis (which is the N-S direction of the magnet in SG), and take only two possible values,

$$S_z = \pm \hbar/2 \tag{2.23}$$

For a given atom entering the SG apparatus, it is impossible to predict whether the outcome will be $+$ or $-$. The SG apparatus on spin is precisely analogous to the birefringent plate for the photon. The analog of a polarizer at angle $\theta$ for the photon is an SG apparatus rotated by an angle $\theta$ with respect to the $z$-axis, and with one of the two outgoing beams blocked.

**(3)** The following experimental set-ups again exemplify the quantum behavior of the spins.
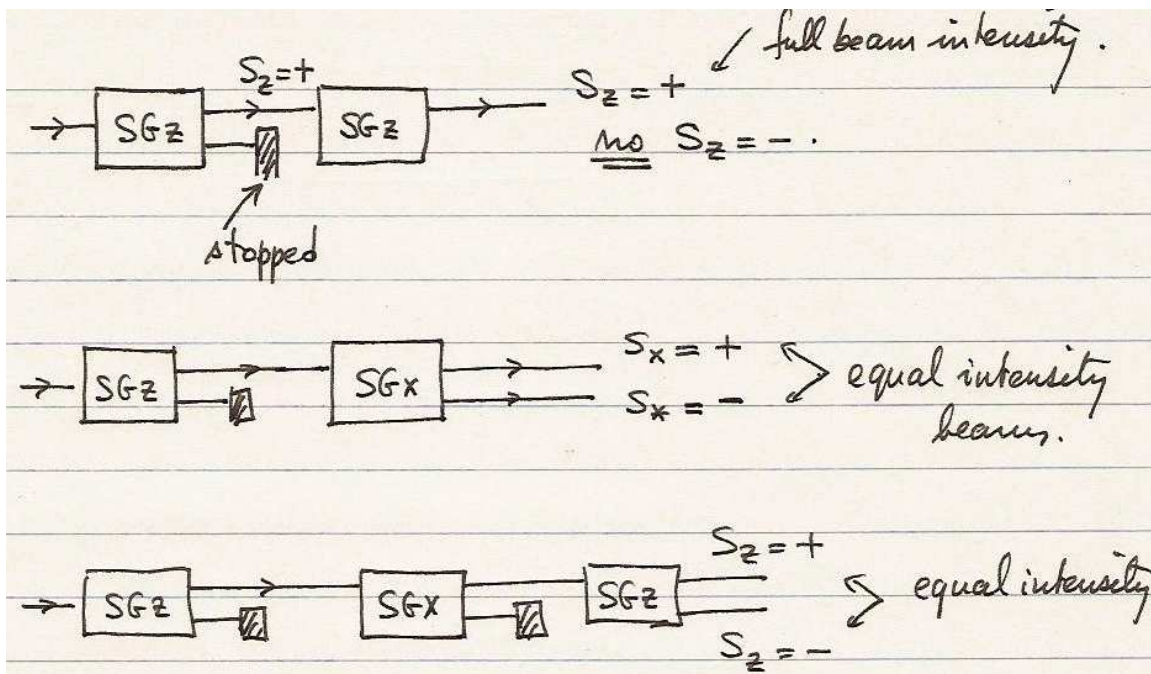


Figure 6: The Stern-Gerlach experiment with multiple SG separators

The first set-up shows that a spin prepared in state $S_z = +\hbar/2$ remains in state $S_z = +\hbar/2$. The second set-up shows that a spin prepared in state $S_z = +\hbar/2$ yields with equal

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probability spins $S_x = \pm\hbar/2$. The third set-up shows how successive SG apparatus in $z$, $x$ and then again in $z$ directions regenerate spins with $S_z = -\hbar/2$ from an incoming beam of purely $S_z = +\hbar/2$.

All these phenomena are accounted for quantitatively by describing the spin as a two-state quantum system, built on a two-dimensional complex vector space with an inner product to yield the transition amplitudes.

# 3 Mathematical Formalism of Quantum Physics

We begin by reviewing the mathematical formalism of quantum physics, including Hilbert spaces of finite and infinite dimensions, and of linear operators acting on Hilbert spaces. Those in hand, we shall give the postulates of quantum physics in the next section.

## 3.1 Hilbert spaces

A Hilbert space $\mathcal{H}$ is a complex vector space, endowed with a Hermitian positive definite inner product, denoted by $(\cdot, \cdot)$. For finite-dimensional $\mathcal{H}$, this definition will be complete, while for infinite-dimensional $\mathcal{H}$, some additional convergence properties will have to be supplied. We shall use the Dirac notation, and denote the vectors in $\mathcal{H}$ by *kets* $|u\rangle, |v\rangle$ etc.

- The fact that $\mathcal{H}$ is a complex vector space requires that

$$
\begin{aligned}
(\alpha + \beta)|u\rangle &= \alpha|u\rangle + \beta|u\rangle \\
\alpha(|u\rangle + |v\rangle) &= \alpha|u\rangle + \alpha|v\rangle \\
(\alpha\beta)|u\rangle &= \alpha(\beta|u\rangle)
\end{aligned}
\tag{3.1}
$$

for all $|u\rangle, |v\rangle \in \mathcal{H}$ and for all $\alpha, \beta \in \mathbf{C}$.

- A Hermitian inner product $(\cdot, \cdot)$ is a map from $\mathcal{H} \times \mathcal{H} \to \mathbf{C}$, such that

$$
\begin{aligned}
(|v\rangle, |u\rangle) &= (|u\rangle, |v\rangle)^* \\
(|u\rangle, \alpha|v\rangle + \beta|w\rangle) &= \alpha\,(|u\rangle, |v\rangle) + \beta\,(|u\rangle, |w\rangle) \\
(\alpha|u\rangle + \beta|v\rangle, |w\rangle) &= \alpha^*\,(|u\rangle, |w\rangle) + \beta^*\,(|v\rangle, |w\rangle)
\end{aligned}
\tag{3.2}
$$

The inner product is linear in the second entry, but *anti-linear* in the first entry. The inner product notation $(\cdot, \cdot)$ is primarily a notation of mathematicians. In physics instead, we use the notation invented by Dirac,

$$
\underset{\text{bra ket}}{\langle v|u\rangle \equiv (|v\rangle, |u\rangle)}
\tag{3.3}
$$

This notation actually also has mathematical significance, as it leads naturally to interpret a *bra* $\langle v|$ as a *linear form on* $\mathcal{H}$. The space of all (continuous) linear forms on $\mathcal{H}$ is by definition the Hilbert space dual to $\mathcal{H}$, and is denoted $\mathcal{H}^+$.

- Positive definiteness of the inner product means that

$$
\begin{aligned}
\langle u|u\rangle = (|u\rangle, |u\rangle) \equiv ||u||^2 &\geq 0 \qquad\qquad \text{for all } |u\rangle \in \mathcal{H} \\
\langle u|u\rangle = 0 \;&\Rightarrow\; |u\rangle = 0
\end{aligned}
\tag{3.4}
$$

Here, $|u\rangle = 0$ stands for the unit element $0$ under the addition of the vector space $\mathcal{H}$.

• The norm on $\mathcal{H}$ provides with a natural notion of distance, which induced the distance topology on $\mathcal{H}$, and allows us to investigate the convergence of sequences in $\mathcal{H}$. The definition of Hilbert space includes the requirement that $\mathcal{H}$ be a *complete space*.

By definition, a space $\mathcal{H}$ is complete if every Cauchy sequence $\{|u_n\rangle\}_{\{n\}} \subset \mathcal{H}$ converges. (Recall that a sequence $\{|u_n\rangle\}_{\{n\}} \subset \mathcal{H}$ is a Cauchy sequence provided $||u_m - u_n|| \to 0$ if $m, n \to \infty$ implies that there exists a $|u\rangle \in \mathcal{H}$ such that the sequence converges to $|u\rangle$, namely $||u_n - u|| \to 0$ as $n \to \infty$.) This property is automatic when the dimension of $\mathcal{H}$ is finite, but is an extra requirement when the dimension is infinite.

• The Hilbert spaces in quantum mechanics are required to be *separable*, which means that they admit a countable orthonormal basis. If the number of orthormal basis vectors of a separable Hilbert space $\mathcal{H}$ is $N < \infty$, then $\mathcal{H}$ is isomorphic to $\mathbf{C}^N$. On the other hand, all separable Hilbert spaces of infinite dimension are isomorphic to one another.

### 3.1.1 Triangle and Schwarz Inequalities

The distance defined by the norm satisfies the triangle inequality,

$$||u + v|| \leq ||u|| + ||v|| \tag{3.5}$$

for all $|u\rangle, |v\rangle \in \mathcal{H}$, which in turn implies the Schwarz inequality,

$$|\langle u|v\rangle| \leq ||u|| \cdot ||v|| \tag{3.6}$$

Both may be shown using the following arguments. If $|v\rangle = 0$, both inequalities hold trivially. Henceforth, we shall assume that $|v\rangle \neq 0$. Positivity of the norm implies that for any complex number $\lambda$, we have

$$0 \leq ||u + \lambda v||^2 = ||u||^2 + |\lambda|^2 ||v||^2 + \lambda \langle u|v\rangle + \lambda^* \langle u|v\rangle^* \tag{3.7}$$

We now choose the phase of $\lambda$ to be such that $\lambda \langle u|v\rangle$ is real and negative; as a result, $\lambda \langle u|v\rangle = -|\lambda||\langle u|v\rangle|$. Using the fact that $|v\rangle \neq 0$, we may choose $|\lambda| = ||u||/||v||$. Substituting the corresponding value for $\lambda$ into (3.7) immediately yields (3.6). Using now $\lambda = 1$ in (3.7) and bounding $|\langle u|v\rangle|$ using the Schwarz inequality readily gives (3.5).

### 3.1.2 The construction of an orthonormal basis

Hilbert spaces of finite dimension and separable Hilbert spaces of infinite dimension share the property that one can construct an orthonormal basis using the Gramm-Schmidt procedure. Let $\{|u_n\rangle\}_n$ be a basis of $\mathcal{H}$, where $n$ either runs over the finite set $\{1, 2, \cdots, N\}$ or over all

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of $\mathbf{N}$ (the set of positive integers). The Gramm-Schmidt procedure goes as follows. We start with the first vector and normalize it,

$$|1\rangle = |u_1\rangle/||u_1|| \tag{3.8}$$

To construct the second vector $|2\rangle$ of the orthonormal basis, we project $|u_2\rangle$ onto the space perpendicular to $|1\rangle$, and normalize the resulting vector,

$$|v_2\rangle = |u_2\rangle - |1\rangle\langle 1|u_2\rangle \qquad\qquad |2\rangle = |v_2\rangle/||v_2|| \tag{3.9}$$

This process may be continued recursively as follows. Given the first $m$ orthonormal vectors $\{|1\rangle, |2\rangle, \cdots, |m\rangle\}$, one constructs $|m+1\rangle$ by the same process,

$$|v_{m+1}\rangle = |u_{m+1}\rangle - \sum_{i=1}^{m} |i\rangle\langle i|u_{m+1}\rangle \qquad\qquad |m+1\rangle = |v_{m+1}\rangle/||v_{m+1}|| \tag{3.10}$$

When the dimension of $\mathcal{H}$ is finite, this process terminates. Separability of the Hilbert space $\mathcal{H}$ in the infinite-dimensional case guarantees that even in this case, the process will converge.

### 3.1.3 Decomposition of an arbitrary vector

Therefore in any finite-dimensional or separable infinite dimensional Hilbert space, we may decompose any vector $|\varphi\rangle$ onto a countable orthonormal basis,

$$|\varphi\rangle = \sum_n c_n|n\rangle \tag{3.11}$$

where $c_n$ are complex numbers given by $\langle n|\varphi\rangle$. It is often convenient to leave the range for $n$ unspecified, so that we can simultaneously deal with the case of finite and infinite dimensions. Since by definition of the Hermitian inner product, we have $\langle \varphi|n\rangle = \langle n|\varphi\rangle^*$, we immediately see that the bra $\langle\varphi|$ dual to the ket $|\varphi\rangle$ has the following decomposition,

$$\langle\varphi| = \sum_n c_n^*\langle n| \tag{3.12}$$

while the norm is given by

$$||\varphi||^2 = \langle\varphi|\varphi\rangle = \sum_n |c_n|^2 \tag{3.13}$$

In finite dimension, this norm is automatically finite for finite values of $c_n$, but this is not so in infinite dimension. Vectors in $\mathcal{H}$ must have finite norm; the requirement of completeness is necessary to guarantee that sequences with finite norm indeed converge to a vector in $\mathcal{H}$ with finite norm. In particular, completeness means that if $||\varphi|| < \infty$, then the sequence

$$|\varphi_N\rangle = \sum_{n=1}^{N} c_n|n\rangle \tag{3.14}$$

converges to $|\varphi\rangle$ and may be used to approximate $|\varphi\rangle$ to arbitrary precision as $N$ grows. More precisely, for any $\epsilon > 0$, there exists an $N$ such that $||\varphi - \varphi_N|| < \epsilon$.

### 3.1.4   Finite-dimensional Hilbert spaces

All Hilbert spaces of finite dimension $N$ are isomorphic to one another. Let $\{|n\rangle\}_{n=1,\cdots,N}$ be an orthonormal basis in an $N$-dimensional Hilbert space $\mathcal{H}$, satisfying $\langle m|n\rangle = \delta_{mn}$. Every vector $|\varphi\rangle$ in $\mathcal{H}$ may be represented by a $1 \times N$ column matrix $\Phi$ whose matrix elements are the complex numbers $\varphi_n = \langle n|\varphi\rangle$ ,

$$|\varphi\rangle \quad \leftrightarrow \quad \Phi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \cdot \\ \cdot \\ \varphi_N \end{pmatrix} \qquad\qquad \langle\varphi| \quad \leftrightarrow \quad \Phi^\dagger = (\, \varphi_1^* \; \varphi_2^* \; \cdots \; \varphi_N^* \,) \qquad (3.15)$$

The inner product of two vectors is given by matrix contraction,

$$(|\psi\rangle, |\varphi\rangle) = \langle\psi|\varphi\rangle = \Psi^\dagger\Phi = \sum_{n=1}^{N} \psi_n^* \varphi_n \qquad (3.16)$$

There is another combination that will be very useful,

$$|\psi\rangle\langle\varphi| \quad \leftrightarrow \quad \Psi\Phi^\dagger = \begin{pmatrix} \psi_1\varphi_1^* & \psi_1\varphi_2^* & \cdots & \psi_1\varphi_N^* \\ \psi_2\varphi_1^* & \psi_2\varphi_2^* & \cdots & \psi_2\varphi_N^* \\ & & \cdots & \\ \psi_N\varphi_1^* & \psi_N\varphi_2^* & \cdots & \psi_N\varphi_N^* \end{pmatrix} \qquad (3.17)$$

Notice that a basis vector $|m\rangle$ corresponds to a column matrix $\Phi$ whose entries are $\varphi_n = \delta_{mn}$.

### 3.1.5   Infinite-dimensional Hilbert spaces

A infinite-dimensional Hilbert space $\mathcal{H}$ in quantum physics will be separable and have a countable orthonormal basis $\{|n\rangle\}_{n\in\mathbf{N}}$. All separable Hilbert spaces are isomorphic to one another, but they may arise in different ways. An arbitrary vector $|\varphi\rangle \in \mathcal{H}$ may be represented by the expansion,

$$|\varphi\rangle = \sum_n c_n|n\rangle \qquad\qquad ||\varphi||^2 = \sum_n |c_n|^2 < \infty \qquad (3.18)$$

where the sum is understood to be over $\mathbf{N}$. The simplest example of an infinite-dimensional separable Hilbert space is given by,

$$L^2 \equiv \{c = (c_1, c_2, c_3, \cdots); \; c_n \in \mathbf{C}\} \qquad\qquad (c, d) \equiv \sum_{n\in\mathbf{N}} c_n^* d_n \qquad (3.19)$$

A more complicated example is provided by spaces of square integrable complex functions on some interval $S$ (or all of) the real line $\mathbf{R}$, defined by

$$L^2(S) \equiv \{f : S \to \mathbf{C}; \ (f,f) < \infty\} \qquad\qquad (f,g) \equiv \int_S dx f(x)^* g(x) \qquad\qquad (3.20)$$

These spaces will be ubiquitous in quantum mechanics. The Fourier transform gives a convenient way of describing $L^2(S)$. For example, on an interval $S = [-\pi\ell, +\pi\ell]$ with periodic boundary conditions (or equivalently a circe of radius $\ell$), we have

$$f(x) = \sum_{m\in\mathbf{Z}} f_m \frac{e^{imx/\ell}}{\sqrt{2\pi\ell}} \qquad\qquad (f,g) = \sum_{m\in\mathbf{Z}} f_m^* g_m \qquad\qquad (3.21)$$

where $g_m$ are the Fourier components of $g$. This shows that $L^2$ and $L^2(S)$ are isomorphic. The basis for $L^2(S)$ used here corresponds to

$$|m\rangle \sim \frac{e^{imx/\ell}}{\sqrt{2\pi\ell}} \qquad\qquad (3.22)$$

and is orthonormal in view of the relation,

$$\int_{-\pi\ell}^{+\pi\ell} dx \left(e^{imx/\ell}\right)^* e^{inx/\ell} = 2\pi\ell \, \delta_{m,n} \qquad\qquad (3.23)$$

which is a standard relation of Fourier analysis.

The Hilbert space $L^2(\mathbf{R})$ must be handled with additional care. Fourier analysis (as well as the limit $\ell \to \infty$ of the above example) suggests a basis given by exponentials $\exp(ikx)$ with $k \in \mathbf{R}$. The problem is that these basis vectors are not square integrable and form a basis which is *not countable*. Nonetheless, countable bases for $L^2(\mathbf{R})$ do exist. A familiar example is provided by the orthonormal basis of wave functions for the harmonic oscillator, $H_n(x)\, e^{-x^2/2}$ where $H_n(x)$ are the Hermite polynomials. Equivalently, one can work with a non-orthonormal but simpler basis given by $x^n e^{-x^2/2}$ for all $n = 0, 1, 2, \cdots, \infty$.

In the physical world, space is not infinite. Using the entire real line $\mathbf{R}$ is an idealization, which often simplifies problems, such as in the thermodynamic limit. In practice, one may resort to approximating $\mathbf{R}$ by a large interval $[-\pi\ell, +\pi\ell]$, subject to certain boundary conditions, and then take the limit.

Alternatively, we shall later on learn how to deal with such non-countable bases.

## 3.2 Linear operators on Hilbert space

A linear operator (or simply operator) $A$ on $\mathcal{H}$ is a linear map from $\mathcal{H}$ to $\mathcal{H}$. Its action on a state $|\varphi\rangle \in \mathcal{H}$ is denoted as follows,

$$A|\varphi\rangle = |A\varphi\rangle \tag{3.24}$$

Successive application of operators involves taking products of operators. The product of operators is generally associative, $A(BC) = (AB)C = ABC$, but is not generally commutative, allowing for $AB \neq BA$.

### 3.2.1 Operators in finite-dimensional Hilbert spaces

Every linear operator $A$ on an $N$-dimensional Hilbert space $\mathcal{H}$ is equivalent to an $N \times N$ matrix, whose entries $A_{mn}$ may be obtained as matrix elements in a given basis, such as the orthonormal basis $\{|n\rangle\}_{n=1,\cdots,N}$ constructed earlier,

$$A_{mn} = \langle m|A|n\rangle \qquad\qquad \langle m|n\rangle = \delta_{mn} \tag{3.25}$$

The product of operators maps to matrix multiplication. If $A_{mn}$ and $B_{mn}$ are the matrix elements of the operators $A$ and $B$ in a certain orthonormal basis $\{|n\rangle\}$ of $\mathcal{H}$, then the matrix elements $(AB)_{mn}$ of the product $AB$ are analogously defined by $(AB)_{mn} = \langle m|AB|n\rangle$. Upon inserting the completeness relation between $A$ and $B$, we find,

$$(AB)_{mn} = \sum_p \langle m|A|p\rangle\langle p|B|n\rangle = \sum_{p=1}^{N} A_{mp}B_{pn} \tag{3.26}$$

which is nothing but the rule of matrix multiplication. The product is associative and generally non-commutative. There is an identity operator $I_{\mathcal{H}}$ which is represented by the unit matrix. A Hermitian operator is represented by a Hermitian matrix $A^\dagger = A$, whose matrix elements satisfy

$$A_{mn} = A^*_{nm} \tag{3.27}$$

for all $m, n = 1, \cdots, N$, while a unitary operator $U$ is defined to satisfy $U^\dagger U = I$.

### 3.2.2 Operators in infinite-dimensional Hilbert spaces

When the dimension of $\mathcal{H}$ is infinite, a linear operator may not be well-defined on all elements of $\mathcal{H}$, but only on a *dense subset*, which is referred to as the *domain* $\mathcal{D}(A)$ of the operator $A$. Take for example the Hilbert space $L^2$, and consider the linear operator $D$ which acts as follows on the states $|n\rangle$,

$$D|n\rangle = n|n\rangle \qquad\qquad n \in \mathbf{N} \tag{3.28}$$

Clearly, $D$ has a well-defined action on every basis vector. But now consider its action on a general vector $|\varphi\rangle \in \mathcal{H}$, with the decomposition of (3.18), and compute the norm of the result. We find,

$$||D|\varphi\rangle||^2 = \sum_n n^2 |c_n|^2 \tag{3.29}$$

If only a finite number of $c_n$ are different from zero, then this norm will be finite. But it is perfectly possible to have $|| |\varphi\rangle ||$ finite, but $|| D|\varphi\rangle || = \infty$. Take for example $c_n = 1/n$, which defines a normalizable vector $|\varphi\rangle$, but for which $D|\varphi\rangle$ is *not normalizable*. In the isomorphic Hilbert space $L^2([-\pi\ell, +\pi\ell])$, this issue appears under a more familiar guise. A function $f$ for which $||f||$ is finite is square normalizable; the operator $D$ is equivalent to taking the derivative of the function $f$ in the Fourier basis. But we know very well that the derivative of a square normalizable function need not be normalizable; in fact it need not be a function at all but could be a Dirac $\delta$-function.

There are many other facts and relations that hold generally true for operators on finite-dimensional Hilbert spaces, but fail for infinite-dimensional ones. A striking example has to do with the nature of the commutator. For two finite dimensional matrices, we always have $\mathrm{tr}[A, B] = 0$, because $\mathrm{tr}AB = \mathrm{tr}BA$. But for operators in Hilbert space, this is more tricky, as may be seen by taking the familiar position and momentum operators, for which $[x, p] = i\hbar$. The rhs of this equation is really multiplied by the identity operator, whose trace is not expected to vanish !!

Subtleties, such as this one, associated with operators acting on infinite dimensional Hilbert spaces, will not be discussed in all generality here. Instead, we shall handle these issues as they arise, more or less on a case by case basis. Beyond that, there is a vast mathematics and mathematical-physics literature on the subject, and things get quite complicated.

## 3.3 Special types of operators

We now generalize and extend the role of certain special operators to a separable Hilbert space $\mathcal{H}$ which may be of finite or of infinite dimension.

- The *identity operator* in $\mathcal{H}$, denoted by $I$ or $I_\mathcal{H}$ maps every $|\varphi\rangle \in \mathcal{H}$ into itself, $I_\mathcal{H}|\varphi\rangle = |\varphi\rangle$. In an orthonormal basis $\{|n\rangle\}_{n=1,\cdots,N}$, it may be expressed as

$$I_\mathcal{H} = \sum_n |n\rangle\langle n| \qquad\qquad \langle m|n\rangle = \delta_{mn} \tag{3.30}$$

- A *projection operator* $P$ is defined to satisfy $P^2 = P$. The identity, and 0 operators are trivially projection operators. A non-trivial projection operator will map all of $\mathcal{H}$ into

a non-trivial subspace $\mathcal{E} \subset \mathcal{H}$, which is itself a Hilbert space. The associated projection operator $P_{\mathcal{E}}$ may be constructed uniquely in terms of an orthonormal basis $\{|\epsilon_p\rangle\}_{\{p\}}$ of $\mathcal{E}$, by

$$P_{\mathcal{E}} = \sum_p |\epsilon_p\rangle\langle\epsilon_p| \tag{3.31}$$

Of special interest is the projection operators onto a single vector $|\alpha\rangle \in \mathcal{H}$, given by

$$P_\alpha = |\alpha\rangle\langle\alpha| \tag{3.32}$$

In quantum theory, $P_\alpha$ plays the role of the analyzer in the photon experiment.

- The *inverse* $A^{-1}$ of an operator $A$ is defined as usual by $A\,A^{-1} = A^{-1}\,A = I_{\mathcal{H}}$.

- The *adjoint* of an operator is defined as follows. Given an operator $A$, with domain $\mathcal{D}(A)$, we define the adjoint operator $A^\dagger$ to be such that for all $|\varphi\rangle \in \mathcal{D}(A)$, we have[3]

$$(|\psi\rangle, A|\varphi\rangle) = (A^\dagger|\psi\rangle, |\varphi\rangle) \qquad \Leftrightarrow \qquad \langle\psi|A|\varphi\rangle = \langle\varphi|A^\dagger|\psi\rangle^* \tag{3.33}$$

For general operators $A$, this relation may not hold for all $|\psi\rangle \in \mathcal{H}$, but will hold only for a dense subset of $\mathcal{H}$, which is, by definition, the domain $\mathcal{D}(A^\dagger)$ of the operator $A^\dagger$. For a finite-dimensional Hilbert space, the adjoint $A^\dagger$ of an operator $A$ is the same as the Hermitian conjugate of that operator, and we have $A^\dagger = (A^*)^t$.

- A *self-adjoint operator* is an operator $A$ whose adjoint $A^\dagger$ satisfies $A^\dagger = A$, and whose domain satisfies $\mathcal{D}(A^\dagger) = \mathcal{D}(A)$. For a finite-dimensional Hilbert space, a self-adjoint operator is simply a Hermitian operator satisfying $A^\dagger = A$. For infinite dimensional Hilbert spaces, self-adjoint is a stronger requirement than Hermitian as the domains have to coincide. Every projection operator is self-adjoint.

- An operator $A$ is a *bounded operator* provided that for all $|\varphi\rangle \in \mathcal{H}$, we have

$$||A|\varphi\rangle||^2 \le C_A ||\varphi||^2 \tag{3.34}$$

Here, $C_A$ is a real positive constant which depends only on the operator $A$, and not on the vector $|\varphi\rangle$. Every operator in a finite-dimensional Hilbert space is automatically a bounded operator. In an infinite-dimensional Hilbert space, bounded operators are the closest in properties to finite-dimensional matrices. In particular, the domain of a bounded operator is the entire Hilbert space $\mathcal{D}(A) = \mathcal{H}$, and its adjoint $A^\dagger$ may be simply defined by

$$(|\psi\rangle, A|\varphi\rangle) = (A^\dagger|\psi\rangle, |\varphi\rangle) \qquad \Leftrightarrow \qquad \langle\psi|A|\varphi\rangle = \langle\varphi|A^\dagger|\psi\rangle^* \tag{3.35}$$

---

[3]The the sake of maximal clarity, we exhibit also the inner product notation here.

for all $|\varphi\rangle, |\psi\rangle \in \mathcal{H}$, while a self-adjoint bounded operator satisfies $\langle\psi|A|\varphi\rangle = \langle\varphi|A|\psi\rangle^*$ for all $|\varphi\rangle, |\psi\rangle \in \mathcal{H}$. A projection operator is always bounded. Unbounded operators will, however, be pervasive in quantum mechanics, and will need to be dealt with.

- An operator $U$ is a *unitary operator* provided that for all $|\varphi\rangle, |\psi\rangle \in \mathcal{H}$, we have

$$(U|\psi\rangle, U|\varphi\rangle) = (|\psi\rangle, |\varphi\rangle) \tag{3.36}$$

for all $|\varphi\rangle, |\psi\rangle \in \mathcal{H}$. Clearly, a unitary operator is a bounded operator with $C_U = 1$, and is invertible. The inverse $U^{-1}$ may be defined by setting $U|\psi\rangle = |u\rangle$, so that $(|u\rangle, U|\varphi\rangle) = (U^{-1}|u\rangle, |\varphi\rangle)$ for all $|\varphi\rangle, |u\rangle \in \mathcal{H}$. Using now the definition of the adjoint of $U$, we see that for a unitary operator, we have

$$U^{-1} = U^\dagger \qquad\qquad U^\dagger U = I_{\mathcal{H}} \tag{3.37}$$

Unitary operators will be key ingredients in quantum mechanics because unitary transformations will preserve transition amplitudes, and represent symmetries.

## 3.4 Hermitian and unitary operators in finite-dimension

Self-adjoint operators will play a central role in quantum mechanics. We now derive some of their key properties. In a finite-dimensional Hilbert space, a Hermitian operator is self-adjoint, and vice versa, and may be represented by a Hermitian matrix.

**Theorem 1**
*(i) The eigenvalues of a self-adjoint operator are real.*
*(ii) Eigenvectors corresponding to two distinct eigenvalues are orthogonal to one another.*
*(iii) A self-adjoint operator may be written as a direct sum of mutually orthogonal projection operators, weighted by the distinct eigenvalues.*

**Proof**
(i) Let $A$ be a Hermitian matrix with eigenvalue $a$ and associated eigenvector $|\varphi\rangle \neq 0$,

$$A|\varphi\rangle = a|\varphi\rangle \tag{3.38}$$

Taking the $\dagger$ of this equation gives $\langle\varphi|A^\dagger = a^*\langle\varphi|$, and using the fact that $A^\dagger = A$, simplifies this equation to $\langle\varphi|A = a^*\langle\varphi|$. Taking the inner product of this equation with $|\varphi\rangle$ and of the eigenvalue equation with $\langle\varphi|$, we obtain,

$$\langle\varphi|A|\varphi\rangle = a\langle\varphi|\varphi\rangle = a^*\langle\varphi|\varphi\rangle \tag{3.39}$$

Since $|\varphi\rangle \neq 0$, we have $\langle\varphi|\varphi\rangle \neq 0$, and hence $a^* = a$, which proves the first assertion.

(ii) Next, let $a' \neq a$ be two distinct eigenvalues (which are both real by (i)),

$$
\begin{aligned}
A|\varphi\rangle &= a|\varphi\rangle \\
A|\varphi'\rangle &= a'|\varphi'\rangle
\end{aligned}
\tag{3.40}
$$

Taking the inner product of the first line with $\langle\varphi'|$ and of the second line by $\langle\varphi|$, and using $\langle\varphi|\varphi'\rangle = \langle\varphi'|\varphi\rangle^*$, and $\langle\varphi|A|\varphi'\rangle = \langle\varphi'|A^\dagger|\varphi\rangle^* = \langle\varphi'|A|\varphi\rangle$, we find that

$$
\langle\varphi'|A|\varphi\rangle = a\langle\varphi|\varphi'\rangle = a'\langle\varphi|\varphi'\rangle
\tag{3.41}
$$

Since $a' \neq a$, we must have $\langle\varphi'|\varphi\rangle = 0$ which proves (ii).

Constructing eigenvalues and eigenvectors in general is difficult, even in finite dimension. If $A$ is an $N \times N$ matrix, the eigenvalues obey the *characteristic equation*,

$$
\det(aI - A) = a^N + c_1 a^{N-1} + c_2 a^{N-2} + \cdots + c_N = 0
\tag{3.42}
$$

where $c_1 = -\mathrm{tr}A$ and $c_N = (-)^N \det A$. Clearly, for Hermitian $A$, all coefficients $c_n$ are real, and all roots are real. Assuming that, given $A$, the roots $a_1, a_2, \cdots, a_N$ of this algebraic equation have been found (possibly numerically), then finding the associated eigenvectors reduces to a linear problem,

$$
(a_n I - A)|\varphi\rangle = 0
\tag{3.43}
$$

which can be solved by standard methods of matrix algebra.

(iii) Finally, a given eigenvalue $a_i$, may have one or several linearly independent eigenvectors, which span the entire eigenspace $\mathcal{E}_i$ associated with $a_i$. By the result of (ii), the eigenspaces associated with distinct eigenvalues are also mutually orthogonal. Therefore, the entire Hermitian matrix equals,

$$
A = \sum_i a_i P_i \qquad\qquad a_i \neq a_j \quad \text{when} \quad i \neq j
\tag{3.44}
$$

where $P_i$ represents the projection operator on eigenspace $\mathcal{E}_i$. The dimension $\dim P_i$ is referred to as the *degeneracy (or multiplicity) of the eigenvalue* $a_i$. This number clearly coincides with the degeneracy of the root $a_i$ in the characteristic equation. In matrix notation, this produces a block-diagonal representation of $A$,

$$
A = \begin{pmatrix}
a_1 I_1 & 0 & 0 & \cdots & 0 \\
0 & a_2 I_2 & 0 & \cdots & 0 \\
0 & 0 & a_3 I_3 & \cdots & 0 \\
& & \cdots & & \\
0 & 0 & 0 & \cdots & a_m I_m
\end{pmatrix}
\tag{3.45}
$$

This proves (iii).

### 3.4.1  Unitary operators

Unitary operators are very closely related to self-adjoint operators. In fact, one proves the following theorem by completely analogous methods,

**Theorem 2**
*(i) The eigenvalues of a unitary operator are pure phases.*
*(ii) Eigenvectors corresponding to two distinct eigenvalues are orthogonal to one another.*
*(iii) A unitary matrix may be written as a direct sum of mutually orthogonal projection operators, weighted by the distinct eigenvalues.*

Thus, a unitary operator $U$ admits a decomposition very analogous to a Hermitian operator, but only the nature of the eigenvalues differs,

$$U = \sum_i e^{i\theta_i} P_i = \begin{pmatrix} e^{i\theta_1} I_1 & 0 & 0 & \cdots & 0 \\ 0 & e^{i\theta_2} I_2 & 0 & \cdots & 0 \\ 0 & 0 & e^{i\theta_3} I_3 & \cdots & 0 \\ & & \cdots & & \\ 0 & 0 & 0 & \cdots & e^{i\theta_m} I_m \end{pmatrix} \tag{3.46}$$

where the angles $\theta_i$ are real and distinct mod $2\pi$, and $I_i$ is the identity matrix in the eigenspace $\mathcal{E}_i$, representing the orthogonal projection operator $P_i$ onto the eigenspace of $U$ with eigenvalue $e^{i\theta_i}$.

### 3.4.2  The exponential map

For any $N \times N$ matrix, and any analytic function function $f(x)$, we defined $f(A)$ by the Taylor expansion of $f$,

$$f(A) = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(0) A^n \tag{3.47}$$

where $f^{(n)}(x)$ is the $n$-th derivative of $f(x)$. Using this definition, it is especially easy to find the function $f$ evaluated on a Hermitian matrix $A$, with the decomposition in terms of orthogonal projectors given in (3.45), and we have

$$f(A) = \sum_i f(a_i) P_i \tag{3.48}$$

The relation between Hermitian and unitary operators may be made explicit by using the exponential function. For any Hermitian matrix $A$, the matrix $U$, uniquely defined by

$$U = e^{iA} \tag{3.49}$$

is a unitary matrix. The statement is readily checked by computing $U^\dagger = e^{-iA^\dagger} = e^{-iA}$. Conversely, any unitary matrix $U$ may be written as the exponential of a Hermitiam matrix $A$, as in (3.49), but the matrix $A$ is not unique, as various shifts by $2\pi$ in $A$ will produce the same $U$. The easiest way to prove this statement is to decompose $U$ into orthogonal projection operators as in (3.46); it is then manifest that the matrix $A$ is then given by (3.45) with $a_i = \phi_i \bmod 2\pi$.

## 3.5   Self-adjoint operators in infinite-dimensional Hilbert spaces

The statements of Theorem 1 have been written in such a way that they essentially also hold for infinite dimensional Hilbert spaces, though the proofs will now differ. In particular, self-adjoint operators will still have real eigenvalues. In statement (iii), the sum over projection operators weighed by eigenvalues need not be a discrete sum, *even in a separable Hilbert space*, but can have discrete and continuous parts, corresponding to the discrete and continuous parts of the spectrum of an operator. Actually, this situation should be familiar from analyzing the spectra of various Hamiltonians in quantum mechanics, such as the Hydrogen atom.

The continuous spectrum arises because all the eigenvectors of an operator need not be normalizable. The simplest case would be the Hamiltonian of the free particle on $\mathbf{R}$, and its associated eigenvalue problem,

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \qquad\qquad H\psi_E(x) = E\psi_E(x) \qquad\qquad (3.50)$$

whose eigenfunctions are $e^{ikx}$ with $E = \hbar^2 k^2/2m$. Although $L^2(\mathbf{R})$ is a perfectly separable Hilbert space, and the operator $H$ is perfectly self-adjoint, the eigenvectors $\psi_E(x)$ are not normalizable on $\mathbf{R}$. This situation is characteristic of the continuous part of a spectrum.

The relation between self-adjoint and unitary operators remains valid for infinite-dimensional Hilbert spaces.

# 4 The Principles of Quantum Physics

The mathematical description of a physical quantum system is in terms of a separable Hilbert space $\mathcal{H}$ and certain linear operators on $\mathcal{H}$.

**Principle 1**  Every *physical state* of a quantum system is represented by a vector in $\mathcal{H}$. Two vectors, $|\varphi\rangle, |\varphi'\rangle \in \mathcal{H}$ correspond to the same physical state if and only if $|\varphi'\rangle = \lambda |\varphi\rangle$ for some non-zero $\lambda \in \mathbf{C}$. Using this equivalence, a physical state is really described by a *ray* in $\mathcal{H}$, and one often chooses $||\varphi|| = 1$.

**Principle 2**  Every *observable* of a physical system is represented by a self-adjoint operator on $\mathcal{H}$. A state $|\phi_i\rangle$ has a definite measured value $a_i$ for an observable $A$ provided $|\phi_i\rangle$ is an eigenvector of $A$,

$$A|\phi_i\rangle = a_i|\phi_i\rangle \tag{4.1}$$

In any quantum system, the outcomes of any experiment on the system are the possible eigenvalues of various observables. States associated with different eigenvalues are orthogonal in view of the fact that $A$ is self-adjoint.

**Principle 3**  Let $|\varphi\rangle$ be an arbitrary state in $\mathcal{H}$, and let $\{|\psi_i\rangle\}$ denote a set of mutually orthogonal states, such as, for example, the eigenstates of an observable. Then, the probability $p$ for measuring the state $|\varphi\rangle$ in one of the states $|\psi_i\rangle$ are given by

$$p\big(|\varphi\rangle \rightarrow |\psi_i\rangle\big) = |\langle\psi_i|\varphi\rangle|^2 \tag{4.2}$$

for normalized states satisfying $\langle\varphi|\varphi\rangle = 1$ and $\langle\psi_i|\psi_j\rangle = \delta_{i,j}$.

**Principle 4**  Time-evolution, also referred to as dynamics, of a quantum system is generated by a self-adjoint Hamiltonian $H$, which is itself an observable associated with the total energy of the system. In the Schrödinger picture of a closed system, the states of the system evolve in time, and the observables are time independent. The Schrödinger equation gives the time evolution of any state $|\varphi(t)\rangle$, according to

$$i\hbar\frac{\partial}{\partial t}|\varphi(t)\rangle = H\,|\varphi(t)\rangle \tag{4.3}$$

In the Heisenberg formulation, the states remain time independent but the observables acquire time-dependence, according to

$$i\hbar\frac{d}{dt}A(t) = [A(t), H] \tag{4.4}$$

The Heisenberg and Schrödinger formulations are equivalent to one another, as we shall confirm shortly.

## 4.1   Conservation of probability

The combination of Principles 2 and 3 specifies the nature of measurement of a general observable $A$. If a quantum system has been prepared in an arbitrary state $|\varphi\rangle$, the measurement of the observable $A$ proceeds as follows.

By Principle 2, only a single eigenvalue $a_i$ of $A$ will be recorded during a single measurement of the observable associated with $A$. (In the photon polarization experiment, any single photon has polarization either along the $x$ or $y$ axis, but not both.) By principle 3, the probability for eigenvalue $a_i$ to be recorded is given by

$$p\big(|\varphi\rangle \to |\phi_i\rangle\big) = |\langle\phi_i|\varphi\rangle|^2 \tag{4.5}$$

provided the eigenvalue $a_i$ is non-degenerate, i.e. has only a single eigenvector $|\phi_i\rangle$. Both states $|\phi_i\rangle$ and $|\varphi\rangle$ are assumed to be normalized here $||\phi_i|| = ||\varphi|| = 1$. More generally, if the eigenvalue $a_i$ is degenerate, let $P_i$ be the projection operator onto the eigenspace $\mathcal{E}_i$ associated with the eigenvalue $a_i$. The total probability $p(a_i|\varphi)$ to record the eigenvalue $a_i$ for the observable $A$ in the state $|\varphi\rangle$ is then given by

$$p(a_i|\varphi) = p\big(|\varphi\rangle \to \mathcal{E}_i\big) = ||P_i\varphi||^2 \tag{4.6}$$

The property of *self-adjointness* of any observable $A$ guarantees that it admits a decomposition into mutually orthogonal projection operators $P_i$ weighted by the corresponding eigenvalues $a_i$ of $A$,

$$A = \sum_i a_i P_i \qquad\qquad \sum_i P_i = I_{\mathcal{H}} \tag{4.7}$$

and the second identity guarantees that this decomposition is complete. As a result, the sum of the probabilities for the state $|\varphi\rangle$ to be recorded in all possible outcomes is 1, since,

$$
\begin{aligned}
\sum_i p(a_i|\varphi) = \sum_i p\big(|\varphi\rangle \to \mathcal{E}_i\big) &= \sum_i ||P_i\varphi||^2 = \sum_i \langle\varphi|P_i^\dagger P_i|\varphi\rangle \\
&= \sum_i \langle\varphi|P_i|\varphi\rangle = \langle\varphi|\varphi\rangle = 1
\end{aligned} \tag{4.8}
$$

This result is, of course, a very important consistency check on the probabilistic interpretation of quantum mechanics.

## 4.2   Compatible versus incompatible observables

Two observables $A$ and $B$ are said to be *compatible* provided $[A, B] = 0$; if $[A, B] \neq 0$, the observable are *incompatible*. For example, the momentum components $p_x$ and $p_y$ are

compatible observables, $[p_x, p_y] = 0$, while the spin components $S_x$ and $S_y$ are not, $[S_x, S_y] = i\hbar S_z$. The role played by compatibility of observables during measurement is expressed by the following,

**Theorem 3**
*(i) Two self-adjoint operators $A$ and $B$, which satisfy $[A, B] = 0$, may be diagonalized in the same basis, i.e. with common eigenspaces;*
*(ii) Two compatible observables may be observed simultaneously.*

**Proof** (i) Since $A$ is self-adjoint, we may decompose it in a sum of projection operators,

$$A = \sum_i a_i P_i \qquad\qquad \sum_i P_i = I_{\mathcal{H}} \tag{4.9}$$

where by assumption, the eigenvalues satisfy $a_i \neq a_j$ when $i \neq j$. By multiplying $B$ to the left and to the right by the identity operator $I_{\mathcal{H}}$, we also have

$$B = \sum_{i,j} P_i B P_j \tag{4.10}$$

The commutator relation is easily computed in this basis,

$$0 = [A, B] = \sum_{i,j} (a_i - a_j) P_i B P_j \tag{4.11}$$

which implies that $P_i B P_j = 0$ whenever $i \neq j$, and as a result

$$B = \sum_i B_i \qquad\qquad B_i = P_i B P_i \tag{4.12}$$

Inside the eigenspace $\mathcal{E}_i$, the projection operator $P_i$ reduces to the identity operator $I_i$ (which manifestly commutes with $B_i$). Since $B_i$ is self-adjoint, it may be written as a direct sum of projection operators weighted by its eigenvalues,

$$B_i = \sum_{m_i} b_{i,m_i} P_{i,m_i} \qquad\qquad \sum_{m_i} P_{i,m_i} = I_i \tag{4.13}$$

where $m_i$ is an index for matrix $B_i$ which labels all the distinct eigenvalues $b_{im_i}$ of $B_i$. The decomposition of both operators is then given by

$$A = \sum_i \sum_{m_i} a_i P_{i,m_i} \qquad\qquad B = \sum_i \sum_{m_i} b_{i,m_i} P_{i,m_i} \tag{4.14}$$

(ii) It is manifest that an observation of $A$ will produce an eigenstate of $A$ $|\phi_i\rangle$ with eigenvalue $a_i$, which with probability 1 will produce one of the eigenstates of $B$ in sector $i$, so that simultaneous measurements of $A$ and $B$ can indeed be made.

## 4.3 Expectation values and quantum fluctuations

If $|\varphi\rangle$ is an eigenstate of an observable $A$ with eigenvalue $a$, then the probability for the outcome $a$ in a measurement of $A$ is unity. If $|\varphi\rangle$ is not an eigenstate of $A$, then $|\varphi\rangle$ cannot be associated with any one of the eigenvalues of $A$, but there is still a probabilistic expectation value for the observable $A$. For a general state $|\varphi\rangle$, any of the eigenvalues $a_i$ of $A$ may be the outcome of a measurement of $A$, but only with a certain probability $p(a_i|\varphi)$, computed in the preceding subsection. The expected outcome in the state $|\varphi\rangle$ of a measurement on $A$ is then the probabilistic expectation value for any of the eigenvalues $a_i$, given by

$$\sum_i a_i \, p(a_i|\varphi) = \sum_i a_i \langle \varphi|P_i|\varphi\rangle = \langle \varphi|A|\varphi\rangle \tag{4.15}$$

The quantity $\langle \varphi|A|\varphi\rangle$, also denoted by $\langle A\rangle_\varphi$, is referred to as *the expectation value of $A$ in the state $|\varphi\rangle$*. As before, it is being assumed that $||\varphi|| = 1$.

In probability theory one is interested in the standard deviation away from an average. Similarly, in quantum physics one is interested in the *average quantum fluctuations away from an expectation value*. One defines the strength of these quantum fluctuations as follows. For any given state $|\varphi\rangle$, subtract the expectation value of the observable to define a new observable which has vanishing expectation value (still in the state $|\varphi\rangle$),

$$A_\varphi \equiv A - \langle A\rangle_\varphi I_\mathcal{H} \qquad\qquad \langle \varphi|A_\varphi|\varphi\rangle = 0 \tag{4.16}$$

The magnitude of the quantum fluctuations is then defined by

$$(\Delta_\varphi A)^2 \equiv \langle \varphi|(A_\varphi)^2|\varphi\rangle = \sum_i \left(a_i - \langle A\rangle_\varphi\right)^2 p(a_i|\varphi) \tag{4.17}$$

Of course, for $|\varphi\rangle$ an eigenstate of the observable $A$, we have $\Delta_\varphi A = 0$, and there are no quantum fluctuations of the observable $A$ in this state.

## 4.4 Incompatible observables, Heisenberg uncertainty relations

Compatible observables may be measured simultaneously on all states. In particular, this means that we can simultaneously have

$$\Delta_\varphi A = \Delta_\varphi B = 0 \tag{4.18}$$

for one and the same state $|\varphi\rangle$, which is then an eigenstate of both $A$ and $B$.

How about two incompatible observables, $A$ and $B$, characterized by $[A, B] \neq 0$ ? Although incompatible observables cannot be measured simultaneously on all states, *it may or may not be possible to measure $A$ and $B$ simultaneously on some subset of all the states.*

The degree to which this is possible is expressed by the Heisenberg uncertainty relations. We begin by defining the following two states,

$$\begin{aligned}
|\alpha\rangle &= A_\varphi |\varphi\rangle \\
|\beta\rangle &= B_\varphi |\varphi\rangle
\end{aligned} \tag{4.19}$$

The Schwarz inequality on these states $|\langle\alpha|\beta\rangle|^2 \leq ||\alpha||^2\,||\beta||^2$ implies

$$\left|\langle A_\varphi B_\varphi\rangle_\varphi\right|^2 \leq \langle A_\varphi^2\rangle_\varphi \langle B_\varphi^2\rangle_\varphi = (\Delta_\varphi A)^2 (\Delta_\varphi B)^2 \tag{4.20}$$

where the last equality was obtained by using the definition of the quantum fluctuations $\Delta_\varphi A$ and $\Delta_\varphi B$ from (4.17). On the lhs, we use the decomposition of the product of operators into commutator and anti-commutator,

$$A_\varphi B_\varphi = \frac{1}{2}[A_\varphi, B_\varphi] + \frac{1}{2}\{A_\varphi, B_\varphi\} \tag{4.21}$$

It is standard that for self-adjoint operators $A$ and $B$, the quantities $i[A, B]$ and $\{A, B\}$ are both self-adjoint. Hence we have

$$\left|\langle A_\varphi B_\varphi\rangle_\varphi\right|^2 = \frac{1}{4}\left|\langle\varphi|[A_\varphi, B_\varphi]|\varphi\rangle\right|^2 + \frac{1}{4}\left|\langle\varphi|\{A_\varphi, B_\varphi\}|\varphi\rangle\right|^2 \tag{4.22}$$

Using the earlier Schwarz inequality for the above relation in which we drop the anti-commutator, and taking the square root gives the inequality,

$$\frac{1}{2}\left|\langle[A, B]\rangle_\varphi\right| \leq (\Delta_\varphi A)\,(\Delta_\varphi B) \tag{4.23}$$

This inequality is the most general form of the Heisenberg uncertainty relations.

**Examples:** A familiar example is when $A$ and $B$ are position $x$ and momentum $p$ operators, satisfying $[x, p] = i\hbar I_\mathcal{H}$. The resulting uncertainty relation is well-known,

$$\frac{1}{2}\hbar \leq \Delta x\,\Delta p \tag{4.24}$$

A less familiar example is provided by angular momentum $[J_x, J_y] = i\hbar J_z$ and cyclic permutations. Let $|\varphi\rangle = |j, m\rangle$ with $-j \leq m \leq j$, then we have

$$\frac{1}{2}|m| \leq (\Delta_\varphi J_x)(\Delta_\varphi J_y) \tag{4.25}$$

In this case, the uncertainty relation clearly depend on the state $|\varphi\rangle$, and quantum fluctuations grow with $m$. In the special states where $m = 0$, the operators $J_x$ and $J_y$ may actually be observed simultaneously, since there $0 \leq (\Delta_\varphi J_x)(\Delta_\varphi J_y)$ even though the operators $J_x$ and $J_y$ do not commute on all states.

## 4.5 Complete sets of commuting observables

For many simple quantum systems, the energy of a state completely specifies that state of the system. This is the case for the 1-dimensional harmonic oscillator, for example. But in more complicated systems, this is no longer the case. At the cost of supplying additional mutually commuting observables, however, it is possible to characterize the state uniquely by the simultaneous eigenvalues of this set of observables.

This concept is familiar, for example, from the description of orbital angular momentum states. An eigenvalue $\ell(\ell + 1)$, for $\ell = 0, 1, 2, \cdots$, of the observable $\mathbf{L}^2$ does not uniquely specify an angular momentum state (except when $\ell = 0$) but leaves a $2\ell+1$-fold degeneration. Supplying the additional observable $L_z$ lifts this degeneracy completely as it supplements $\ell$ with the eigenvalue $m$ of $L_z$ such that $-\ell \leq m \leq +\ell$. The pair $(\ell, m)$ now completely and uniquely specifies all quantum states. Another example, which builds on this one, is provided by the Hydrogen atom, whose states may be completely specified by the quantum numbers $(n, \ell, m)$, ignoring the spins of the nucleus and of the electron.

The above construction may be generalized to more complicated quantum systems. One defines a *complete set of commuting observables* of a system, as a set of observables,

$$A_1, A_2, \cdots, A_n \tag{4.26}$$

(1) such that they mutually commute, $[A_i, A_j] = 0$ for all $i, j = 1, \cdots, n$;
(2) and such that the eigenspaces common to $A_1, A_2, \cdots, A_n$ are all one-dimensional.

The fact that the eigenspaces are all one-dimensional means precisely that there is a one-to-one map between the simultaneous eigenvalues $(a_1, a_2, \cdots, a_n)$ and a basis of states in $\mathcal{H}$. The set of eigenvalues $(a_1, a_2, \cdots, a_n)$ which describes the states of $\mathcal{H}$ uniquely is referred to as the set of *quantum numbers* of that state.

Complete sets of commuting observables can be trivial. For example, given an orthonormal basis of states $|n\rangle$, for $n \in \mathbf{N}$, the following is a complete set of commuting observables,

$$P_n = |n\rangle\langle n| \qquad\qquad n \in \mathbf{N} \tag{4.27}$$

where $P_n$ is the orthogonal projection operators on a single state $|n\rangle$. The possible eigenvalues of the operators are 0 and 1, and would provide a digital numbering of all the basis vectors in $\mathcal{H}$. Describing all the states of the harmonic oscillator this way would not be very efficient.

Given an operator $A$, any function $f(A)$ will commute with $A$. Also, given two mutually commuting operators $A_1$ and $A_2$, the product $A_1 A_2$ commutes with $A_1$ and $A_2$. Neither $f(A)$, nor $A_1 A_2$, however, produce information not already contained in $A$, or in $A_1$ and $A_2$. Therefore, the most interesting complete sets of commuting operator will be the most economical ones in which the operators are functionally independent from one another.

# 5   Some Basic Examples of Quantum Systems

It is will be very useful for later studies to examine some of the most fundamental quantum systems beyond the two-state models. They will include some finite systems with more than 2 states, time-dependent 2-state systems like NMR, the 1-dimensional harmonic oscillator, and the angular momentum algebra.

## 5.1   Propagation in a finite 1-dimensional lattice

One of the most fundamental *models* consists of states propagating on a 1-dimensional lattice consisting of $N$ sites. We label the lattice sites by an integer $n = 1, 2, \cdots, N$. The Hilbert space is spanned by the basis states $|n\rangle$. A state $|n\rangle$ may be thought of as representing the quantum system where the "particle" is at site $n$ with probability 1, and probability 0 to be on any of the $N$ other sites. Such states are naturally orthogonal, and may be chosen orthonormal, $\langle m|n\rangle = \delta_{m,n}$ for $m, n = 1, 2, \cdots, N$.

A simple example of such a system is provided by an electron propagating on a lattice of atoms, ions or molecules. In reality, there will not just be one electron, but many. Also, the electron will be free to move in more than one dimension, and will have electromagnetic and spin interactions as well. In this model, all these extra effects will be omitted in favor of just to 1-dimensional location of the electron. An example with $N = 6$ is provided by the Benzene molecule, where 3 electrons approximately freely move over a 6-atom ring. In this case the lattice is naturally periodic. More generally, the model can describe propagation of electrons along long chains of atoms, ions or molecules with $N \gg 1$. If only bulk properties are of interest, we are free to impose convenient boundary conditions on this lattice. We choose these to be periodic, which allows for the simplest treatment. Therefore, it is often convenient to identify $|N + 1\rangle = |1\rangle$.

The dynamics of the quantum system is governed by the Schrödinger equation, in terms of a Hamiltonian $H$ for the system. We want to use physical arguments to try and retain only the most important dynamical information in $H$, and omit all else. To do this, we study the Schrödinger equation. Any state $|\psi(t)\rangle$ may be decomposed onto the basis $\{|n\rangle\}_n$,

$$|\psi(t)\rangle = \sum_{n=1}^{N} c_n(t)|n\rangle \qquad\qquad c_n(t) = \langle n|\psi(t)\rangle \qquad\qquad (5.1)$$

The Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H \ |\psi(t)\rangle \qquad\qquad (5.2)$$

determines the time-evolution of the probability amplitudes $c_n(t)$, as a function of the matrix elements of the Hamiltonian. To show this, take the inner product of the above Schrödinger

equation with $\langle n|$,

$$i\hbar\frac{\partial}{\partial t}c_n(t) = \langle n|H|\psi(t)\rangle = \sum_{m=1}^{N}\langle n|H|m\rangle c_m(t) \tag{5.3}$$

To obtain the second equality, we have inserted the identity operator, represented as a sum over the basis, $I = \sum_m |m\rangle\langle m|$.

The simplest non-trivial Hamiltonian for a 1-dimensional periodic lattice retains only the effects of nearest neighbors in the lattice. For example, given that an electron is initially on site $|n\rangle$ with probability 1, it is natural to include only the simplest effects, namely that there must be some probability for the electron the remain on site $|n\rangle$, and some probability to move the electron from site $|n\rangle$ to its nearest neighboring sites $|n+1\rangle$ or $|n-1\rangle$. The simplest choice is such that

$$\begin{aligned} \langle n|H|n\rangle &= A_0 \\ \langle n|H|n\pm 1\rangle &= -A_1 \end{aligned} \tag{5.4}$$

where both $A_0$ and $A_1$ are real, and all other matrix elements are zero. It is convenient to write the Hamiltonian as follows,

$$H = A_0\,I - A_1\,T - A_1\,T^\dagger \tag{5.5}$$

where $I$ is the identity operator, and $T$, and $T^\dagger$ are given by

$$T = \sum_{n=1}^{N}|n+1\rangle\langle n| \qquad\qquad T^\dagger = \sum_{n=1}^{N}|n\rangle\langle n+1| \tag{5.6}$$

and where we continue to use the periodicity $|N+1\rangle = |1\rangle$ of the lattice.

### 5.1.1  Diagonalizing the translation operator

The operator $T$ has a remarkably simple interpretation, which may be gathered by applying $T$ to an arbitrary state

$$\begin{aligned} T|n\rangle &= |n+1\rangle & n = 1,\cdots,N-1 \\ T|N\rangle &= |1\rangle \end{aligned} \tag{5.7}$$

Clearly, $T$ translates the system by one lattice spacing forward, and $T^\dagger = T^{-1}$ translates it backwards by one lattice spacing. As a result, we have $T^N = I$. Since $[H,T] = 0$, translations are a symmetry of the Hamiltonian, as the physical picture indeed suggests. It also means that the operators $H$ and $T$ may be diagonalized simultaneously. Since the

operator $T$ is simpler than $H$, it will be advantageous to diagonalize it first. Since $T$ is unitary, its eigenvalues are pure phases $e^{i\varphi_m}$. We shall denote the corresponding eigenstates by $|k_m; T\rangle$; we include the label $T$ inside the state ket, because these kets will form a basis in which $T$ is diagonal and this basis is different from the basis $|n\rangle$. The label $T$ is included to make this distinction clear. Thus we have,

$$T|k_m; T\rangle = e^{-i\varphi_m}|k_m; T\rangle \tag{5.8}$$

From $T^N = I$, we have $N\varphi_m \equiv 0 \pmod{2\pi}$. The eigenvalues are all distinct, and we have

$$\varphi_m = 2\pi m/N \qquad\qquad m = 0, 1, \cdots, N-1 \tag{5.9}$$

This leads to $N$ orthogonal eigenstates (since $T$ is unitary), and gives an explicit construction of all the normalized eigenstates of $T$,

$$|k_m; T\rangle = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{+in\varphi_m}|n\rangle \qquad\qquad m = 0, 1, \cdots, N-1 \tag{5.10}$$

These states are usually referred to as *Bloch states*.

### 5.1.2 Position and translation operator algebra

We may define a *position operator* $X$ on this finite lattice by introducing a physical lattice spacing $a$ into the problem. The origin of position is arbitrary, which allows us to leave an arbitrary additive constant $x_0$ in the eigenvalues,

$$X|n\rangle = (an + x_0)|n\rangle \tag{5.11}$$

Clearly, this operator is self-adjoint and indeed corresponds to an observable. The physical length of the lattice is then $L = aN$. The translation operator $T$ now has the physical interpretation of shifting the system forward by one lattice spacing $a$. Since the action of $T$ and $X$ is known on all states, we can compute the action of $T$ on $X$,

$$\begin{aligned} T^\dagger X T|n\rangle &= T^\dagger X|n+1\rangle = T^\dagger(a(n+1) + x_0)|n+1\rangle \\ &= (a(n+1) + x_0)|n\rangle = (X + a)|n\rangle \end{aligned} \tag{5.12}$$

This equation being valid on all states, we conclude that

$$T^\dagger X T = X + aI \tag{5.13}$$

which makes full intuitive sense: the action of the translation generator indeed shifts the position eigenvalues all by $a$. Of course, what is not well-accounted for here is the fact that $X$ is really a periodic variable, defined only mod $aN$. To account for this periodicity, a more appropriate operator would be $e^{2\pi iX/(Na)}$.

### 5.1.3 The spectrum and generalized Hamiltonians

We are guaranteed that $H$ is diagonalizable in this basis; in fact it is already diagonal, and we readily evaluate the eigenvalues of $H$:

$$H|k_m;T\rangle = E_m|k_m;T\rangle \qquad\qquad E_m = A_0 - 2A_1\cos\varphi_m \qquad\qquad (5.14)$$

Remarkably, it is very easy to include next to nearest neighbor interactions and so on. We would do this by including in $H$ terms which have higher powers of the translation operator. Including next to nearest neighbor interactions would produce the Hamiltonian,

$$H = A_0\,I - A_1 T - A_1 T^{-1} - A_2 T^2 - A_2 T^{-2} \qquad\qquad (5.15)$$

By construction, this Hamiltonian is also already diagonal in the basis $|k_m;T\rangle$, and we may read off the eigenvalues,

$$E_m = A_0 - 2A_1\cos\varphi_m - 2A_2\cos 2\varphi_m \qquad\qquad (5.16)$$

### 5.1.4 Bilateral and reflection symmetric lattices

The periodic lattice has a natural reflection symmetry. This symmetry is often useful in performing practical calculations. For example, in the subsequent subsections, we shall be led to consider the limit $N \to \infty$, which is more easily represented in symmetric form. Here, we shall recast the periodic lattice with $N$ sites in a manifestly reflection symmetric way. The rearrangement depends on whether $N$ is even or odd; it will be convenient to define $\nu \equiv [N/2]$, where $[\ ]$ stands for the integer part. To exhibit the reflection symmetry of the periodic lattice, it suffices to choose $x_0$ of the preceding subsection as follows,

$$x_0 = -\nu a \qquad\qquad \tilde{n} = n - \nu \qquad\qquad (5.17)$$

Here, we have also shifted the label $n$ to a symmetric label $\tilde{n}$. For $N$ odd, the states $|\nu\rangle$ and $|-\nu\rangle$ are different from one another, and the range of $\tilde{n}$ labeling independent states $|\tilde{n}\rangle$ is as follows, $-\nu \le \tilde{n} \le \nu$. For $N$ even, the states $|-\nu\rangle$ and $|\nu\rangle$ are to be identified $|-\nu\rangle = |\nu\rangle$, and the range of $\tilde{n}$ labeling independent states $|\tilde{n}\rangle$ is instead $-\nu < \tilde{n} \le \nu$.

For example, when $N$ is odd, we have $N = 2\nu + 1$, and the phases $\varphi_m$ may be chosen symmetrically as follows,

$$\varphi_m = 2\pi m/N \qquad\qquad m = -\nu, \cdots, 0, \cdots, \nu \qquad\qquad (5.18)$$

The Bloch states are then given by

$$|k_m;T\rangle = \frac{1}{\sqrt{N}}\sum_{\tilde{n}=-\nu}^{\nu} e^{+i\tilde{n}\varphi_m}|\tilde{n}\rangle \qquad\qquad m = -\nu, \cdots, 0, \cdots, \nu \qquad\qquad (5.19)$$

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## 5.2 Propagation in an infinite 1-dimensional lattice

Keeping the lattice spacing $a$ fixed, we may let the physical extent of the lattice become infinite by letting $N \to \infty$, so that also $L = Na \to \infty$. To do this symmetrically about the origin, we use the results of the last subsection, but we shall drop the tildes on $n$. As $N \to \infty$, the spectrum of the position operator remains discrete, with eigenstates $|n\rangle$, and linearly spaced by the lattice spacing $a$. Its only modification as $N \to \infty$ is that the spectrum of $X$ extends to larger and larger values.

The translation operator, however, now acquires a continuous spectrum, since its eigenvalues $e^{i\varphi_m} = e^{2\pi im/N}$ become increasingly dense on the unit circle. We represent the eigenvalues in terms of the physical quantity of momentum $p$, or equivalently, of wave number $k$, which is related to momentum by $p = \hbar k$,

$$\frac{\varphi_m}{a} \to k \qquad\qquad -\frac{\pi}{a} \leq k \leq +\frac{\pi}{a} = k_c \tag{5.20}$$

The range of the momentum or wave number is characteristic of propagation on a lattice, and is referred to as the *Brillouin zone*. The eigenstates $|k; T\rangle$ of the translation operator become labeled by a continuous parameter $k$. To take the limit properly, however, the discrete normalization of the states $|k_m; T\rangle$ must be changed to a continuum normalization,

$$|k_m; T\rangle \sqrt{Na} = |k; T\rangle \qquad\qquad ka = \varphi_m \tag{5.21}$$

With this new normalization, the states $|k; T\rangle$ are now given by an infinite sum,

$$|k; T\rangle = \sqrt{a} \sum_{n=-\infty}^{+\infty} e^{inak} |n\rangle \tag{5.22}$$

The completeness relation on the momentum states now involves an integral rather than a discrete sum,

$$I = \int_{-k_c}^{+k_c} \frac{dk}{2\pi} \, |k; T\rangle\langle k; T| \tag{5.23}$$

It may be verified explicitly by using the expression for $|k; T\rangle$ in terms of $|n\rangle$, and the formula,

$$\int_{-k_c}^{+k_c} \frac{dk}{2\pi} \, a \, e^{iak(n-n')} = \delta_{nn'} \tag{5.24}$$

The normalization of the momentum states must now also be carried out in the continuum, and may be deduced directly from the completeness relation itself. Applying the completeness relation to an arbitrary state $|k'; T\rangle$, we have

$$|k'; T\rangle = \int_{-k_c}^{+k_c} \frac{dk}{2\pi} \, |k; T\rangle \, \langle k; T|k'; T\rangle \tag{5.25}$$

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This relation must hold for all states $|k'; T\rangle$, and it means that

$$\langle k; T | k'; T \rangle = 2\pi \delta(k' - k) \qquad\qquad k, k' \in [-k_c, k_c] \qquad (5.26)$$

where $\delta(k - k')$ is the *Dirac $\delta$-function*. It is generally defined by the relation

$$f(x) = \int dy \; \delta(x - y) \; f(y) \qquad\qquad (5.27)$$

for any dense set of infinitely differentiable functions $f(x)$ (strictly speaking with the extra technical assumption of compact support). It is instructive to verify this relation directly from the expression of $|k; T\rangle$ in terms of $|n\rangle$,

$$\langle k'; T | k; T \rangle = a \sum_{n=-\infty}^{+\infty} e^{ina(k-k')} \qquad\qquad (5.28)$$

This gives us a convenient representation of the $\delta$-function,

$$2\pi \delta(k - k') = a \sum_{n=-\infty}^{+\infty} e^{ina(k-k')} \qquad\qquad k, k' \in [-k_c, k_c] \qquad (5.29)$$

We conclude by taking the limit of the energy eigenvalues of the lattice Hamiltonian in the $N \to \infty$ limit. It is given by

$$E_k = A_0 - 2A_1 \cos(ka) - 2A_2 \cos(2ka) \qquad\qquad k \in [-k_c, k_c] \qquad (5.30)$$

This is a very general result for the propagation of free waves on a lattice with spacing $a$.

## 5.3  Propagation on a circle

Another way of taking the limit $N \to \infty$ is obtained by keeping the physical size of the system $Na = 2\pi L$ finite. For fixed $L$, the lattice spacing must then tend to 0 as follows, $a = 2\pi L/N$. This time, the momentum operator retains a discrete spectrum, and the position operator acquires a continuous spectrum. We choose $x_0 = -\pi(N+1)L$, such that

$$an + x_0 = x \qquad\qquad -\pi L \leq x \leq +\pi L \qquad (5.31)$$

It is clear from the conjugation relation of $X$ and $T$ that as $a \to 0$, the operator $T$ approaches the identity operator linearly in $a$. We define the momentum operator $P$ by

$$T = I - i\frac{a}{\hbar}P + \mathcal{O}(a^2) \qquad\qquad (5.32)$$

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The translation equation $T^\dagger X T = X + aI$ then allows us to compute the commutator

$$[X, P] = i\hbar I \tag{5.33}$$

The position eigenstates become labeled by the continuous eigenvalues of the position operator, and including the appropriate continuum normalization factor of $N$, we have

$$|n\rangle \sqrt{N/(2\pi L)} = |x; X\rangle \qquad an + x_0 = x$$
$$X|x; X\rangle = x|x; X\rangle \tag{5.34}$$

We have included the label $X$ in the kets $|x; X\rangle$ to make it clear that the basis of states corresponds to eigenstates of the operator $X$. Since the operator $P$ is manifestly diagonal in the same basis where $T$ is diagonal, we may interchangeably use the notations $|k_m; T\rangle = |k_m; P\rangle$. The relation between momentum and position eigenstates becomes,

$$P|k_m; P\rangle = \hbar k_m |k_m; P\rangle \qquad\qquad |k_m; P\rangle = \int_{-\pi L}^{+\pi L} dx \, e^{ixk_m} \, |x; X\rangle \tag{5.35}$$

The momentum eigenvalues $p_m = \hbar k_m$ remain finite and discrete during this limit, since

$$k_m = \frac{\varphi_m}{a} = \frac{2\pi m}{Na} = \frac{m}{L} \qquad\qquad m \in \mathbf{Z} \tag{5.36}$$

The completness relations are now,

$$I = \sum_{m \in \mathbf{Z}} |k_m; P\rangle\langle k_m; P| = \int_{-\pi L}^{+\pi L} dx \, |x; X\rangle\langle x; X| \tag{5.37}$$

from which it follows that the inner product relations between $|x; X\rangle$ states are

$$\langle x; X|x'; X\rangle = \delta(x - x') \tag{5.38}$$

We conclude by producing the energy levels for this problem. Since $\varphi_m = ak_m$, all the phases tend to 0 as $a \to 0$, and all energy levels would be then degenerate. To make things more interesting, we can choose a more interesting limit, where

$$A_0 = 2A_2 = \frac{\hbar^2}{Ma^2} \tag{5.39}$$

for a fixed parameter $M$. As a result, the limiting energy levels are given by

$$E_m = \frac{(p_m)^2}{2M} \tag{5.40}$$

which is the standard kinetic energy formula for a free particle on a circle, and the parameter $M$ should be thought of as the mass.

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## 5.4 Propagation on the full line

In the problem of propagation on the circle, we may finally take the infinite volume limit where $L \to \infty$. This limit is identical to the limit where the lattice spacing $a \to 0$ is taken in the problem of propagation on the infinite lattice. Both position and momentum operators now have continuous spectra,

$$[X, P] = i\hbar I \qquad\qquad X|x; X\rangle = x|x; X\rangle \qquad\qquad x \in \mathbf{R}$$
$$P|k; P\rangle = \hbar k|k; P\rangle \qquad\qquad k \in \mathbf{R} \qquad (5.41)$$

Since the operators $X$ and $P$ are self-adjoint, their eigenvalues are real, and the eigenspaces corresponding to different eigenvalues are orthogonal to one another. The normalization of each eigenstate may be chosen at will, since a quantum state corresponds to a vector in Hilbert space, up to an overall complex multiplicative factor. The normalizations of the two sets of basis vectors $|x; X\rangle$ and $|k; P\rangle$ may be chosen independently of one another. It will be convenient to choose them as follows,

$$\langle x'; X|x; X\rangle = \delta(x' - x)$$
$$\langle k'; P k; P\rangle = 2\pi\delta(k' - k) \qquad (5.42)$$

As a result, the completeness relations are completely determined (a complete derivation of these results, for any Hamiltonian, will be given in section 5.5),

$$I = \int_{\mathbf{R}} dx \; |x; X\rangle\langle x; X| = \int_{\mathbf{R}} \frac{dk}{2\pi} \; |k; P\rangle\langle k; P| \qquad (5.43)$$

The overlap between a state in the $X$-basis, and a state in the $P$-basis, is given by,

$$\langle x; X|k; P\rangle = e^{+ikx}$$
$$\langle k; P|x; X\rangle = e^{-ikx} \qquad (5.44)$$

The energy relation is

$$E_p = \frac{p^2}{2M} \qquad (5.45)$$

Notice that the completeness relation is just the formula for the Fourier transform.

$$\langle x'; X|x; X\rangle = \delta(x - x') = \int_{\mathbf{R}} \frac{dk}{2\pi}\langle x'; X|k; P\rangle\langle k; P|x; X\rangle = \int_{\mathbf{R}} \frac{dk}{2\pi} \; e^{ik(x'-x)} \qquad (5.46)$$

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### 5.4.1 The Dirac $\delta$-function

The defining relation for the Dirac $\delta$-function on the real line is such that for all test functions $f$ (a test function belongs to a dense set of $C^\infty$ functions on $\mathbf{R}$ with compact support, often called the Schwartz space), we have

$$\int_{-\infty}^{+\infty} dx \delta(x-y)f(x) = f(y) \tag{5.47}$$

It follows immediately that $\delta(x)$ has support only at $x = 0$, so that $\delta(x) = 0$ unless $x = 0$, so that $x\delta(x) = 0$ for all $x$, and that

$$\int_{-\infty}^{+\infty} dx \delta(x-y) = 1 \tag{5.48}$$

for all $y$. The Dirac $\delta$-function may be viewed as a limit of a sequence of continuous or smooth functions $\delta_n(x)$, which converge in the sense that their pairing against any function in the Schwartz space converges. Examples of such sequences are

$$
\begin{aligned}
\delta_n(x) &= \begin{cases} 0 & |x| > 1/(2n) \\ n & |x| < 1/(2n) \end{cases} \\
\delta_n(x) &= \frac{n}{\sqrt{\pi}} e^{-n^2 x^2} \\
\delta_n(x) &= \frac{n}{\pi} \frac{1}{1 + n^2 x^2}
\end{aligned}
\tag{5.49}
$$

Derivatives of $\delta(x)$ may be defined by using the rule that the derivative and the integral commute with one another. Since the test functions have compact support, one may always integrate by parts under the integral without producing boundary terms. The defining relation of the derivative $\delta'(x-y) = \partial_x \delta(x-y)$ is by

$$\int_{-\infty}^{+\infty} dx \delta'(x-y)f(x) = -f'(y) \tag{5.50}$$

As a result, we have for example,

$$x\delta'(x) = -\delta(x) \tag{5.51}$$

Dirac $\delta$-functions may be multiplied under certain restricted conditions, essentially when their supports are appropriately weighed. For example, we have the following integral formulas,

$$\int_{-\infty}^{+\infty} dy \, \delta(x-y) \, \delta(y-z) = \delta(x-z) \tag{5.52}$$

but the product $\delta(x)\delta(x)$ is not defined.

## 5.5 General position and momentum operators and eigenstates

Given self-adjoint position and momentum operators, denoted respectively $X$ and $P$, which satisfy the canonical commutation relation $[X, P] = i\hbar I$, there are a number of *general results that may be deduced without appeal to a specific Hamiltonian.* These results will be derived here in all generality.

- The *translation operator* $T(a)$ is defined for any real $a \in \mathbf{R}$ by,

$$T(a) = \exp\left(-i\frac{a}{\hbar}P\right) \tag{5.53}$$

Self-adjointness of $P$ and reality of $a$ and $\hbar$ imply that $T(a)$ is unitary, and satisfies

$$T(a)^\dagger T(a) = T(a)T(a)^\dagger = I \tag{5.54}$$

The properties of the exponential imply the following $U(1)$ group composition property,

$$T(a)T(b) = T(a+b) \tag{5.55}$$

Using the Baker-Campbell-Haussdorff formula, $e^A B e^{-A} = e^{Ad_A} B$ where the *adjoint map* is defined by $Ad_A B = [A, B]$, the definition of $T(a)$, and the canonical commutation relations, it follows,

$$T(a)^\dagger X T(a) = X + aI \tag{5.56}$$

More generally, we have $T(a)^\dagger f(X)T(a) = f(X + aI)$ for any analytic function $f$. Taking $a$ infinitesimal, $T(a) \sim I - iaP/\hbar$, or equivalently $P$, generates infinitesimal translations in $X$.

- Since $X$ and $P$ are self-adjoint, *each operator separately* may be diagonalized, with real eigenvalues. The corresponding eigenvalues will be denoted $x$ and $\hbar k$ respectively, and the eigenstates will be denoted as follows,

$$\begin{aligned} X|x; X\rangle &= x|x; X\rangle \\ P|k; P\rangle &= \hbar k|k; P\rangle \end{aligned} \tag{5.57}$$

Self-adjointness also implies that orthogonality of eigenstates associated with distinct eigenvalues, namely $\langle x'; X|x; X\rangle = 0$ for $x' \neq x$, and $\langle k'; P|k; P\rangle = 0$ for $k' \neq k$. The normalization of the states may be fixed, in part, by choosing the following relations,

$$\begin{aligned} \langle x'; X|x; X\rangle &= \delta(x' - x) \\ \langle k'; P|k; P\rangle &= 2\pi\delta(k' - k) \end{aligned} \tag{5.58}$$

This choice of normalization uniquely determines the completeness relation, and we have[4]

$$
\begin{aligned}
I &= \int_{\mathbf{R}} dx \, |x; X\rangle\langle x; X| \\
I &= \int_{\mathbf{R}} \frac{dk}{2\pi} \, |k; P\rangle\langle k; P|
\end{aligned}
\tag{5.59}
$$

Note that the normalization of (5.58) fixes the "norm" of the states, but not their relative phases, which are left undetermined. The proofs of both completeness relations are similar, so we shall carry out explicitly only the first one. Denote the result of the $x$-integral by $A$,

$$
A = \int_{\mathbf{R}} dx \, |x; X\rangle\langle x; X|
\tag{5.60}
$$

Now apply the operator to a ket $|y; X\rangle$,

$$
\begin{aligned}
A|y; X\rangle &= \int_{\mathbf{R}} dx \, |x; X\rangle\langle x; X|y; X\rangle \\
&= \int_{\mathbf{R}} dx \, |x; X\rangle\delta(x - y) = |y; X\rangle
\end{aligned}
\tag{5.61}
$$

In going from the first line to the second, we have used the normalization of the position eigenstates, defined above. Since this relation holds *for all* $y$, and $|y; X\rangle$ spans a basis, it must be that $A = I$ by its very definition.

• The overlaps of the position and momentum eigenstates may be determined by computing the matrix element $\langle k; P|T(x)|0; X\rangle$ in two different ways, namely by letting $T(a)$ act either on the left or on the right, and we find,

$$
\langle k; P|x; X\rangle = \langle k; P|T(x)|0; X\rangle = e^{-ikx}\phi(k)
\tag{5.62}
$$

where $\phi(k) = \langle k; P|0; X\rangle$. As a result, we have

$$
\begin{aligned}
\langle k; P|x; X\rangle &= \phi(k)\, e^{-ikx} \\
\langle x; X|k; P\rangle &= \phi(k)^*\, e^{+ikx}
\end{aligned}
\tag{5.63}
$$

The function $\phi(k)$ may be determined, in part, from the completeness relations, as follows,

$$
\begin{aligned}
\langle k'; P|k; P\rangle &= \int_{\mathbf{R}} dx \langle k'; Px; X\rangle\langle x; X|k; P\rangle \\
&= \phi(k')^*\phi(k) \int_{\mathbf{R}} dx \, e^{i(k-k')x} \\
&= 2\pi\delta(k' - k)|\phi(k)|^2
\end{aligned}
\tag{5.64}
$$

---

[4]The choice of normalization in (5.58) is not unique. One might have multiplied $\delta(x' - x)$ by function $f(x)$, and $\delta(k' - k)$ by an independent function $\tilde{f}(k)$. As a result, the completeness relations of (5.59) will be replaced by $dx \to dx/f(x)$ and $dk \to dk/\tilde{f}(k)$. The choice we have adopted in (5.58) is, for almost all applications, the simplest one, and it is almost universally adopted in the literature. (One exception is when $\mathbf{R}$ carries a general Riemannian metric, not just the flat Euclidean metric as we have here.)

so that $|\phi(k)| = 1$. The phase of $\phi(k)$ is not determined by the normalization conditions (5.58). The simplest choice is given by $\phi(k) = 1$, and it is this choice that we adopt.

• Matrix elements of the operators $X$ and $P$ between a general state $|\psi\rangle$ and the position or momentum eigenstates may be derived in a similar manner. It is customary to define the position and momentum space *wave functions* respectively by,

$$
\begin{aligned}
\psi(x) &\equiv \langle x; X|\psi\rangle \\
\tilde{\psi}(k) &\equiv \langle k; P|\psi\rangle
\end{aligned}
\tag{5.65}
$$

All other matrix elements may be expressed in terms of these wave functions. Thus, one has for example,

$$
\begin{aligned}
\langle x; X|X|\psi\rangle &= x\psi(x) \\
\langle k; P|P|\psi\rangle &= \hbar k\tilde{\psi}(k) \\
\langle x; X|P|\psi\rangle &= -i\hbar\frac{\partial}{\partial x}\psi(x) \\
\langle k; P|X|\psi\rangle &= i\frac{\partial}{\partial k}\tilde{\psi}(k)
\end{aligned}
\tag{5.66}
$$

Matrix elements between general states $|\phi\rangle$ and $|\psi\rangle$, with wave functions respectively $\phi(x)$, and $\psi(x)$, may be calculated analogously,

$$
\begin{aligned}
\langle\psi|X|\phi\rangle &= \int_{\mathbf{R}} dx\, \psi(x)^*\langle x; X|X|\phi\rangle = \int_{\mathbf{R}} dx\, x\psi(x)^*\phi(x) \\
\langle\psi|P|\phi\rangle &= \int_{\mathbf{R}} dx\, \psi(x)^*\langle x; X|P|\phi\rangle = -i\hbar\int_{\mathbf{R}} dx\, \psi(x)^*\frac{\partial\phi(x)}{\partial x}
\end{aligned}
\tag{5.67}
$$

## 5.6 The harmonic oscillator

The 1-dimensional harmonic oscillator for the position $X$ and momentum $P$ operators is given by the Hamiltonian

$$
H = \frac{1}{2M}P^2 + \frac{1}{2}M\omega^2 X^2
\tag{5.68}
$$

where $[X, P] = i\hbar$. The constants $M$ and $\omega$ are respectively the mass and the frequency, while the combination $K = M\omega^2$ is the spring constant. The importance of the harmonic oscillator derives from the fact that it may be used as an approximation for the Hamiltonian with a general potential $V$, considered around one of the minima $x_0$ of $V$, where,

$$
V(x) = V(x_0) + \frac{1}{2}V''(x_0)(x - x_0)^2 + \cdots
\tag{5.69}
$$

The solution to the harmonic oscillator problem will then provide an approximation to the problem for general potential $V$ for reasonably low energies.

Of course, one may derive the spectrum of the harmonic oscillator by solving the Schrödinger equation. The harmonic oscillator actually provides the perfect example of a system that may be solved much more directly using operator methods. The techniques we shall present also will also illustrate more directly how the principles of quantum mechanics may be applied.

### 5.6.1 Lowering and Raising operators

We begin by reformulating the harmonic oscillator in terms of *lowering and raising operators* $a$ and $a^\dagger$, defined as follows,

$$
\begin{aligned}
a &= \frac{1}{\sqrt{2M\omega\hbar}}\Big(M\omega\,X + i\,P\Big) \\
a^\dagger &= \frac{1}{\sqrt{2M\omega\hbar}}\Big(M\omega\,X - i\,P\Big)
\end{aligned}
\tag{5.70}
$$

For self-adjoint operators $X$ and $P$, clearly $a^\dagger$ is the adjoint operator of $a$, as the notation indeed indicates. This change of variables has been chosen so that

$$
H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) \qquad\qquad [a, a^\dagger] = 1
\tag{5.71}
$$

The terminology of *lowering and raising operators* for $a$ and $a^\dagger$, derives from the fact that they satisfy the following commutation relations with the Hamiltonian $H$,

$$
\begin{aligned}
[H, a] &= -\hbar\omega\,a \\
[H, a^\dagger] &= +\hbar\omega\,a^\dagger
\end{aligned}
\tag{5.72}
$$

For this simple system, there are no possible degeneracies and the Hamiltonian by itself may be used to span the complete set of commuting observables. One may verify that no operator built from $x$ and $p$ commutes with $H$, lest it be functions of $H$. Thus, any state $|n\rangle$ may be uniquely labeled by its energy $E_n$,

$$
H|n\rangle = E_n|n\rangle
\tag{5.73}
$$

Applying the operators $a$ and $a^\dagger$ respectively lowers and raises the energy of a state by $\hbar\omega$,

$$
\begin{aligned}
H\,a\,|n\rangle &= \Big(a\,H + [H, a\,]\Big)|n\rangle = (E_n - \hbar\omega)\,a|n\rangle \\
H\,a^\dagger|n\rangle &= \Big(a^\dagger H + [H, a^\dagger]\Big)|n\rangle = (E_n + \hbar\omega)a^\dagger|n\rangle
\end{aligned}
\tag{5.74}
$$

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Next, we show that the operator $H$ is bounded from below by $\frac{1}{2}\hbar\omega$. Indeed, take any normalized state $|\psi\rangle$, and compute the expectation value of $H$,

$$\langle\psi|H|\psi\rangle = \frac{1}{2}\hbar\omega + \hbar\omega\langle\psi|a^\dagger a|\psi\rangle = \frac{1}{2}\hbar\omega + \hbar\omega||a\psi||^2 \geq \frac{1}{2}\hbar\omega \tag{5.75}$$

Hence all eigenvalues of $H$ must be greater than or equal to $\frac{1}{2}\hbar\omega$.

### 5.6.2 Constructing the spectrum

Now here is the crucial step that will allow us to solve this system without ever solving a differential equation. Consider a normalized state $|n\rangle$ with energy $E_n$. Since $a$ lowers the energy by $\hbar\omega$, it follows that $a^k|n\rangle$ should have energy $E_n - k\hbar\omega$. But for sufficiently large $k$, this energy would dip below the bound $\frac{1}{2}\hbar\omega$, which is not possible. Thus, it must be that for some values of $k > 0$, the state $a^k|n\rangle$ is actually zero, and the spectrum must contain a state which is annihilated by $a$. We shall denote this state by $|0\rangle$,

$$a|0\rangle = 0 \qquad \Rightarrow \qquad E_0 = \frac{1}{2}\hbar\omega \tag{5.76}$$

The state $|0\rangle$ is the ground state; it is the unique state of lowest energy $E_0$, which actually saturates the lower bound on the expectation value of the Hamiltonian. All other states are then obtained by multiple application of the raising operator $a^\dagger$, and we find,

$$|n\rangle \sim \left(a^\dagger\right)^n|0\rangle \qquad \Rightarrow \qquad E_n = \hbar\omega\left(n + \frac{1}{2}\right) \tag{5.77}$$

which is indeed the entire harmonic oscillator spectrum for $n \geq 0$.

Since the states $|E_n\rangle$ for different $n$ belong to different eigenvalues of the self-adjoint operator $H$, they are automatically orthogonal. We shall also assume that they are normalized, $\langle m|n\rangle = \delta_{m,n}$. The matrix elements of the operators $a$ and $a^\dagger$ are as follows,

$$\begin{aligned} a^\dagger|n\rangle &= \sqrt{n+1}\,|n+1\rangle \\ a|n\rangle &= \sqrt{n}\,|n-1\rangle \end{aligned} \tag{5.78}$$

Or equivalently, we have $\langle m|a|n\rangle = \sqrt{n}\delta_{m,n-1}$.

### 5.6.3 Harmonic oscillator wave functions

The wave function $\psi_n(x) = \langle x; X|n\rangle$ for a state $|n\rangle$ may also be computed simply. We start with the ground state, which satisfies

$$\langle x; X|a|0\rangle = \frac{1}{\sqrt{2M\hbar\omega}}\langle x; X|(M\omega X + iP)|0\rangle = 0 \tag{5.79}$$

Since we have (see section 5.5 for the derivation),

$$\langle x; X|X|\psi\rangle = x\psi(x) \qquad\qquad \langle x; X|P|\psi\rangle = -i\hbar\frac{\partial}{\partial x}\psi(x) \qquad (5.80)$$

The ground state wave function is found to obey the first order differential equation,

$$\left(\frac{\partial}{\partial x} + \frac{M\omega}{\hbar}x\right)\psi_0(x) = 0 \qquad (5.81)$$

The unique solution is given by

$$\psi_0(x) = \left(\frac{M\omega}{\pi\hbar}\right)^{\frac{1}{4}}\exp\left\{-\frac{M\omega}{2\hbar}x^2\right\} \qquad (5.82)$$

where we have included the proper normalization factor.

Finally, recall that the wave functions for excited states are given by the ground state wave function multiplied by Hermite polynomials. This can also be recovered directly from the operator formalism. To simplify notation, we use the scaled coordinate $z = x(M\omega/\hbar)^{\frac{1}{2}}$, in terms of which we have

$$a = \frac{1}{\sqrt{2}}\left(z + \frac{\partial}{\partial z}\right) \qquad\qquad a^\dagger = \frac{1}{\sqrt{2}}\left(z - \frac{\partial}{\partial z}\right) \qquad (5.83)$$

As a result,

$$\psi_n(x) = \frac{1}{\sqrt{n!\, 2^n}}\left(z - \frac{\partial}{\partial z}\right)^n\psi_0(z) \sim H_n(x)e^{-\frac{1}{2}z^2} \qquad (5.84)$$

and it follows that $H_{n+1}(z) = 2zH_n(z) - H_n'(z)$, which is a convenient way to define the Hermite polynomials (up to an overall normalization).

## 5.7   The angular momentum algebra

Both orbital angular momentum and spin satisfy the same angular momentum algebra. We shall denote the general operators of angular momentum by $\mathbf{J}$, so that its components satisfy the angular momentum algebra,

$$[J_x, J_y] = i\hbar J_z \qquad [J_y, J_z] = i\hbar J_x \qquad [J_z, J_x] = i\hbar J_y \qquad (5.85)$$

A slightly more convenient notation is to use numerical subscripts for the axes, and let $J_1 = J_x$, $J_2 = J_y$, and $J_3 = J_z$, so that the algebra can be written in a single vector equation,

$$[J_i, J_j] = i\hbar\sum_{k=1}^{3}\varepsilon_{ijk}J_k \qquad (5.86)$$

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where $\varepsilon_{ijk}$ is totally antisymmetric in $i, j, k$ and is normalized to $\varepsilon_{123} = 1$.

We now study all possible quantum systems on which the angular momentum algebra can be realized. Since the rotations generate symmetries of a quantum system, they must be realized on the quantum system in terms of unitary operators. The infinitesimal generators of these unitary transformations are precisely the angular momentum operators $J_1, J_2, J_3$ which must be self-adjoint operators, i.e. observables. The commutation relations of the $J's$ indeed respect their self-adjointness.

### 5.7.1  Complete set of commuting observables

The angular momentum algebra possesses an operator (other than $0$ or $I$) which commutes with all three $J_i$, $i = 1, 2, 3$, namely the Casimir operator

$$\mathbf{J}^2 = J_1^2 + J_2^2 + J_3^2 \tag{5.87}$$

Any other operator which commutes with all three $J_i$, $i = 1, 2, 3$ must be functionally dependent on $\mathbf{J}^2$. In this sense, $\mathbf{J}^2$ is unique. Given the self-adjointness of the $J_i$, $i = 1, 2, 3$, it is manifest that $\mathbf{J}^2$ is also self-adjoint, and thus an observable.

To construct the Hilbert space $\mathcal{H}$ of a quantum system, we identify a complete set of commuting observables, and then simultaneously diagonalize these observables to find a basis for $\mathcal{H}$. Assuming that the Hilbert space $\mathcal{H}$ contains one and only one state associated with each set of quantum numbers leads to an "irreducible quantum system". Mathematically, this means that we will find an "irreducible representation" of the angular momentum algebra. A general quantum system associated with the angular momentum algebra may be reducible, i.e. it can be decomposed as a direct sum of a number of irreducible systems.

We choose one of the generators, say $J_3$ as the first observable. Clearly, no non-zero linear combination of $J_1$ and $J_2$ commutes with $J_3$, but the Casimir operator $\mathbf{J}^2$ does commute with $J_3$. This is a standard result that a complete basis for all angular momentum states may be parametrized by the quantum numbers of $J_3$ and $\mathbf{J}^2$. We shall label the states by $|j, m\rangle$ where $j, m \in \mathbf{R}$, since they correspond to eigenvalues of observables.

$$\begin{aligned} \mathbf{J}^2 |j, m\rangle &= \lambda(j)\hbar^2 |j, m\rangle \\ J_3 |j, m\rangle &= m\hbar |j, m\rangle \end{aligned} \tag{5.88}$$

The factors of $\hbar$ have been pulled out for later convenience.

### 5.7.2  Lowering and raising operators

We introduce *lowering and raising operators* as follows,

$$J_\pm = J_1 \pm iJ_2 \tag{5.89}$$

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Given that $J_1$ and $J_2$ are self-adjoint, the operators $J_\pm$ are not self-adjoint, but are instead the adjoints of one another,

$$(J_+)^\dagger = J_- \qquad\qquad (J_-)^\dagger = J_+ \qquad\qquad (5.90)$$

In terms of these operators, the angular momentum algebra assumes the form,

$$[J_3, J_\pm] = \pm\hbar J_\pm \qquad \Leftrightarrow \qquad J_3 J_\pm = J_\pm(J_3 \pm \hbar)$$
$$[J_+, J_-] = +2\hbar J_3 \qquad\qquad\qquad\qquad\qquad (5.91)$$

Since $\mathbf{J}^2$ commutes with $J_\pm$, the value $j$ or $\lambda(j)$ remains unchanged upon applying $J_\pm$ to a state $|\lambda(j), m\rangle$. The $m$-value will be lowered or raised, since

$$J_3\, J_\pm\, |j, m\rangle = \hbar(m \pm 1) J_\pm |j, m\rangle \qquad\qquad (5.92)$$

### 5.7.3  Constructing the spectrum

Our goal is to realize the angular momentum algebra of a Hilbert space. Since $\lambda(j)$ and $m$ label different eigenvalues of self-adjoint operators, the corresponding eigenstates are orthogonal, and we may normalize them by requiring

$$\langle j, m | j', m' \rangle = \delta_{j,j'}\delta_{m,m'} \qquad\qquad (5.93)$$

We shall now show that, given $j$, the range for the eigenvalue $m$ must be bounded. To do so, express $\mathbf{J}^2$ in terms of $J_3$ and $J_\pm$,

$$
\begin{aligned}
\mathbf{J}^2 &= \frac{1}{2}(J_+ J_- + J_- J_+) + J_3^2 \\
&= J_+ J_- + J_3^2 - \hbar J_3 \\
&= J_- J_+ + J_3^2 + \hbar J_3 \qquad\qquad (5.94)
\end{aligned}
$$

Now, both the operators $J_+ J_-$ and $J_- J_+$ are positive, since for all $j, m$,

$$
\begin{aligned}
\langle j, m | J_+ J_- | j, m \rangle = ||J_- | j, m \rangle||^2 &= \hbar^2[\lambda(j) - m^2 + m] \geq 0 \\
\langle j, m | J_- J_+ | j, m \rangle = ||J_+ | j, m \rangle||^2 &= \hbar^2[\lambda(j) - m^2 - m] \geq 0 \qquad (5.95)
\end{aligned}
$$

Clearly, given $\lambda(j)$, the values of $m$ are bounded from above and from below. But since successive application of $J_+$ would raise $m$ indefinitely, there must be a state with value $m = m_+$ which is annihilated by $J_+$. Similarly, since successive application of $J_-$ would lower $m$ indefinitely, there must be a state with value $m = m_-$ which is annihilated by $J_-$. By construction, we will have $m_+ \geq m_-$, and

$$
\begin{aligned}
J_+ |j, m_+\rangle = 0 \qquad\qquad &\langle j, m_+ | j, m_+ \rangle = 1 \\
J_- |j, m_-\rangle = 0 \qquad\qquad &\langle j, m_- | j, m_- \rangle = 1 \qquad\qquad (5.96)
\end{aligned}
$$

The norms of $J_\pm|j, m_\pm\rangle$ were already computed earlier, and thus require that

$$
\begin{aligned}
\lambda(j) - m_+(m_+ + 1) &= 0 \\
\lambda(j) - m_-(m_- - 1) &= 0
\end{aligned}
\tag{5.97}
$$

Eliminating $\lambda(j)$ gives a relation directly between $m_+$ and $m_-$, $(m_+ + m_-)(m_+ - m_- + 1) = 0$. Since we have $m_+ - m_- \geq 0$, the second parenthesis never vanishes, and we must have $m_- = -m_+$. We assumed that the quantum system was irreducible, so that for given $j$, all states with different $m$ are mapped into one another under $J_\pm$. Thus, successively applying $J_-$ to $|j, m_+\rangle$ must ultimately yield the state $|j, m_-\rangle$. Since the number of times $J_-$ is being applied is of clearly an integer, we must have that $m_+ - m_- = 2m_+$ is a positive or zero integer. We define $j$ to be this integer or half-integer $j \equiv m_+$, so that

$$
\lambda(j) = j(j+1) \qquad\qquad 2j + 1 \in \mathbf{N}
\tag{5.98}
$$

The integer $2j + 1$ is the dimension of the Hilbert space $\mathcal{H}_j$ for this irreducible quantum system, since the number of basis vectors $|j, m\rangle$ with $m = -j, -j+1, -j+2, \cdots, j-1, j$ is precisely $2j + 1$. For later convenience, we list the matrix elements of all the operators,

$$
\begin{aligned}
\mathbf{J}^2|j, m\rangle &= j(j+1)\,\hbar^2\,|j, m\rangle \\
J_3|j, m\rangle &= m\,\hbar\,|j, m\rangle \\
J_+|j, m\rangle &= \sqrt{(j-m)(j+m+1)}\,\hbar\,|j, m+1\rangle \\
J_-|j, m\rangle &= \sqrt{(j-m+1)(j+m)}\,\hbar\,|j, m-1\rangle
\end{aligned}
\tag{5.99}
$$

## 5.8  The Coulomb problem

The Coulomb problem involves a single mobile charged particle in the electro-static potential of a fixed central charge. In Hydrogen-like atoms, for example, the fixed charge is a nucleus and the mobile charge is an electron. The Coulomb potential is then attractive and produces bound states. But it also covers systems in which the mobile charge is a proton or a positron, so that no bound states exist. For the time being, effects of spin are neglected. The Schrödinger equation for the Coulomb problem with charges $q_1$ and $q_2$ is given by,

$$
-\frac{\hbar^2}{2m}\Delta\psi_E(\mathbf{r}) + \frac{q_1 q_2}{r}\psi_E(\mathbf{r}) = E\psi_E(\mathbf{r})
\tag{5.100}
$$

As for any spherically symmetric problem, we work in spherical coordinates $r, \theta, \phi$, in terms of which the Laplace operator takes the form,

$$
\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) - \frac{\mathbf{L}^2}{\hbar^2 r^2}
\tag{5.101}
$$

The operator $\mathbf{L}^2$ may be expressed solely in terms of the coordinates $\theta$ and $\phi$, but we shall not need its explicit form here. Instead, we specialize to a definite eigenstate of $\mathbf{L}^2$, labeled by its eigenvalue $\hbar^2 \ell(\ell+1)$, with $\ell = 0, 1, 2, \cdots$, corresponding to $s$, $p$, $d$-waves etc respectively. The remaining equation for the radial wave function $\varphi_{\ell,E}(r)$ takes the form,

$$-\frac{\hbar^2}{2m}\left(\varphi_{\ell,E}'' + \frac{2}{r}\varphi_{\ell,E}' - \frac{\ell(\ell+1)}{r^2}\varphi_{\ell,E}\right) + \frac{q_1 q_2}{r}\varphi_{\ell,E} = E\varphi_{\ell,E} \qquad (5.102)$$

It is always a good idea to extract all dimensionful quantities, and leave a differential equation in terms of dimensionless variables. To do so, we rescale $r$ by

$$r = \lambda x \qquad\qquad \lambda^2 = \pm\frac{\hbar^2}{2mE} \qquad (5.103)$$

where we have the $+$ sign for scattering states with $E > 0$, and $-$ for bound states with $E < 0$. The equation is then governed by a single dimensionless parameter for fixed $\ell$,

$$\varepsilon = \frac{2mq_1 q_2 \lambda}{\hbar^2} \qquad (5.104)$$

and takes the final form in terms of the reduced radial wave function $f_{\ell,\varepsilon}(x) = \varphi_{\ell,E}(r)/r$, given as follows,

$$x^2 f_{\ell,\varepsilon}'' - \ell(\ell+1)f_{\ell,\varepsilon} - \varepsilon x f_{\ell,\varepsilon} \pm x^2 f_{\ell,\varepsilon} = 0 \qquad (5.105)$$

### 5.8.1 Bound state spectrum

For the bound state problem, the sign is $-$, and solutions that are normalizable at $\infty$ must behave as $e^{-x}$ and at zero like $x^{\ell+1}$. Extracting this behavior then leaves,

$$f_{\ell,\varepsilon}(x) = g_{\ell,\varepsilon}(x)x^{\ell+1}e^{-x} \qquad (5.106)$$

where $g_{\ell,\varepsilon}(x)$ now satisfies the equation,

$$xg_{\ell,\varepsilon}'' + (2\ell + 2 - 2x)g_{\ell,\varepsilon}' - (2 + 2\ell - \varepsilon)g_{\ell,\varepsilon} = 0 \qquad (5.107)$$

The solutions leading to normalizable wave functions are polynomial in $x$. To admit a polynomial solution of degree $\nu$ requires the relation

$$\varepsilon = 2(\ell + 1 + \nu) \equiv 2n \qquad (5.108)$$

We find the well-known result that the spectrum of bound states of the Coulomb problem is in fact independent of $\ell$, and depends only on the principal quantum number $n$, as defined above. Substituting these values into the above formulas to obtain the energy, we find,

$$E_n = -\frac{1}{2}mc^2 \frac{1}{n^2} \frac{q_1^2 q_2^2}{\hbar^2 c^2} \qquad (5.109)$$

For an electron we have $q_1 = -e$, and for a nucleus of with $Z$ protons we have $q_2 = Ze$. In addition, in cgs units (which is what we have been using here), the combination

$$\alpha = \frac{e^2}{\hbar c} \tag{5.110}$$

is dimensionless and is referred to as the *fine structure constant*, with value approximately given by $\alpha = 1/137.04$. Thus, the bound state energy levels of this system are given by,

$$E_n = -\frac{1}{2}mc^2\alpha^2 Z^2 \tag{5.111}$$

which is equivalent to the standard formula.

The solutions $g_{\ell,2n}(x)$ for $n$ integer are *associated Laguerre polynomials*, denoted $L^p_{q-p}(x)$, and given in terms of Laguerre polynomials $L_q(x)$ by,

$$
\begin{aligned}
g_{\ell,2n}(x) &= L^{2\ell+1}_{n-\ell-1}(x) \\
L^p_{q-p}(x) &= (-1)^p \frac{d^p}{dx^p} L_q(x) \\
L_q(x) &= e^x \frac{d^q}{dx^q}\left(x^q e^{-x}\right)
\end{aligned} \tag{5.112}
$$

The spherical harmonics, which are the final ingredient of the full wave functions of the Coulomb problem, will be derived explicitly in the chapter on angular momentum.

### 5.8.2   Scattering spectrum

The equation is now,

$$x^2 f''_{\ell,\varepsilon} - \ell(\ell+1)f_{\ell,\varepsilon} - \varepsilon x f_{\ell,\varepsilon} + x^2 f_{\ell,\varepsilon} = 0 \tag{5.113}$$

The asymptotic behavior of the solutions as $x \to \infty$ is given by an oscillatory exponential $e^{\pm ix}$, as is expected for a scattering problem. Since the differential equation is real, its two independent solutions may be taken to be complex conjugates of one another, so we shall choose the asymptotic behavior to be $e^{-ix}$. Extracting also the familiar factor of $x^{\ell+1}$ for regularity at $x = 0$, we have

$$f_{\ell,\varepsilon}(x) = g_{\ell,\varepsilon}(x)x^{\ell+1}e^{ix} \tag{5.114}$$

so that the equation becomes,

$$xg''_{\ell,\varepsilon} + (2\ell + 2 - 2ix)g'_{\ell,\varepsilon} - (2i(\ell+1) + \varepsilon)\, g_{\ell,\varepsilon} = 0 \tag{5.115}$$

This equation is of a well-known form, namely that of a confluent hypergeometric function, or Kummer function,

$$g_{\ell,\varepsilon}(x) = M\left(\ell + 1 - \frac{i\varepsilon}{2}, 2\ell + 2, 2ix\right) \tag{5.116}$$

To get a better idea of what these functions are, it is useful to give an integral representation,

$$M(a, b, z) = \frac{\Gamma(b)}{\Gamma(b-a)\Gamma(a)} \int_0^1 dt\, e^{tz}\, t^{a-1}(1-t)^{b-a-1} \tag{5.117}$$

Most of the essential properties of $M$, such as its asymptotics for large and small $z$, may be read off directly from this representation.

## 5.9 Self-adjoint operators and boundary conditions

The precise definition of self-adjointness is not just a matter of mathematical sophistication, but instead has physical consequences. On the one hand, a given differential operator may allow for inequivalent domains, resulting in inequivalent physical spectra. On the other hand, an operator that "looks" self-adjoint, but is not actually self-adjoint, may not have a real spectrum, and/or mutually orthogonal eigenspaces associated with distinct eigenvalues. We illustrate these possibilities below with the help of some concrete examples.

### 5.9.1 Example 1: One-dimensional Schrödinger operator on half-line

Consider a 1-dim quantum system given by the following Hamiltonian,

$$H_1 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \tag{5.118}$$

As an operator on complex functions on the real line, and for a "reasonable" potential $V(x)$, the Hamiltonian $H_1$ is self-adjoint. The domain $\mathcal{D}(H_1)$ may be taken to be the sub-space of $L^2(\mathbf{R})$ consisting of infinitely differentiable functions (denoted $C^\infty$) which vanish at $x = \pm\infty$. Self-adjointness then follows from the fact that all functions in $\mathcal{D}(H_1)$ vanish at $x = \pm\infty$.

As an operator on functions on $x \in [0, +\infty]$, the Hamiltonian $H_1$ may be self-adjoint for certain choices of the domain, but not for others. The key relation is as follows,

$$(\psi, H_1\phi) - (H_1\psi, \phi) = \frac{\hbar^2}{2m}j(0) \tag{5.119}$$

where $j(x)$ is the probability current density, defined by

$$j(x) = \phi(x)\frac{d\psi^*}{dx}(x) - \psi^*(x)\frac{d\phi}{dx}(x) \tag{5.120}$$

The operator $H_1$ will be self-adjoint if a domain $\mathcal{D}(H_1)$ can be chosen for the functions $\psi$ and $\phi$ such that $j(0) = 0$ for *any pair* $\psi, \phi \in \mathcal{D}(H_1)$. This will be the case if the domain is defined to be the subspace of $C^\infty$ functions which obey

$$\psi(0) + \lambda \frac{d\psi}{dx}(0) = 0 \tag{5.121}$$

for a given real constant $\lambda$. Note that $\lambda = 0$ and corresponds to Dirichlet boundary conditions, while $\lambda = \infty$ corresponds to Neumann boundary conditions. Thus, $\lambda$ parametrizes an *interpolation between Dirichlet and Neumann boundary conditions*, and for each value of $\lambda$, $H_1$ is self-adjoint.

The spectrum of $H_1$ depends on $\lambda$ even though, at face value, the differential operator $H_1$ of (5.118) does not involve $\lambda$. Consider, for example, the problem with a potential $V(x) = 0$ for $0 \le x < \ell$, and $V(x) = +\infty$ for $x \ge \ell$, and solve for the eigenvalues $E$ of $H_1$. To satisfy the vanishing boundary condition at $x = \ell$, we must have

$$\psi(x) = \sin k(x - \ell) \qquad\qquad E = \frac{\hbar^2 k^2}{2m} \tag{5.122}$$

where $k$ can be any positive real number. Enforcing also the $\lambda$-dependent boundary condition (5.121) at $x = 0$ renders the spectrum of $k$ discrete, and requires,

$$\mathrm{tg}(k\ell) = \lambda k \tag{5.123}$$

We recover the special cases,

$$\lambda = 0 \qquad\qquad k_n = \frac{2n\pi}{2\ell} \qquad\qquad n = 1, 2, 3, \cdots$$

$$\lambda = \infty \qquad\qquad k_n = \frac{(2n-1)\pi}{2\ell} \tag{5.124}$$

For intermediate values of $\lambda$, the solutions are transcendental, and may be determined graphically. They clearly interpolate between the above cases. Thus, the spectrum depends on the precise domain, through the boundary conditions.

### 5.9.2 Example 2: One-dimensional momentum in a box

Next, consider the 1-dim quantum system given by the Hamiltonian,

$$H_2 = i\hbar c \frac{d}{dx} \tag{5.125}$$

As an operator on functions on the real line, $H_2$ is self-adjoint. But what happens when we attempt to put the system in a box ? For example, can $H_2$ be self-adjoint when acting on functions on the finite interval $[0, \ell]$ with $\ell > 0$ ?

Before launching into any math, let's solve the Schrödinger equation for $H_2$,

$$i\hbar\frac{\partial}{\partial t}\psi(t,x) = i\hbar c\frac{\partial}{\partial x}\psi(t,x) \tag{5.126}$$

or equivalently

$$\left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}\right)\psi(t,x) = 0 \tag{5.127}$$

The general solution of this equation is $\psi(t,x) = f(x - ct)$ for any function $f$ of one variable. The wave function corresponds to a purely right-moving particle. The Schrödinger equation turns out to be so restrictive that no left-moving particles can be allowed in the spectrum. We now immediately see why imposing a boundary condition on this Hamiltonian could be problematic. Both Dirichlet and Neumann boundary conditions would correspond to a reflection of waves, which cannot happen. The only allowed boundary condition on an interval would be periodic boundary conditions, since the right-moving wave could then freely continue to travel without having to be reflected.

This may be seen concretely on the interval $[0, \ell]$, as follows,

$$(\psi, H_2\phi) - (H_2\psi, \phi) = i\hbar c\Big(\psi(x)^*\phi(x)\Big)\Big|_{x=0}^{x=\ell} \tag{5.128}$$

Self-adjointness of $H_2$ requires the vanishing of the right hand side. If we require $\psi(\ell) = \psi(0) = 0$, then $\phi(\ell)$ and $\phi(0)$ can take any values, so this choice of domain does not lead to a self-adjoint $H_2$. Assuming now that $\psi(0) \neq 0$, and $\phi(0) \neq 0$, the vanishing of (5.128) is equivalent to,

$$\frac{\psi^*(\ell)}{\psi^*(0)}\frac{\phi(\ell)}{\phi(0)} = 1 \tag{5.129}$$

whose general solution is given by the Bloch wave periodicity condition,

$$\begin{aligned}\psi(\ell) &= e^{i\theta}\psi(0)\\ \phi(\ell) &= e^{i\theta}\phi(0)\end{aligned} \tag{5.130}$$

for a real parameter $\theta$. The spectrum of $H_2$ again depends on $\theta$, since the eigenstate wave functions are given by

$$\psi_n(x) = e^{ik_n x} \qquad k_n = (\theta + 2\pi n)/\ell \qquad n \in \mathbf{Z} \tag{5.131}$$

The eigenvalues of $H_2$ are then given by $-\hbar c k_n$, and are real. Notice that the eigenfunctions are also mutually orthogonal for distinct $n$, as we indeed expect from a self-adjoint operator.

### 5.9.3 Example 3: One-dimensional Dirac-like operator in a box

A lesson we have learned from Example 2 is that the momentum operator corresponds to a quantum system of left-movers only, (and no right-movers), a situation that vitiates the possibility of imposing any reflecting boundary conditions. We may double the number of degrees of freedom, however, and include one left-moving and one right-moving degree of freedom. Thus, we consider doublets of wave functions $\psi_1$ and $\psi_2$,

$$\psi \equiv \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \qquad\qquad \phi \equiv \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \tag{5.132}$$

with Hermitean inner product,

$$(\psi, \phi) = \int_0^\ell dx \, (\psi_1^* \phi_1 + \psi_2^* \phi_2) \, (x) \tag{5.133}$$

and Hamiltonian (here we use the standard notation $\partial_x \equiv \partial/\partial x$),

$$H_3 = \hbar c \begin{pmatrix} 0 & \partial_x \\ -\partial_x & 0 \end{pmatrix} \tag{5.134}$$

It is straightforward to evaluate the combinations,

$$\begin{aligned}
(H_3\psi, \phi) &= \hbar c \int_0^\ell dx \Big( \partial_x \psi_2^* \phi_1 - \partial_x \psi_1^* \phi_2 \Big)(x) \\
(\psi, H_3\phi) &= \hbar c \int_0^\ell dx \Big( \psi_1^* \partial_x \phi_2 - \psi_2^* \partial_x \phi_1 \Big)(x)
\end{aligned} \tag{5.135}$$

and

$$(H_3\psi, \phi) - (\psi, H_3\phi) = \hbar c \Big( \psi_2 \phi_1(\ell) - \psi_1^* \phi_2(\ell) - \psi_2 \phi_1(0) + \psi_1^* \phi_2(0) \Big) \tag{5.136}$$

Self-adjointness of $H_3$ requires this combination to vanish. This may be achieved by imposing, for example, the *MIT bag boundary conditions* (which were introduced to model quarks confined to nucleons),

$$\begin{aligned}
\phi_2(\ell) &= \lambda_\ell \phi_1(\ell) & \phi_2(0) &= \lambda_0 \phi_1(0) \\
\psi_2(\ell) &= \lambda_\ell \psi_1(\ell) & \psi_2(0) &= \lambda_0 \psi_1(0)
\end{aligned} \tag{5.137}$$

for two real independent constants $\lambda_0$ and $\lambda_\ell$. The spectrum of $H_3$ is now real, but does depend upon $\lambda_0$ and $\lambda_\ell$.

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# 6    Quantum Mechanics Systems

Quantum systems associated with systems of classical mechanics are fundamental. In fact, it is for these systems that we write the Schrödinger equation; they will also admit a formulation in terms of functional integrations over all possible paths, to be discussed in 221B. It is useful to begin with a brief review of Lagrangian and Hamiltonian mechanics.

## 6.1    Lagrangian mechanics

At a most basic level, we describe systems by the time-evolution of the individual particles that make up the system. Particle $n$ is characterized in classical mechanics by its position $\mathbf{r}_n(t)$ at any given time $t$. It is a fact of Nature that its basic laws involve equations that are first or second order in time derivatives, but not higher. Newton's force law $\mathbf{F} = M\mathbf{a}$, for example, is second order in time derivatives. As a result, the initial conditions of a classical system are the positions $\mathbf{r}_n$ and velocities $\dot{\mathbf{r}}_n$ of each of its constituent particles. The laws of physics then yield the positions at later times.

The starting point of Lagrangian mechanics is a set of *generalized positions* $q_i$ with $i = 1, \cdots, N$, describing all the degrees of freedom of classical particles. For $n$ particles in 3-dimensional space, for example, we use $N = 3n$ generalized position variables $q_i$. The associated generalized velocities are denoted by $\dot{q}_i = dq_i/dt$. Under the assumption of at most second order time derivative evolution equations, Lagrangian mechanics will be completely specified by a single function,

$$L(q, \dot{q}; t) = L(q_1, \cdots, q_N, \dot{q}_1, \cdots, \dot{q}_N; t) \tag{6.1}$$

referred to as *the Lagrangian*. The associated Euler-Lagrange equations

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0 \qquad\qquad i = 1, \cdots, N \tag{6.2}$$

arise as the solution to a variational principle of the action functional

$$S[q] = S[q_1, \cdots, q_N] = \int_{t_1}^{t_2} dt\, L(q_1, \cdots, q_N, \dot{q}_1, \cdots, \dot{q}_N; t) \tag{6.3}$$

The notation $S[q_1, \cdots, q_N]$ indicated that $S$ is a functional of the path $(q_1(t), \cdots, q_N(t))$ spanned for $t \in [t_1, t_2]$. To derive the Euler-Lagrange equations from the action, we perform a variation $\delta q_i(t)$ on the path $q_i(t)$, keeping the end points fixed,

$$\delta q_i(t_1) = \delta q_i(t_2) = 0 \tag{6.4}$$

The variation is then computed using standard chain rule,

$$
\begin{aligned}
\delta S[q] &= S[q + \delta q] - S[q] \\
&= \int_{t_1}^{t_2} dt \Big( L(q + \delta q, \dot{q} + \delta \dot{q}; t) - L(q, \dot{q}; t) \Big) \\
&= \int_{t_1}^{t_2} dt \sum_i \Big( \frac{\partial L}{\partial q_i} \delta q_i + \frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i \Big)
\end{aligned}
\tag{6.5}
$$

Using now the fact that

$$
\delta \dot{q}_i = \frac{d}{dt} \delta q_i
\tag{6.6}
$$

integrating by parts and using the vanishing boundary conditions, we are left with

$$
\delta S[q] = \int_{t_1}^{t_2} dt \sum_i \Big( -\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} + \frac{\partial L}{\partial q_i} \Big) \delta q_i
\tag{6.7}
$$

Finally, requiring that a path be stationary amounts to requiring that a small variation around the path leaves the action unchanged $\delta S[q] = 0$, which clearly is equivalent to the Euler-Lagrange equations.

In the simplest examples, the Lagrangian is the difference between kinetic and potential energy $V$ of the generalized positions,

$$
L_V = \frac{1}{2} \sum_{i=1}^{N} m_i \dot{q}_i^2 - V(q_1, \cdots, q_N)
\tag{6.8}
$$

for which the Euler-Lagrange equations are

$$
m_i \ddot{q}_i = -\frac{\partial V}{\partial q_i}
\tag{6.9}
$$

In a slightly more complicated example, we have the Lagrangian of a charged particle in 3 space dimensions in the presence of an electric $\mathbf{E}(\mathbf{r}, t)$ and magnetic field $\mathbf{B}(\mathbf{r}, t)$, which derive from an electric potential $\Phi(\mathbf{r}, t)$ and vector field $\mathbf{A}(\mathbf{r}, t)$ as follows,

$$
\mathbf{E} = -\vec{\nabla}\Phi - \frac{\partial \mathbf{A}}{\partial t} \qquad\qquad \mathbf{B} = \vec{\nabla} \times \mathbf{A}
\tag{6.10}
$$

The associated Lagrangian for a particle with electric charge $e$, mass $m$, and position $\mathbf{r}$ is,

$$
L_A = \frac{1}{2} m \dot{\mathbf{r}}^2 - e\Phi(\mathbf{r}, t) + e\mathbf{A}(\mathbf{r}, t) \cdot \dot{\mathbf{r}}
\tag{6.11}
$$

Check that the Euler-lagrange equation coincides with the Lorentz force law

$$
m\ddot{\mathbf{r}} = e\mathbf{E}(\mathbf{r}, t) + e\dot{\mathbf{r}} \times \mathbf{B}(\mathbf{r}, t)
\tag{6.12}
$$

## 6.2 Hamiltonian mechanics

Returning to the general case, with Lagrangian $L(q, \dot{q}; t)$, one defines the *momentum* $p_i$ *canonically conjugate to* $q_i$ as follows,

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \tag{6.13}$$

For the simplest systems, like the Lagrangian $L_V$, the canonical momentum coincides with the mechanical momentum, given by mass times velocity, $p_i = m_i \dot{q}_i$. But for more complicated Lagrangians, like $L_A$, the two quantities differ, and one has in this case $\mathbf{p} = m\dot{\mathbf{r}} + e\mathbf{A}$.

We shall assume that the relation $p_i = p_i(q, \dot{q}; t)$ is invertible,[5] so that the generalized velocities can be obtained uniquely as a function of the generalized coordinates and momenta,

$$\dot{q}_i = \dot{q}_i(q, p; t) \tag{6.14}$$

The Hamiltonian is now defined as the Legendre transform of the Lagrangian,

$$H(q, p; t) = \sum_{i=1}^{N} p_i \dot{q}_i - L(q, \dot{q}; t) \tag{6.15}$$

with the understanding that the velocities are eliminated in favor of $q$ and $p$ on the rhs using (6.14). The space of all allowed positions $q_i$ and momenta $p_i$ is referred to as *phase space*. Hamiltonian mechanics is formulated in terms of time evolution equations (or flows) on phase space.

The Hamilton equations are obtained as follows. Under a general variation of $q$ and $p$, the rhs above transforms as,

$$\delta H = \sum_i \left( \delta p_i \dot{q}_i + p_i \delta \dot{q}_i - \frac{\partial L}{\partial q_i} \delta q_i - \frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i \right) \tag{6.16}$$

Notice that the second and fourth terms on the rhs cancel by the very definition of $p_i$. Alternatively, the variation of $H$ in terms $p$ and $q$ only gives,

$$\delta H = \sum_i \left( \frac{\partial H}{\partial q_i} \delta q_i + \frac{\partial H}{\partial p_i} \delta p_i \right) \tag{6.17}$$

Comparing the two expressions for $\delta H$ and using the Euler-Lagrange equation gives the Hamilton equations,

$$\frac{\partial H}{\partial q_i} = -\dot{p}_i \qquad\qquad \frac{\partial H}{\partial p_i} = \dot{q}_i \tag{6.18}$$

---

[5]There are many physically interesting Lagrangians where this relation is not invertible. These systems are referred to as having *constraints*.

Since the number of dynamical variables on phase space has been doubled up, Hamilton's equations are now first order.

There is a somewhat formal structure on phase space, the *Poisson bracket* which is very useful for quantum mechanics. For any two functions $a(q, p)$ and $b(q, p)$, it is defined by

$$\{a, b\} \equiv \sum_{i=1}^{N} \left( \frac{\partial a}{\partial q_i} \frac{\partial b}{\partial p_i} - \frac{\partial a}{\partial p_i} \frac{\partial b}{\partial q_i} \right) \tag{6.19}$$

The Poisson bracket is linear in $a$ and $b$, anti-symmetric under interchange of its arguments $\{a, b\} = -\{b, a\}$, acts as a derivative in each argument,

$$\{a, bc\} = \{a, b\}c + \{a, c\}b \tag{6.20}$$

and satisfies the Jacobi identity,

$$\{\{a, b\}, c\} + \{\{b, c\}, a\} + \{\{c, a\}, b\} = 0 \tag{6.21}$$

It also satisfies the elementary relation

$$\{q_i, p_j\} = \delta_{i,j} \tag{6.22}$$

The time derivative of any function $A(q, p; t)$ may be expressed simply via Poisson brackets,

$$\frac{d}{dt} a(q, p; t) = \frac{\partial}{\partial t} a(q, p; t) + \sum_i \left( \frac{\partial a}{\partial q_i} \dot{q}_i + \frac{\partial a}{\partial p_i} \dot{p}_i \right) \tag{6.23}$$

Using Hamilton's equations to obtain $\dot{q}_i$ and $\dot{p}_i$, we have

$$\frac{d}{dt} a(q, p; t) = \frac{\partial}{\partial t} a(q, p; t) + \{a, H\} \tag{6.24}$$

In particular, Hamilton's equations may be recast in the following form,

$$\begin{aligned} \dot{q}_i &= \{q_i, H\} \\ \dot{p}_i &= \{p_i, H\} \end{aligned} \tag{6.25}$$

## 6.3   Constructing a quantum system from classical mechanics

There are two general procedures for associating a quantum system with a system of classical mechanics. The first is via the *correspondence principle* which produces a Hilbert space, a set of observables and a Hamiltonian from a classical mechanics system in the Hamiltonian

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formulation. A second is via the *functional or path integral* which directly produces probability amplitudes from a classical mechanics system in the Lagrangian formulation; this method will be discussed in the next section.

Let the classical mechanics system be given by a Hamiltonian $H(q, p)$ on a phase space $q_i, p_j$, with $i, j = 1, \cdots, N$,

$$\{q_i, p_j\} = \delta_{i,j} \qquad\qquad \dot{a}(q, p) = \{a, H\} \qquad\qquad (6.26)$$

The correspondence principle states that, to this classical system, there corresponds a quantum system with the following observables,

| classical variable | | Quantum Observable |
|:---:|:---:|:---:|
| $q_i$ | $\rightarrow$ | $Q_i$ |
| $p_i$ | $\rightarrow$ | $P_i$ |
| $a(p, q)$ | $\rightarrow$ | $A(P, Q)$ |
| $\{a, b\}$ | $\rightarrow$ | $-\dfrac{i}{\hbar}[A, B]$ | (6.27) |

In particular, the classical Hamiltonian has a quantum counterpart $H(P, Q)$, and the Poisson bracket relations between $q_i$ and $p_j$ become the canonical commutation relations,

$$[Q_i, P_j] = i\hbar\delta_{i,j} \qquad\qquad [Q_i, Q_j] = [P_i, P_j] = 0 \qquad\qquad (6.28)$$

The correspondence principle maps the Hamilton time-evolution equations into the Schrödinger equation for observables, i.e. given in the Heisenberg formulation,

$$i\hbar\frac{d}{dt}A = [A, H] + i\hbar\frac{\partial}{\partial t}A \qquad\qquad (6.29)$$

The evolution operator may be used to translate the Heisenberg formulation into the Schrödinger formulation.

## 6.4 Schrödinger equation with a scalar potential

In the usual *position realization* of the canonical commutation relations, given by

$$Q_i = q_i \qquad\qquad P_i = -i\hbar\frac{\partial}{\partial q_i} \qquad\qquad (6.30)$$

the Hilbert space is that of of square integrable functions of $q_i$. The simplest non-relativistic classical mechanical systems, given in terms of a potential $V(q)$, with Hamiltonian,

$$H(\mathbf{q}, \mathbf{p}) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{q}) \qquad\qquad (6.31)$$

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have a unique quantum Hamiltonian, given by the correspondence principle,

$$H(\mathbf{Q}, \mathbf{P}) = \frac{\mathbf{P}^2}{2m} + V(\mathbf{Q}) \tag{6.32}$$

In the position representation of $Q_i$ and $P_i$, the Hamiltonian becomes a differential operator acting on wave functions. The time-dependent Schrödinger equation then becomes,

$$i\hbar \frac{\partial \psi(\mathbf{q}, t)}{\partial t} = -\frac{\hbar^2}{2m} \Delta_{\mathbf{q}} \psi(\mathbf{q}.t) + V(\mathbf{q})\psi(\mathbf{q}, t) \tag{6.33}$$

where $\Delta = \Delta_{\mathbf{q}}$ is the standard Laplace operator on functions of $\vec{q}$, defined by

$$\Delta = \Delta_{\mathbf{q}} \equiv \sum_{i=1}^{N} \frac{\partial^2}{\partial q_i \partial q_i} \tag{6.34}$$

Specializing to energy eigenvalues and eigenfunctions,

$$\psi(\mathbf{q}, t) = e^{-iEt/\hbar} \psi_E(\mathbf{q}) \tag{6.35}$$

we recover the standard time-independent Schrödinger equation,

$$-\frac{\hbar^2}{2m} \Delta \psi_E(\mathbf{q}) + V(\mathbf{q})\psi_E(\mathbf{q}) = E\psi_E(\mathbf{q}) \tag{6.36}$$

## 6.5 Uniqueness questions of the correspondence principle

But note that this standard realization is *not unique*. For example, we could just as well have chosen the *momentum realization* of the canonical commutation relations, in which we would have instead, $P_i = p_i$ and $Q_i = +i\hbar \partial/\partial p_i$. The Hilbert space is simply the space of square integrable functions of $p_i$. Such alternative realizations are sometimes really useful. Suppose we had to solve the very bizarre looking quantum system for the Hamiltonian,

$$H = \frac{C_1}{|\mathbf{P}|} + C_2 \mathbf{X}^2 \tag{6.37}$$

In the momentum realization, the problem is actually just the Coulomb problem !!

For the simplest classical mechanical systems, the corresponding quantum system is unique, but this need not be so in general. Suppose, for example, that the classical Hamiltonian contained not just a potential of $q$, but also an interaction of the type $2p^2 U(p)$ for some function $U$. There are clearly two (and in fact an infinite number) of inequivalent ways of writing down a corresponding (self-adjoint) quantum interaction. For example,

$$2pU(q)p \quad \neq \quad p^2 U(q) + U(q)p^2 \tag{6.38}$$

From classical mechanics, there is no way to decide. On the quantum side, both produce self-adjoint Hamiltonians. This *ordering ambiguity* almost never matters much in quantum mechanics but it does play a crucial role in quantum field theory.

# 7  Charged particle in an electro-magnetic field

Of fundamental importance is the problem of an electrically charged particle in the presence of electro-magnetic fields. To construct the Schrödinger equation for this system, we use the correspondence principle. We start from the classical Lagrangian for a non-relativistic particle with mass $m$, and electric charge $e$, in the presence of a general electro-magnetic field, given in terms of the electric potential $\Phi$ and the vector potential $\mathbf{A}$,

$$L(\mathbf{r}, \dot{\mathbf{r}}, t) = \frac{1}{2} m \dot{\mathbf{r}}^2 - e\Phi(\mathbf{r}, t) + e\mathbf{A}(\mathbf{r}, t) \cdot \dot{\mathbf{r}} \tag{7.1}$$

We allow the electro-magnetic fields to be time-dependent as this would be required, for example, when dealing with a charged particle in the presence of an electro-magnetic wave. The momentum $\mathbf{p}$ canonically conjugate to $\mathbf{r}$ is given by,

$$\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{r}}} = m\dot{\mathbf{r}} + e\mathbf{A}(\mathbf{r}, t) \tag{7.2}$$

The Hamiltonian is then obtained by eliminating $\dot{\mathbf{r}}$ in favor of $\mathbf{p}$ is the expression,

$$H = \mathbf{p} \cdot \dot{\mathbf{r}} - L(\mathbf{r}, \dot{\mathbf{r}}, t) \tag{7.3}$$

This problem is algebraic; it is easily carried out explicitly, and we find,

$$H(\mathbf{r}, \mathbf{p}, t) = \frac{1}{2m} \Big( \mathbf{p} - e\mathbf{A}(\mathbf{r}, t) \Big)^2 + e\Phi(\mathbf{r}, t) \tag{7.4}$$

By the correspondence principle, we promote the classical variables $\mathbf{r}$ and $\mathbf{p}$ to operators obeying canonical commutation relations. The time-dependent Schrödinger equation in the position realization is then given by,

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = \frac{1}{2m} \Big( -i\hbar \nabla_{\mathbf{r}} - e\mathbf{A}(\mathbf{r}, t) \Big)^2 \psi(\mathbf{r}, t) + e\Phi(\mathbf{r}, t)\psi(\mathbf{r}, t) \tag{7.5}$$

In the remainder of this chapter, we proceed to exhibiting the gauge invariance of this equation, and then studying applications to constant fields, Landau levels, the Aharonov-Bohm effect, and the quantization conditions for Dirac magnetic monopoles.

## 7.1  Gauge transformations and gauge invariance

Recall that the electric and magnetic fields are given in terms of $\Phi$ and $\mathbf{A}$ by

$$\mathbf{B} = \nabla \times \mathbf{A} \qquad\qquad \mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \nabla\Phi \tag{7.6}$$

Under gauge transformations,

$$\mathbf{A} \to \mathbf{A}' = \mathbf{A} + \nabla\theta \qquad\qquad \Phi \to \Phi' = \Phi - \frac{\partial\theta}{\partial t} \qquad\qquad (7.7)$$

the fields $\mathbf{B}$ and $\mathbf{E}$ are invariant (i.e. $\mathbf{B} \to \mathbf{B}' = \mathbf{B}$ and $\mathbf{E} \to \mathbf{E}' = \mathbf{E}$) for an arbitrary function $\theta = \theta(\mathbf{r}, t)$. The classical Lagrangian transforms as follows,

$$L \to L' = L + e\Big(\dot{r} \cdot \nabla\theta + \frac{\partial\theta}{\partial t}\Big) = L' + \frac{d(e\theta)}{dt} \qquad\qquad (7.8)$$

As a result, the classical action $S = \int dt\, L$ is invariant (except for boundary effects) and hence the classical mechanics of a charged particle is invariant under such gauge transformations. This is of course well-known, since the equations of motion reduce to

$$m\ddot{\mathbf{r}} = e\mathbf{E}(\mathbf{r}, t) + e\dot{\mathbf{r}} \times \mathbf{B}(\mathbf{r}, t) \qquad\qquad (7.9)$$

which are manifestly gauge invariant.

The Schrödinger equation (7.5) is now *invariant* since the fields $\mathbf{A}$ and $\Phi$ are clearly changed under the transformation, but (7.5) is instead *covariant* provided we also transform the wave function by,

$$\psi(\mathbf{r}, t) \to \psi'(\mathbf{r}, t) = e^{i\gamma\theta}\psi(\mathbf{r}, t) \qquad\qquad (7.10)$$

for some constant $\gamma$, which remains to be determined. To see how this works, we use the gauge transformation rules of (19.6) and (7.10) to derive the following intermediate formulas,

$$
\begin{aligned}
\Big(-i\hbar\nabla_{\mathbf{r}} - e\mathbf{A}'\Big)\psi' &= e^{i\gamma\theta}\Big(-i\hbar\nabla_{\mathbf{r}} - e\mathbf{A}\Big)\psi + e^{i\gamma\theta}(\hbar\gamma + e)(\nabla\theta)\psi \\
\Big(i\hbar\partial_t - e\Phi'\Big)\psi' &= e^{i\gamma\theta}\Big(i\hbar\partial_t - e\Phi(\mathbf{r}, t)\Big)\psi + e^{i\gamma\theta}(\hbar\gamma + e)(\partial_t\theta)\psi
\end{aligned}
\qquad (7.11)
$$

For the value

$$\gamma = -\frac{e}{\hbar} \qquad\qquad (7.12)$$

the second terms on the right hand side cancel, and we see that these particular combinations (referred to as *gauge covariant derivatives*) transform exactly in the same manner that the wave function $\psi$ did in (19.6). As a result, the full Schrödinger equation transforms just as $\psi$ did, and this property is referred to as *covariance* of the equation.

## 7.2 Constant Magnetic fields

An important special case is when the electric and magnetic fields are constant in time, and uniform in space, so that

$$\mathbf{A}(\mathbf{r}, t) = \frac{1}{2}\mathbf{B} \times \mathbf{r} \qquad\qquad \Phi(\mathbf{r}, t) = -\mathbf{E} \cdot \mathbf{r} \qquad\qquad (7.13)$$

Here, we have chosen a particular convenient gauge. The Hamiltonian is then time-independent, and we may specialize to the eigenfunctions $\psi_E(\mathbf{r})$ at fixed energy $E$, which now obey the time-independent Schrödinger equation,

$$\frac{1}{2m}\left(-i\hbar\nabla_{\mathbf{r}} - \frac{1}{2}e\mathbf{B} \times \mathbf{r}\right)^2 \psi_E(\mathbf{r}) - e\mathbf{E} \cdot \mathbf{r}\psi_E(\mathbf{r}) = E\psi_E(\mathbf{r}) \qquad (7.14)$$

This system is akin to a harmonic oscillator problem. Instead of trying to solve the Schrödinger equation explicitly (in terms of Hermite polynomials etc), we shall fully exploit its relation with the harmonic oscillator and solve for the spectrum using operator methods.

In fact, we will set $\mathbf{E} = 0$, concentrating on the purely magnetic problem. Choosing the $z$-axis to coincide with the direction of $\mathbf{B}$, the problem may be reduced to a 2-dimensional one, since motion along the $z$-direction is insensitive to the magnetic field. To make the problem even more interesting, we add a harmonic oscillator with frequency $\omega$. Thus, the effective Hamiltonian of the system is now,

$$H = \frac{1}{2m}\left(p_x + \frac{1}{2}eBy\right)^2 + \frac{1}{2m}\left(p_y - \frac{1}{2}eBx\right)^2 + \frac{1}{2}m\omega^2(x^2 + y^2) \qquad (7.15)$$

Combining terms of the form $x^2 + y^2$, we may recast $H$ as follows,

$$H = \frac{1}{2m}(p_x^2 + p_y^2) - \frac{eB}{2m}(xp_y - yp_x) + \frac{1}{2}m\omega_B^2(x^2 + y^2) \qquad (7.16)$$

where we have defined the frequency $\omega_B$ by,

$$\omega_B^2 = \omega^2 + \frac{e^2B^2}{4m^2} \qquad (7.17)$$

We recognize the middle term in $H$ as the orbital angular momentum operator $L_z$. Clearly, this term commutes with $H$ and may be diagonalized simultaneously with $H$.

### 7.2.1 Map onto harmonic oscillators

To solve this system, we introduce the following harmonic oscillator combinations,

$$\begin{aligned} a_1 &= \frac{1}{\sqrt{2m\hbar\omega_B}}(ip_x + m\omega_B x) \\ a_2 &= \frac{1}{\sqrt{2m\hbar\omega_B}}(ip_y + m\omega_B y) \end{aligned} \qquad (7.18)$$

and their adjoints $a_1^\dagger$ and $a_2^\dagger$. By construction they obey canonical commutation relations $[a_i, a_j^\dagger] = \delta_{ij}$ for $i, j = 1, 2$, while $[a_1, a_2] = [a_1^\dagger, a_2^\dagger] = 0$. Re-expressing the Hamiltonian in terms of these oscillators, we find,

$$H = \hbar\omega_B \left(a_1^\dagger a_1 + a_2^\dagger a_2 + 1\right) + i\frac{eB\hbar}{2m}\left(a_1^\dagger a_2 - a_2^\dagger a_1\right) \tag{7.19}$$

Finally, we make the following orthonormal change of variables from $a_{1,2}$ to $a_\pm$,

$$a_\pm \equiv \frac{1}{\sqrt{2}}(a_1 \pm ia_2) \tag{7.20}$$

and their conjugates. These oscillators still obey canonical commutation relations,

$$[a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0 \qquad\qquad [a_i, a_j^\dagger] = \delta_{i,j} \qquad i, j = +, - \tag{7.21}$$

Using the following relations (the $\pm$ signs are correlated),

$$2a_\pm^\dagger a_\pm = a_1^\dagger a_1 + a_2^\dagger a_2 \pm i\left(a_1^\dagger a_2 - a_2^\dagger a_1\right) \tag{7.22}$$

the Hamiltonian may be recast as follows,

$$H = \frac{1}{2}\hbar\omega_+\left(1 + 2a_+^\dagger a_+\right) + \frac{1}{2}\hbar\omega_-\left(1 + 2a_-^\dagger a_-\right) \tag{7.23}$$

where the combinations $\omega_\pm$ are defined by

$$\omega_\pm = \omega_B \pm \left|\frac{eB}{2m}\right| \geq 0 \tag{7.24}$$

We have now achieved our goal: the magnetic field Hamiltonian has been expressed in terms of two independent harmonic oscillator variables $a, b$.

To solve for the spectrum is straightforward. The ground state $|0,0\rangle$ satisfies $a_\pm|0,0\rangle = 0$, and the excited states are given by

$$|n_+, n_-\rangle = \mathcal{N}(n_+, n_-)\,(a_+)^{n_+}(a_-)^{n_-}\,|0,0\rangle \qquad\qquad n_\pm \geq 0 \tag{7.25}$$

where $\mathcal{N}$ is the normalization factor. The corresponding eigenvalue is simply,

$$E(n_+, n_-) = \frac{1}{2}\hbar\omega_+(1 + 2n_+) + \frac{1}{2}\hbar\omega_-(1 + 2n_-) \tag{7.26}$$

Two different states $|n_+, n_-\rangle$ and $|n_+', n_-'\rangle$ will be degenerate provided

$$\omega_+(n_+' - n_+) + \omega_-(n_-' - n_-) = 0 \tag{7.27}$$

Since $n_\pm, n_\pm'$ are integers, this relation can have solutions if and only if $\omega_-/\omega_+$ is *rational* (including the value 0). If this is the case, we write $\omega_\pm = k_\pm\omega_0$ where $k_+ > 0$ and $k_- \geq 0$ are relatively prime integers. All states degenerate with $|n_+, n_-\rangle$ are then given by $|n_+ + nk_-, n_- - nk_+\rangle$ for any integer $n$ such that $n_- \geq nk_+$. If $\omega_- = 0$, namely $\omega = 0$, this degeneracy is infinite, as $n$ can take an infinite number of different values, while if $\omega_- > 0$, the degeneracy is necessarily finite.

## 7.3    Landau Levels

For a charged particle in a magnetic field without the harmonic oscillator present, we have $\omega = 0$ and $\omega_- = 0$, and the spectrum becomes infinitely degenerate, since the energies do not depend upon $n_-$ any more. Alternatively, as $\omega = 0$, we have

$$[H, a_-] = [H, a_-^\dagger] = 0 \tag{7.28}$$

For each value of $n_+$, there is a *Landau level* with an infinite degeneracy. The algebra of $a_-$ and $a_-^\dagger$ represent the symmetry algebra of this degeneracy. Of course, in any physical system, space is not truly of infinite extent and the magnetic field is not quite uniform. Nonetheless, this infinite degeneracy makes the Landau levels an incredibly interesting phenomenon.

### 7.3.1    Complex variables

The wave functions in each Landau level exhibit remarkable properties. To exhibit these properties, we change to complex variables. The $x, y$ parts of the combinations $a_\pm$ correspond to forming the complex variables

$$z = \frac{1}{\sqrt{2}}(x + iy) \qquad\qquad p_z = \frac{1}{\sqrt{2}}(p_x - ip_y)$$
$$\bar{z} = \frac{1}{\sqrt{2}}(x - iy) \qquad\qquad p_{\bar{z}} = \frac{1}{\sqrt{2}}(p_x + ip_y) \tag{7.29}$$

which satisfy the canonical commutation relations,

$$\begin{aligned}
[z, p_z] = [\bar{z}, p_{\bar{z}}] &= i\hbar \\
[z, p_{\bar{z}}] = [\bar{z}, p_z] &= 0
\end{aligned} \tag{7.30}$$

and as a result,

$$p_z = -i\hbar\frac{\partial}{\partial z} \qquad\qquad p_{\bar{z}} = -i\hbar\frac{\partial}{\partial \bar{z}} \tag{7.31}$$

The oscillators now become,

$$a_+ = \frac{1}{\sqrt{2m\hbar\omega_B}}\Big(ip_{\bar{z}} + m\omega_B z\Big) \qquad\qquad a_+^\dagger = \frac{1}{\sqrt{2m\hbar\omega_B}}\Big(-ip_z + m\omega_B \bar{z}\Big)$$
$$a_- = \frac{1}{\sqrt{2m\hbar\omega_B}}\Big(ip_z + m\omega_B \bar{z}\Big) \qquad\qquad a_-^\dagger = \frac{1}{\sqrt{2m\hbar\omega_B}}\Big(-ip_{\bar{z}} + m\omega_B z\Big) \tag{7.32}$$

Since $\omega = 0$, the Hamiltonian depends only on $a_+$ and $a_+^\dagger$, $H = \hbar\omega_B(2a_+^\dagger a_+ + 1)$. The lowest Landau level $|0, n_-\rangle$ is characterized by $a_+|0, n_-\rangle = 0$. The wave functions of the lowest

Landau level satisfy the differential equation

$$\left(\frac{\partial}{\partial\bar{z}} + \frac{m\omega_B}{\hbar}z\right)\psi_{(0)}(z,\bar{z}) = 0 \tag{7.33}$$

Its general solution is straightforward (since as a differential equation in $\bar{z}$, you may think of $z$ as a constant coefficient), and we get

$$\psi(z,\bar{z}) = \varphi(z)\psi_{(0)}(z,\bar{z}) \qquad\qquad \psi^{(0)}(z,\bar{z}) = \exp\left\{-\frac{m\omega_B}{\hbar}|z|^2\right\} \tag{7.34}$$

where $\varphi(z)$ is an arbitrary complex analytic function of $z$. Actually, $\varphi(z)$ cannot has poles since they would lead to non-square integrable wave functions. Also, assuming that $\psi(z,\bar{z})$ is single-valued, it follows that $\varphi(z)$ must be single-valued, and thus cannot have branch cuts. Therefore, $\varphi(z)$ must be single-valued and holomorphic throughout the complex plane. A basis for such functions is obtained by polynomials (and square integrable Taylor expandable functions by completeness). Notice that all such polynomial functions are obtained by applying $a_-^\dagger$ repeatedly to the ground state $\psi_{(0)}$ of both $a_+$ and $a_-$, since we have

$$\psi_{(n_-)} \sim (a_-^\dagger)^{n_-}\psi_{(0)}(z,\bar{z}) \sim z^{n_-}\psi_{(0)}(z,\bar{z}) \tag{7.35}$$

This agrees with general principles that the group theory of $a_-, a_-^\dagger$ must precisely reproduce the normalizable spectrum.

## 7.4 The Aharonov-Bohm Effect

The classical equations of motion governing a charged particle in an electro-magnetic field involve the fields $\mathbf{B}$ and $\mathbf{E}$, even though both the Lagrangian and the Hamiltonian must be formulated not in terms of $\mathbf{B}$ and $\mathbf{E}$, but rather in terms of the gauge potentials $\Phi$ and $\mathbf{A}$. The quantum equations are based on the Hamiltonian (or on the Lagrangian if one uses path integral methods), and necessarily involves the gauge potentials $\Phi$ and $\mathbf{A}$. This difference leads to measurable effects, of which the most striking are the Aharonov-Bohm effects.

### 7.4.1 The scattering Aharonov-Bohm effect

Consider a beam of particles of charge $e$, moving in a plane perpendicular to an infinite impenetrable straight solenoid with a non-zero magnetic flux $\Phi_B$. One may realize impenetrability by requiring the presence of a potential $V(\mathbf{r})$ which is infinite inside the solenoid, and vanishes outside. Although the particles can propagate only *outside* the solenoid, where $\mathbf{B} = 0$, the presence of the solenoid produces measurable interference effects. Outside the

solenoid, the gauge potential $\mathbf{A}$ must satisfy $\nabla \times \mathbf{A} = 0$. Nonetheless, the gauge potential cannot vanish outside, because we have in view of Stokes' theorem,

$$\oint_C d\mathbf{l} \cdot \mathbf{A} = \int d^2\mathbf{s} \cdot \mathbf{B} = \Phi_B \tag{7.36}$$

where the surface integral $\int d^2\mathbf{s}$ is over the domain enclosed by the curve $C$, which includes the inside of the solenoid (see figure 7).
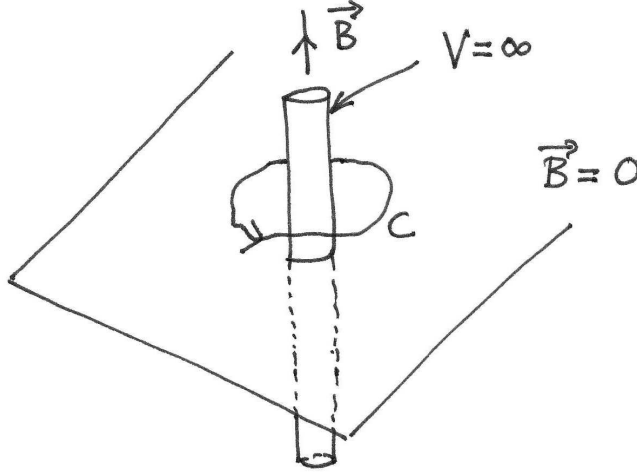


Figure 7: Aharonov-Bohm scattering set-up

A simple solution for the gauge potential is given in cylindrical coordinates $r, \theta, z$ by

$$\mathbf{A}(\mathbf{r}) = \frac{\mathbf{n}_\theta \Phi_B}{2\pi r} \tag{7.37}$$

where $\mathbf{n}_\theta$ is the unit vector along the direction of varying $\theta$, and $r$ is the distance from the center of the solenoid. The wave function for the system is now determined by the following Schrödinger equation,

$$\frac{1}{2m}\left(-i\hbar\nabla - e\mathbf{A}(\mathbf{r})\right)^2 \psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{7.38}$$

To solve this equation, we notice that, outside of the solenoid, $\mathbf{A}$ is actually a gradient,

$$\mathbf{A}(\mathbf{r}) = \nabla\left(\frac{\theta\Phi_B}{2\pi}\right) \tag{7.39}$$

which in particular explains why $\mathbf{B} = 0$ there. The transformation function is not, however, a single-valued function, which is why $\mathbf{A}$ is not quite an honest gauge transformation of

$\mathbf{A} = 0$. Nonetheless, we can use this property to solve the Schrödinger equation, by setting

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) \exp\left\{-i\theta \frac{e\Phi_B}{2\pi\hbar}\right\} \tag{7.40}$$

where $\psi_0(\mathbf{r})$ now satisfies the Schrödinger equation in the absence of any gauge fields,

$$\frac{1}{2m}\left(-i\hbar\nabla\right)^2 \psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{7.41}$$

Imagining now two localized wave packets, with wave functions $\psi_\pm(\mathbf{r})$ traveling parallel into the solenoid from infinity (where we shall choose $\theta = 0$), one packet traveling on the left and one traveling on the right of the solenoid. After passing the solenoid and proceeding far away from the solenoid, the left wave packet is characterized by $\theta = \pi$, which the right packet is characterized by $\theta = -\pi$. Thus asymptotically we have

$$\psi_\pm(\mathbf{r}) \to \psi_0(\mathbf{r}) \exp\left\{\mp i\frac{e\Phi_B}{2\hbar}\right\} \tag{7.42}$$

The total wave function $\psi_+ + \psi_-$ exhibits interference, which is constructive when

$$e\Phi_B = 2\pi\hbar n \tag{7.43}$$

for any integer $n$, and destructive then $n - 1/2$ is an integer. This is a measurable outcome, which has been confirmed by experiment.

### 7.4.2 The bound state Aharonov-Bohm effect

In this set-up a spinless charged particle is constrained to move between two impenetrable concentric cylinders with radii $R_+ > R_-$, impenetrability being again enforced by the presence of a potential $V(\mathbf{r})$ which vanishes for $R_- < |\mathbf{r}| < R_+$ and is infinite otherwise. Inside the small cyclinder, we have a magnetic flux $\Phi_B$, and in between the two cylinders, the magnetic field vanishes (see figure 8).

We shall show that, although the particle is always in a region with $\mathbf{B} = 0$, nonetheless its energy spectrum depends on $\Phi_B$. The gauge potential $\mathbf{A}$ is as in (7.37) and the wave function satisfies (7.38). This time, we work out the Schrödinger equation is cyclindrical coordinates $r, \theta$. The gradient in these coordinates is given by

$$\nabla = \mathbf{n}_r \frac{\partial}{\partial r} + \frac{\mathbf{n}_\theta}{r}\frac{\partial}{\partial \theta} \tag{7.44}$$

where $\mathbf{n}_r$ and $\mathbf{n}_\theta$ are unit vectors in the $r$ and $\theta$ directions respectively. The set-up is invariant under rotations (i.e. translations in $\theta$), so that the angular momentum operator
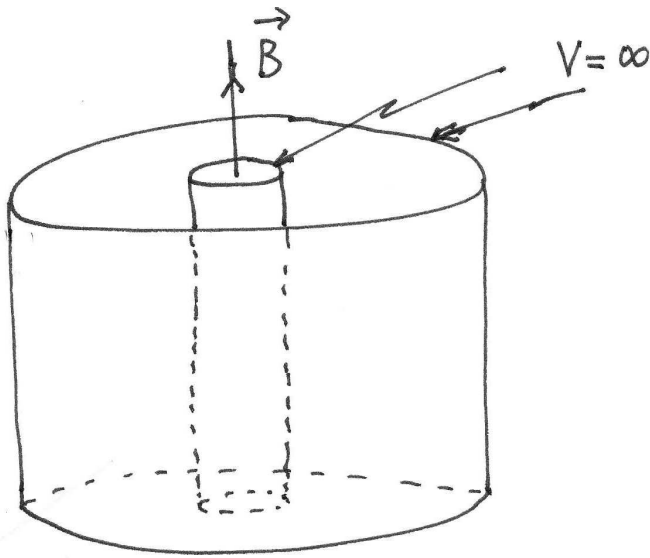
Figure 8: Aharonov-Bohm bound state set-up

$L_z = -i\hbar\partial/\partial\theta$ commutes with the Hamiltonian, and may be diagonalized simultaneously. Thus, we are interested in wave functions for fixed angular momentum $\ell$,

$$\psi(\mathbf{r}) = \psi_\ell(r)\, e^{i\ell\theta} \tag{7.45}$$

The covariant derivative acts as follows,

$$-i\hbar\nabla\psi(\mathbf{r}) - e\mathbf{A}(\mathbf{r})\psi(\mathbf{r}) = -i\hbar e^{i\ell\theta}\left(\mathbf{n}_r\frac{\partial}{\partial r} + \frac{\mathbf{n}_\theta}{r}\left(i\ell + i\nu\right)\right)\psi_\ell(r) \tag{7.46}$$

where we have defined the combination

$$\nu = \frac{e\Phi_B}{2\pi\hbar} \tag{7.47}$$

The radial part of the Schrödinger equation becomes,

$$r^2\psi_\ell'' + r\psi_\ell' + \left(k^2r^2 - (\ell+\nu)^2\right)\psi_\ell = 0 \tag{7.48}$$

The infinite potential $V$ outside $R_- < r < R_+$ imposes the following boundary conditions,

$$\psi_\ell(R_+) = \psi_\ell(R_-) = 0 \tag{7.49}$$

The differential equation is of the Bessel kind, and can be easily solved in terms of those functions. Before we do so, however, much can already be deduced from inspection of (7.48). The most striking property is that the equation depends only on the combination $\ell + \nu$, not on $\ell$ and $\nu$ separately. In particular, the effect of adding a single flux quantum, $\nu = 1$, simply has the effect of moving the spectrum up by one unit of angular momentum, $\ell \to \ell + 1$, but leaving the entire spectrum (for all angular momenta) unchanged. This confirms our earlier

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discovery for the scattering Aharonov-Bohm effect, that the presence of an integer number of basic flux quanta has no measurable effects. For a half flux quantum $\nu = 1/2$, the particle is quantized as a spin 1/2 fermion ! Denoting by $E_0$ the ground state energy for $\ell + \nu = 0$, then adding angular momentum will increase the energy. In figure 9, we show a qualitative picture of how the ground state energy depends on $\nu$. Note that for $|\nu| < 1/2$, the ground state has $\ell = 0$, but as $\nu$ is increased, the ground state is achieved successively for $\ell = -1, \ell = -2, \cdots$.
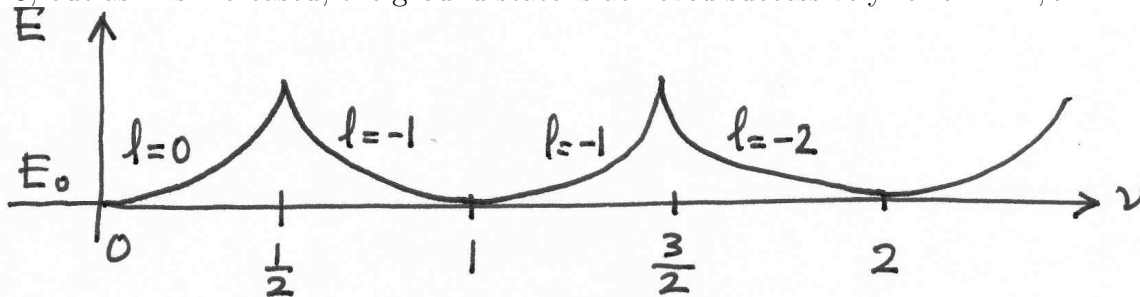


Figure 9: Energy of the ground state for the bound state Aharonov-Bohm effect

Finally, for completeness, we obtain the full spectrum using Bessel functions. The two linearly independent solutions of (7.48) are the Bessel functions $J_{|\ell+\nu|}(kr)$ and $N_{|\ell+\nu|}(kr)$, with small $r$ asymptotics given respectively by $r^{|\ell+\nu|}$ and $r^{-|\ell+\nu|}$. The general solution to (7.48) is then given by,

$$\psi_\ell(r) = \alpha J_{|\ell+\nu|}(kr) + \beta N_{|\ell+\nu|}(kr) \tag{7.50}$$

The boundary conditions impose a quantization condition on $k$,

$$J_{|\ell+\nu|}(kR_+)N_{|\ell+\nu|}(kR_-) - J_{|\ell+\nu|}(kR_-)N_{|\ell+\nu|}(kR_+) = 0 \tag{7.51}$$

In the limit where the inner cylinder has small radius, $R_- \to 0$, we may neglect the second term in this equation, since $J_{|\ell+\nu|}(kR_-) \to 0$ then, and we are left with the condition $J_{|\ell+\nu|}(kR_+) = 0$, so that $kR_+$ is given by the zeros of the Bessel function $J_{|\ell+\nu|}$. Analysis with Maple, for example, readily confirms numerically that the corresponding energies indeed do depend upon $\nu$.

## 7.5 The Dirac magnetic monopole

The existence of a fundamental quantum of magnetic flux has an immediate application to the theoretical existence of *magnetic monopoles* in quantum mechanics. One of Maxwell's equations, $\vec{\nabla} \cdot \mathbf{B} = 0$, states that, classically, there exist no magnetic monopoles. The electric counterpart of this equation is $\vec{\nabla} \cdot \mathbf{E} = \rho$, where $\rho$ is the electric charge density, which can

of course be non-zero. If we had a magnetic pointlike charge $g$ at the origin $\mathbf{x} = 0$, then its magnetic field would be given by

$$\vec{\nabla} \cdot \mathbf{B} = 4\pi g \delta^{(3)}(\mathbf{x}) \qquad\qquad \mathbf{B} = g\,\frac{\mathbf{x}}{|\mathbf{x}|^3} \tag{7.52}$$

where we usually refer to $g$ as the *magnetic charge*. Of course, classical Maxwell's equations do not allow for $g \neq 0$, and we conclude that magnetic monopoles cannot exists as solutions to the classical Maxwell equations.

Dirac proposed that, nonetheless, magnetic monopoles can exist quantum mechanically. To see this, imagine a magnetic field pointing outward radially, as above, combined with magnetic flux brought in from $\infty$ through an infinitesimally thin solenoid, or *Dirac string*. If the incoming flux matches the outgoing radial flux, then flux is conserved and the magnetic field configuration obeys $\vec{\nabla} \cdot \mathbf{B} = 0$ everywhere.

Dirac's remarkable observation is that if the magnetic flux $4\pi g$ of the solenoid is actually an integer multiple of the fundamental magnetic flux quantum $\Phi_B^{(0)} = 2\pi\hbar/e$, then the Dirac string will be unobservable by any charged particle whose charge is an integer multiple of $e$. This gives the famous Dirac quantization condition on the magnetic charge $g$,

$$4\pi g = n\Phi_B^{(0)} \qquad \Leftrightarrow \qquad g = n\,\frac{\hbar}{2e} \tag{7.53}$$

It is not too hard to write down the required gauge potential assuming that the Dirac string is either along the positive $z$-axis (corresponding to potential $A_-$ which is regular in the lower hemisphere) or the negative $z$-axis (corresponding to potential $A_+$ which is regular in the lower hemisphere),

$$\mathbf{A}_\pm = -g\,\frac{\cos\theta \mp 1}{r\sin\theta}\,\mathbf{n}_\phi \tag{7.54}$$

in the usual spherical coordinates $r, \theta, \phi$, and $\mathbf{n}_\phi$ is the unit vector tangent to the direction of $\phi$ variation. The difference between these two vector potentials is given by

$$\mathbf{A}_+ - \mathbf{A}_- = \frac{2g}{r\sin\theta}\,\mathbf{n}_\phi \tag{7.55}$$

Recalling the expression for the gradient in spherical coordinates,

$$\vec{\nabla}\Lambda = \frac{\partial\Lambda}{\partial r}\,\mathbf{n}_r + \frac{1}{r}\frac{\partial\Lambda}{\partial\theta}\,\mathbf{n}_\theta + \frac{1}{r\sin\theta}\frac{\partial\Lambda}{\partial\phi}\,\mathbf{n}_\phi \tag{7.56}$$

we see that the difference is actually the gradient of the angle $\phi$,

$$\mathbf{A}_+ - \mathbf{A}_- = \vec{\nabla}\Lambda \qquad\qquad \Lambda = 2g\phi \tag{7.57}$$

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In other words, the difference is a gauge transformation that moves the Dirac string from one location to another. Wu and Yang gave an interpretation of this construction in terms of fiber bundles. In particular, the Dirac magnetic monopole construction is closely related to the Hopf fibration of $S^2$ by a circle $S^1$ giving total space $S^3$. Coincidentally, Dirac invented the magnetic monopole in exactly the same year as Hopf did his work on fiber bundles. It took about 40 years before the connection between these two problems was understood.

# 8 Theory of Angular Momentum

In a subsequent chapter, we shall study symmetry transformations in quantum systems in a systematic manner. In this chapter, we shall concentrate on rotations, which is one of the most important cases, both practically and conceptually, and work out the addition of angular momentum.

## 8.1 Rotations

Rotations in 3-dimensional real space may be defined as follows. Let $X$ be the column matrix of the real coordinates $x_1, x_2, x_3$ of 3-dimensional space. The length squared $\ell^2(X)$, or norm, of $X$ is defined by,

$$\ell^2(X) = x_1^2 + x_2^2 + x_3^2 = X^t X \tag{8.1}$$

An *orthogonal transformation* is defined to be a real linear map $X \to X' = MX$ which preserves the length of every vector $X$. This requires $(X')^t(X') = (MX)^t(MX) = X^t X$, for all $X$, or equivalently

$$M^t M = I \tag{8.2}$$

The space of all $M$ forms a group under multiplication, which is denoted by $O(3)$.

Actually, the group $O(3)$ consists of two disconnected components. To see this, we take the determinant of $M^t M = I$, which yields $\det M = \pm 1$. The component with $\det M = 1$ corresponds to *rotations*, which we shall henceforth denote by the letter $R$ instead of $M$. Thus, the group of rotations $R$ in 3-dimensional space is defined by,

$$R^t R = I \qquad\qquad \det R = 1 \tag{8.3}$$

and is usually referred to as $SO(3)$. The $O$ stands for orthogonal (expressed $R^t R = I$), while the $S$ indicates the determinant condition. The element $M = -I$ belongs to $O(3)$, but not to $SO(3)$, since $\det(-I) = -1$. Thus, $M = -I$ is NOT a rotation. Instead, it is a space *parity transformation*, usually denoted by $\mathcal{P}$. As a result of the multiplicative property of the determinant, any element $M$ of $O(3)$ with $\det M = -1$ may be expressed as $M = -R$ where $R$ is a rotation.

Rotations in $n$-dimensional real space may be defined analogously. Let $X$ be the column matrix of the real coordinates $x_1, x_2, \cdots, x_n$, and $\ell^2(X)$ its norm, defined by $\ell^2(X) = X^t X$. Orthogonal transformations are defined as the linear maps $X \to X' = MX$ which leave $\ell^2(X)$ invariant for all $X$, and form a group $O(n)$ of $n \times n$ matrices $M$ satisfying $M^t M = I$. Rotations $R$ in $n$-dimensional space correspond to the component $\det R = 1$, and form the

group $SO(n)$. The element $-I$ always belongs to $O(n)$, and belongs to $SO(n)$ for $n$ even, but not for $n$ odd. Therefore, one may define a parity transformation $\mathcal{P}$ for all $n$ as reflecting only the last coordinate, leaving the others unchanged. Any $M$ with $\det M = -1$ may then be decomposed as $M = \mathcal{P}R$, where $R$ is a proper rotation.

All rotations in $SO(3)$ may be parametrized by 3 real parameters. A convenient way of choosing those is to pick a direction around which to rotate by specifying a unit vector $\mathbf{n} = (n_1, n_2, n_3)$, and then further specify the angle $\omega$ by which to rotate around $\mathbf{n}$. One may write down the rotation matrix explicitly,

$$R(\mathbf{n}, \omega) = \exp\left\{\omega\, \mathbf{n} \cdot \mathbf{T}\right\} \tag{8.4}$$

where the matrices $T_1$, $T_2$, $T_3$ are given by

$$T_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \qquad T_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \qquad T_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{8.5}$$

The matrices $\mathbf{T}$ are real antisymmetric. The rotation $R(\mathbf{n}, \omega)$ applied to an arbitrary vector $\mathbf{v}$ is given by

$$
\begin{aligned}
R(\mathbf{n}, \omega)\mathbf{v} &= \mathbf{v}\cos\omega + \mathbf{v}(\mathbf{n}\cdot\mathbf{v})\,(1 - \cos\omega) + \mathbf{n}\times\mathbf{v}\sin\omega \\
&= \mathbf{v} + \omega\,\mathbf{n}\times\mathbf{v} + \mathcal{O}(\omega^2)
\end{aligned}
\tag{8.6}
$$

Note that, because the matrices $T_1, T_2, T_3$ are traceless, we automatically have $\det R(\mathbf{v}, \omega) = 1$ for all $\mathbf{v}, \omega$. Thus, the operation of space parity reversal $R = -I$ cannot be represented by the above exponential parametrization. The reason is that the element with $\det R = 1$ and $\det R = -1$ are disconnected from one another, and not continuously connected by rotations.

The matrices $T_1, T_2, T_3$ satisfy the following commutation relations,

$$[T_1, T_2] = T_3 \qquad\qquad [T_2, T_3] = T_1 \qquad\qquad [T_3, T_1] = T_2 \tag{8.7}$$

It is convenient to summarize these relations by using the totally antisymmetric tensor $\varepsilon_{abc}$,

$$[T_a, T_b] = \sum_{c=1}^{3} \varepsilon_{abc} T_c \qquad\qquad \varepsilon_{123} = 1 \tag{8.8}$$

where $a, b, c = 1, 2, 3$. It is more usual to work with Hermitean or self-adjoint operators, and to include also a unit of $\hbar$ for proper units of angular momentum,

$$[L_a, L_b] = i\,\hbar \sum_{c=1}^{3} \varepsilon_{abc} L_c \qquad\qquad L_a = i\,\hbar\, T_a \tag{8.9}$$

and the rotations are now represented by

$$R(\mathbf{n}, \omega) = \exp\left\{-\frac{i}{\hbar}\omega\, \mathbf{n} \cdot \mathbf{L}\right\} \tag{8.10}$$

It is in this form that we shall most often use rotations.

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## 8.2   The Lie algebra of rotations – angular momentum

The rotation group $SO(3)$ (as well as all $SO(n)$ groups) is actually a *Lie group*, which means that its group elements can be parametrized in a continuous and differentiable manner by real parameters, such as $\omega$ and $\mathbf{n}$, or also just by the entries of the matrices $R$.

The Norwegian mathematician Sophus Lie (1842 - 1899) proved two remarkable theorems about Lie groups. Lie's first theorem states that if the group multiplication is continuous and once differentiable, then it is real analytic (i.e. infinitely differentiable and completely given by its Taylor series expansion).

Lie's second theorem is equally powerful. It states the equivalence (up to certain global topological issues, which we will mention later) of Lie groups and Lie algebras.

A Lie algebra is obtained from a Lie group by Taylor series expanding the group around its identity element. We are, of course, already familiar with doing this for rotations by a small angle $\omega$,

$$R(\mathbf{n}, \omega) = I - \frac{i}{\hbar}\omega\, \mathbf{n} \cdot \mathbf{L} + \mathcal{O}(\omega^2) \tag{8.11}$$

The quantities $\mathbf{L}$ are the generators of the Lie algebra, and the multiplication law of $SO(3)$ matrices yielding again orthogonal matrices then translates into the commutation relations (8.9), while the associativity translates into the Jacobi identity,

$$[L_a, [L_b, L_c]] + [L_b, [L_c, L_a]] + [L_c, [L_a, L_b]] = 0 \tag{8.12}$$

Lie proved that, conversely, if we have a Lie algebra defined by its commutation relations (generalizing (8.9)) which satisfy the Jacobi identity, then there exists a unique globally well-defined *simply connected* Lie group, of which it is the Lie algebra. Practically, this means that essentially all operations and constructions may be carried out at the level of the Lie algebra, and we are then guaranteed that they will nicely carry over to the whole Lie group. The advantage of the Lie algebra is that it is much much easier to handle.

## 8.3   General Groups and their Representations

A group $G_{,*}$ consists of a set $G$ and a multiplication law $*$ satisfying the following axioms,

1. The multiplication closes: $g_1 * g_2 \in G$ for all $g_1, g_2 \in G$;

2. Associativity, $(g_1 * g_2) * g_3 = g_1 * (g_2 * g_3) = g_1 * g_2 * g_3$ for all $g_1, g_2, g_3 \in G$;

3. $G$ contains an identity element $e$ such that $e * g = g * e = g$ for all $g \in G$;

4. Every $g \in G$ has an inverse $g^{-1}$ so that $g * g^{-1} = g^{-1} * g = e$.

Examples of groups include $\mathbf{Z}_{,+}$; $\mathbf{Q}_{,+}$; $\mathbf{R}_{,+}$; $\mathbf{C}_{,+}$; $\mathbf{Q}^0_{,\times}$; $\mathbf{R}^0_{,\times}$; $\mathbf{C}^0_{,\times}$; as well as the group of all $m \times n$ matrices under addition, and the group of all invertible $n \times n$ matrices under multiplication, a group denoted $Gl(n)$. These groups are all infinite groups, namely having a infinite set of elements. The quintessential example of a finite group is the group $\mathcal{S}_n$ of permutations acting on any set of $n$ distinct elements. The crystallographic groups are other finite groups.

A *representation $\rho$ of dimension $N$ of the group $G$* is a map $\rho$ from $G$ into the group of $N \times N$ invertible matrices, $Gl(N)$,

**1'** Group multiplication carries over to multiplication of matrices
$\rho(g_1 * g_2) = \rho(g_1)\rho(g_2)$ for all $g_1, g_2 \in G$;

**2'** Associativity is automatic for matrices;

**3'** The image of $e$ is the unit matrix, $\rho(e) = I$;

**4'** The image of the inverse is the inverse matrix, $\rho(g^{-1}) = \big(\rho(g)\big)^{-1}$.

In other words, a representation of a group $G$ gives a representation of the elements of $G$ and of the group multiplication law $*$ in terms of $N \times N$ matrices.

One distinguishes the following special types of representations,

- The *trivial representation* $\rho(g) = I$ for all $g \in G$;

- A *faithful representation* is such that the map $\rho$ is injective;

- A *real representation* is such that $\rho(g)$ is a real $N \times N$ matrix for all $g \in G$;

- A *complex representation* is such that $\rho(g)$ is complex for at least one $g \in G$;

- A *unitary representation* is such that $\rho(g)^\dagger \rho(g) = I$ for all $g \in G$.

Representations allow us to represent the action of an abstract group concretely on a linear vector space, such as a Hilbert space in quantum mechanics.

## 8.4   General Lie Algebras and their Representations

A Lie algebra $\mathcal{G}$ is a linear vector space, endowed with a bilinear pairing, usually denoted as the commutator. The defining properties are as follows; for all $X_1, X_2, X_3 \in \mathcal{G}$, we have,

1. The commutator is antisymmetric, $[X_1, X_2] = -[X_2, X_1]$, and belongs to $\mathcal{G}$;

2. Bilinearity $[\lambda_1 X_1 + \lambda_2 X_2, X_3] = \lambda_1[X_1, X_3] + \lambda_2[X_2, X_3]$ for $\lambda_1, \lambda_2 \in \mathbf{C}$;

3. The Jacobi identity $[X_1, [X_2, X_3]] + [X_2, [X_3, X_1]] + [X_3, [X_1, X_2]] = 0$ holds;

A representation $D$ of a Lie algebra $\mathcal{G}$ is a map from $\mathcal{G}$ into $N \times N$ matrices such that for all $X_1, X_2 \in \mathcal{G}$, we have,

**1'** $D([X_1, X_2]) = [D(X_1), D(X_2)]$;

**2'** $D(\lambda_1 X_1 + \lambda_2 X_2) = \lambda_1 D(X_1) + \lambda_2 D(X_2)$, and it follows that $D(0) = 0$;

**3'** The Jacobi identity is automatically obeyed on matrices.

## 8.5 Direct sum and reducibility of representations

Consider two representations $\rho^{(1)}$ and $\rho^{(2)}$ of a group $G$, or any two representations $D^{(1)}$ and $D^{(2)}$ of a Lie algebra $\mathcal{G}$, with $\rho^{(i)}, D^{(i)}$ of dimension $N_i$. We form the direct sum representations as follows,

$$
\left( \rho^{(1)} \oplus \rho^{(2)} \right)(g) = \begin{pmatrix} \rho^{(1)}(g) & 0 \\ 0 & \rho^{(2)}(g) \end{pmatrix}
$$

$$
\left( D^{(1)} \oplus D^{(2)} \right)(X) = \begin{pmatrix} D^{(1)}(X) & 0 \\ 0 & D^{(2)}(X) \end{pmatrix} \tag{8.13}
$$

It is immediate to see that $\rho^{(1)} \oplus \rho^{(2)}$ is a representation of $G$, and that $D^{(1)} \oplus D^{(2)}$ is a representation of $\mathcal{G}$, both of dimension $N = N_1 + N_2$.

A representation $\rho$ of $G$ (similarly $D$ of $\mathcal{G}$) is *reducible* if $\rho$ can be written as the direct sum of two representations of $G$,

$$
\rho = \rho^{(1)} \oplus \rho^{(2)} \qquad\qquad \dim \rho^{(1)}, \dim \rho^{(2)} \neq 0 \tag{8.14}
$$

A representation $\rho$ of $G$ is *irreducible* if it is not reducible.

## 8.6 The irreducible representations of angular momentum

During our study of the quantum system of angular momentum, we have already identified all the irreducible representations of $SO(3)$. They are labeled by the total angular momentum $j$, such that the eigenvalue of $\mathbf{J}^2$ is $\hbar^2 j(j+1)$. We shall denote these representations by $D^{(j)}$. Since they are representations, they satisfy the same algebra as the $J$,

$$
\left[ D^{(j)}(J_a), D^{(j)}(J_b) \right] = i\hbar \sum_{c=1}^{3} \varepsilon_{abc} D^{(j)}(J_c) \qquad\qquad \dim D^{(j)} = 2j + 1 \tag{8.15}
$$

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By a widely used abuse of notation, one usually does not write the symbol $D^{(j)}$, and this sometimes leads to some confusion as to what a representation really is.

It is a good exercise to compute the representation matrices in the lowest dimensional representations. This is done with the help of the matrix elements,

$$\left(D^{(j)}(J_a)\right)_{m',m} = \langle j, m'|J_a|j, m\rangle \tag{8.16}$$

which in turn may be carried out by using the formulas[6]

$$\begin{aligned} J_3|j, m\rangle &= m\hbar|j, m\rangle \\ J_\pm|j, m\rangle &= \sqrt{(j \mp m)(j \pm m + 1)}\,\hbar|j, m \pm 1\rangle \end{aligned} \tag{8.17}$$

This allows us to compute

$$\begin{aligned} \left(D^{(j)}(J_3)\right)_{m',m} &= m\hbar\delta_{m',m} \\ \left(D^{(j)}(J_+)\right)_{m',m} &= \sqrt{(j-m)(j+m+1)}\,\hbar\,\delta_{m',m+1} \\ \left(D^{(j)}(J_-)\right)_{m',m} &= \sqrt{(j+m)(j-m+1)}\,\hbar\,\delta_{m',m-1} \end{aligned} \tag{8.18}$$

From these formula, it is manifest that each of these representations is irreducible. We obviously have $D^{(0)} = 0$, the trivial representation. Next, we find, for $j = 1/2$,

$$\begin{aligned} \left(D^{(\frac{1}{2})}(J_3)\right) &= \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ \left(D^{(\frac{1}{2})}(J_+)\right) &= \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad \left(D^{(\frac{1}{2})}(J_1)\right) = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \left(D^{(\frac{1}{2})}(J_-)\right) &= \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \qquad \left(D^{(\frac{1}{2})}(J_2)\right) = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \end{aligned} \tag{8.19}$$

which are just the Pauli matrices for spin $1/2$. Next, for $j = 1$, we find,

$$\begin{aligned} \left(D^{(1)}(J_3)\right) &= \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \\ \left(D^{(1)}(J_+)\right) &= \sqrt{2}\hbar\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \qquad \left(D^{(1)}(J_1)\right) = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \\ \left(D^{(1)}(J_-)\right) &= \sqrt{2}\hbar\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \qquad \left(D^{(1)}(J_2)\right) = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \end{aligned} \tag{8.20}$$

---

[6]Recall our notations of $J_\pm = J_1 \pm iJ_2$.

Finally, we need to make a change of basis to compare these representation matrices with the ones found earlier, and we have

$$D^{(1)}(J_a) = S L_a S^\dagger \tag{8.21}$$

where the unitary change of basis is given by

$$S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i & 0 \\ 0 & 0 & -\sqrt{2} \\ -1 & -i & 0 \end{pmatrix} \tag{8.22}$$

## 8.7 Addition of two spin 1/2 angular momenta

We begin with the simplest case of two spin $1/2$ angular momenta, $\mathbf{S}_1$ and $\mathbf{S}_2$. The basic assumption is that the two spin $1/2$ degrees of freedom are completely independent from one another. We may think of the spins of two electrons, whose states are independent from one another. The commutation relations are

$$
\begin{aligned}
[S_{ia}, S_{ib}] &= i\hbar \sum_{c=1}^{3} \varepsilon_{abc} S_{ic} && i = 1, 2 \\
[S_{1a}, S_{2b}] &= 0
\end{aligned}
\tag{8.23}
$$

The Hilbert spaces of states $\mathcal{H}_i$ for each system admit the following basis vectors,

$$\mathcal{H}_i \qquad |i, \pm\rangle \qquad\qquad i = 1, 2 \tag{8.24}$$

The dimension of each Hilbert space is 2, and the total number of states for the combined system of two spins is their product, namely 4. The Hilbert space of the total system $\mathcal{H}$ thus has dimension 4. A natural basis of states for $\mathcal{H}$ is given by the tensor product of the basis states for each spin $1/2$ system,

$$
\begin{aligned}
\mathcal{H} \qquad & |1, +\rangle \otimes |2, +\rangle \qquad & |1, +\rangle \otimes |2, -\rangle \\
& |1, -\rangle \otimes |2, +\rangle \qquad & |1, -\rangle \otimes |2, -\rangle
\end{aligned}
\tag{8.25}
$$

The total Hilbert space $\mathcal{H}$ is thus the tensor product of the factors,

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \tag{8.26}$$

The spin operators extend to this tensor product Hilbert space as follows. The first spin operator $\mathbf{S}_1$ really only acts on the first factor in the tensor product and it is the identity

in the second factor. For the second spin operator, the roles are reversed, and it acts as the identity. One may summarize this by

$$\begin{aligned}
\mathbf{S}_1 \quad \text{on} \quad \mathcal{H}_1 \quad &\rightarrow \quad \mathbf{S}_1 \otimes I_2 \quad \text{on} \quad \mathcal{H} \\
\mathbf{S}_2 \quad \text{on} \quad \mathcal{H}_2 \quad &\rightarrow \quad I_1 \otimes \mathbf{S}_2 \quad \text{on} \quad \mathcal{H}
\end{aligned} \tag{8.27}$$

In this way, both operators are now defined on the same Hilbert space $\mathcal{H}$, and may be added to obtain total spin,

$$\mathbf{S} = \mathbf{S}_1 \otimes I_2 + I_1 \otimes \mathbf{S}_2 \quad \text{or simply} \quad \mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2 \tag{8.28}$$

but the latter, although commonly used, is a bit of an abuse of notation.

It is straightforward to check that $\mathbf{S}$ satisfies the angular momentum algebra as well. By definition, $\mathbf{S}$ gives a 4-dimensional representation of $SO(3)$. The question is now whether this representation is reducible or not, and if it is reducible what its irreducible components are.

To shed light on this question, we first calculate the total $S^3 = S^z$ of each basis state. Fortunately, the states have been arranged so that they are eigenstates of $S^3$, with eigenvalues $m$, and we get

$$\begin{aligned}
m &= +1 & &|1, +\rangle \otimes |2, +\rangle \\
m &= 0 & &|1, +\rangle \otimes |2, -\rangle, \ |1, -\rangle \otimes |2, +\rangle \\
m &= -1 & &|1, -\rangle \otimes |2, -\rangle
\end{aligned} \tag{8.29}$$

There is a single state with $m = \pm 1$, which indicates that this 4-dimensional representation contains the $j = 1$ irreducible representation of $SO(3)$. Thus, we identify

$$\begin{aligned}
|j = 1, m = +1\rangle &= |1, +\rangle \otimes |2, +\rangle \\
|j = 1, m = -1\rangle &= |1, -\rangle \otimes |2, -\rangle
\end{aligned} \tag{8.30}$$

The way we can get all the states of this representation is by starting with these states, and applying $S^-$ successively. Since

$$\begin{aligned}
S_{i-}|i, +\rangle &= \hbar|i, -\rangle & S_{i-}|i, -\rangle &= 0 \\
S_{i+}|i, -\rangle &= \hbar|i, +\rangle & S_{i+}|i, +\rangle &= 0
\end{aligned} \tag{8.31}$$

we have

$$\begin{aligned}
S_-|j = 1, m = +1\rangle &= \sqrt{2}\hbar|j = 0, m = 0\rangle \\
&= (S_{1-} \otimes I_2 + I_1 \otimes S_{2-})|1, +1\rangle \otimes |2, +\rangle \\
&= \hbar|1, -\rangle \otimes |2, +\rangle + \hbar|1, +\rangle \otimes |2, -\rangle
\end{aligned} \tag{8.32}$$

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As a result, we find that the state $|j = 1, m = 0\rangle$ of the total system is given by

$$|j = 1, m = 0\rangle = \frac{1}{\sqrt{2}}\Big(|1, -\rangle \otimes |2, +\rangle + |1, +\rangle \otimes |2, -\rangle\Big) \tag{8.33}$$

We may check the consistency of this process by applying $S^-$ once more,

$$
\begin{aligned}
S_-|j = 1, m = 0\rangle &= \hbar\sqrt{2}|j = 1, m = -1\rangle \\
&= (S_{1-} \otimes I_2 + I_1 \otimes S_{2-})\frac{1}{\sqrt{2}}\Big(|1, -\rangle \otimes |2, +\rangle + |1, +\rangle \otimes |2, -\rangle\Big) \\
&= \hbar\sqrt{2}|1, -\rangle \otimes |2, -\rangle \tag{8.34}
\end{aligned}
$$

and this is in agreement with our earlier identification.

The remaining linear combination of the four states which is orthogonal to the three $j = 1$ states may be normalized and is given by

$$\frac{1}{\sqrt{2}}\Big(|1, -\rangle \otimes |2, +\rangle - |1, +\rangle \otimes |2, -\rangle\Big) \tag{8.35}$$

This state is clearly annihilated by all three components of $\mathbf{S}$, and thus corresponds to the unique $|j = 0, m = 0\rangle$ state. Thus, we have proven by explicit calculation that

$$D^{(1/2)} \otimes D^{(1/2)} = D^{(1)} \oplus D^{(0)} \tag{8.36}$$

## 8.8   Addition of a spin 1/2 with a general angular momentum

We shall now study the addition of a spin 1/2 with a general angular momentum $\mathbf{J}_1$ and $\mathbf{S}_2$, which commute with one another,

$$[J_{1a}, S_{2b}] = 0 \qquad\qquad a, b = 1, 2, 3 \tag{8.37}$$

The system 1, we shall restrict attention to the irreducible representation of spin $j_1$, while for system 2, it is the irreducible representation of spin 1/2. The associated Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ are of dimensions $2j_1 + 1$ and 2 respectively, and a canonical basis of states is given by

$$
\begin{array}{lll}
\mathcal{H}_1 & |j_1, m_1\rangle & m_1 = -j_1, -j_1 + 1, \cdots, j_1 - 1, j_1 \\
\mathcal{H}_2 & |2, \pm\rangle & 
\end{array} \tag{8.38}
$$

A basis for the total Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ is given by the tensor product of these basis vectors,

$$
\begin{array}{lll}
\mathcal{H} & |j_1, m_1\rangle \otimes |2, +\rangle & m_1 = -j_1, -j_1 + 1, \cdots, j_1 - 1, j_1 \\
& |j_1, m_1\rangle \otimes |2, -\rangle & 
\end{array} \tag{8.39}
$$

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Total angular momentum may be defined on $\mathcal{H}$ just as we did when we added two spin $1/2$ systems,

$$\mathbf{J} = \mathbf{J}_1 \otimes I_2 + I_1 \otimes \mathbf{S}_2 \tag{8.40}$$

The basis states of $\mathcal{H}$ may be organized according to eigenvalues $m$ of $J_3 = J_z$,

$$
\begin{array}{ll}
m = j_1 + \dfrac{1}{2} & |j_1, j_1\rangle \otimes |2, +\rangle \\[2mm]
m = j_1 - \dfrac{1}{2} & |j_1, j_1\rangle \otimes |2, -\rangle, \ |j_1, j_1 - 1\rangle \otimes |2, +\rangle \\[2mm]
m = j_1 - \dfrac{3}{2} & |j_1, j_1 - 1\rangle \otimes |2, -\rangle, \ |j_1, j_1 - 2\rangle \otimes |2, +\rangle \\
\quad \cdots & \quad \cdots \\[2mm]
m = -j_1 + \dfrac{1}{2} & |j_1, -j_1 + 1\rangle \otimes |2, -\rangle, \ |j_1, -j_1\rangle \otimes |2, +\rangle \\[2mm]
m = -j_1 - \dfrac{1}{2} & |j_1, -j_1\rangle \otimes |2, -\rangle
\end{array} \tag{8.41}
$$

There is a unique highest $J_3$ state with $j = j_1 + 1/2$, so the tensor product contains once the representation $j = j_1 + 1/2$, and we identity

$$
\begin{aligned}
|j, +j\rangle &= |j_1, +j_1\rangle \otimes |2, +\rangle \\
|j, -j\rangle &= |j_1, -j_1\rangle \otimes |2, -\rangle
\end{aligned} \tag{8.42}
$$

Acting with $J_- = J_{1-} + S_{2-}$, we obtain all the states of this representation exactly once. For example, at the level $m = j_1 - 1/2$, we obtain,

$$
\begin{aligned}
J_-|j, +j\rangle &= \hbar\sqrt{2j_1}|j, j - 1\rangle \\
&= \left(J_{1-} \otimes I_2 + I_1 \otimes S_{2-}\right)|j_1, j_1\rangle \otimes |2, +\rangle \\
&= \hbar\sqrt{2j_1}|j_1, j_1 - 1\rangle \otimes |2, +\rangle + \hbar|j_1, j_1\rangle \otimes |2, -\rangle
\end{aligned} \tag{8.43}
$$

As a result, we obtain a formula for the state

$$|j, j - 1\rangle = \frac{1}{\sqrt{2j}}\left(\sqrt{2j_1}|j_1, j_1 - 1\rangle \otimes |2, +\rangle + |j_1, j_1\rangle \otimes |2, -\rangle\right) \tag{8.44}$$

At each value of $m = -j, \cdots, +j$, there is exactly one state belonging to the representation $j$. At $m = j - 1$, the linear combination orthogonal to $|j, j - 1\rangle$ is given by

$$\frac{1}{\sqrt{2j}}\left(|j_1, j_1 - 1\rangle \otimes |2, +\rangle - \sqrt{2j_1}|j_1, j_1\rangle \otimes |2, -\rangle\right) \tag{8.45}$$

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The state has $m = j - 1$, but also is annihilated by $J_+$, and so it is the highest $m$ state of the representation with total angular momentum $j_1 - \frac{1}{2}$. Thus, the tensor product decomposes as follows,

$$D^{(j_1)} \otimes D^{(1/2)} = D^{(j_1+1/2)} \oplus D^{(j_1-1/2)} \qquad\qquad j_1 \geq \frac{1}{2} \qquad (8.46)$$

## 8.9  Addition of two general angular momenta

We shall now carry out the addition of two general angular momenta, with irreducible representations of spins $j_1$ and $j_2$, and associated Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$. The tensor product basis of the tensor product $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ is given by

$$
\begin{array}{lll}
\mathcal{H}_1 & |j_1, m_1\rangle & m_1 = -j_1, \, -j_1 + 1, \cdots, j_1 - 1, \, j_1 \\
\mathcal{H}_2 & |j_2, m_2\rangle & m_2 = -j_2, \, -j_2 + 1, \cdots, j_2 - 1, \, j_2 \\
\mathcal{H} & |j_1, m_1\rangle \otimes |j_2, m_2\rangle & \text{''}
\end{array} \qquad (8.47)
$$

Total angular momentum $\mathbf{J}$ is defined by

$$\mathbf{J} = \mathbf{J}_1 \otimes I_2 + I_1 \otimes \mathbf{J}_2 \qquad (8.48)$$

At total $J^3 = J^z$ eigenvalue $m$, we have

$$
\begin{array}{ll}
m = j_1 + j_2 & |j_1, j_1\rangle \otimes |j_2, j_2\rangle \\
m = j_1 + j_2 - 1 & |j_1, j_1\rangle \otimes |j_2, j_2 - 1\rangle, \; |j_1, j_1 - 1\rangle \otimes |j_2, j_2\rangle \\
m = j_1 + j_2 - 2 & |j_1, j_1\rangle \otimes |j_2, j_2 - 2\rangle, \; |j_1, j_1 - 1\rangle \otimes |j_2, j_2 - 1\rangle, \; |j_1, j_1 - 2\rangle \otimes |j_2, j_2\rangle \\
\quad \cdots & \quad \cdots \\
m = -j_1 - j_2 & |j_1, -j_1\rangle \otimes |j_2, -j_2\rangle
\end{array} \qquad (8.49)
$$

The unique state with the highest value of $m = j_1 + j_2$ belongs to the irreducible representation $D^{(j)}$ with $j = j_1 + j_2$. Thus, we may identify

$$
\begin{aligned}
|j, +j\rangle &= |j_1, j_1\rangle \otimes |j_2, j_2\rangle \\
|j, -j\rangle &= |j_1, -j_1\rangle \otimes |j_2, -j_2\rangle
\end{aligned} \qquad (8.50)
$$

By applying the lowering operator $J_- = J_{1-} \otimes I_2 + I_1 \otimes J_{2-}$ to this state, we find

$$
\begin{aligned}
J_-|j, +j\rangle &= \hbar\sqrt{2j}\,|j, j - 1\rangle \\
&= \left( J_{1-} \otimes I_2 + I_1 \otimes J_{2-} \right) |j_1, j_1\rangle \otimes |j_2, j_2\rangle \\
&= \hbar\sqrt{2j_1}\,|j_1, j_1 - 1\rangle \otimes |j_2, j_2\rangle + \hbar\sqrt{2j_2}\,|j_1, j_1\rangle \otimes |j_2, j_2 - 1\rangle \qquad (8.51)
\end{aligned}
$$

As a result, we have

$$|j, j - 1\rangle = \frac{1}{\sqrt{2j}} \left( \sqrt{2j_1} |j_1, j_1 - 1\rangle \otimes |j_2, j_2\rangle + \sqrt{2j_2} |j_1, j_1\rangle \otimes |j_2, j_2 - 1\rangle \right) \tag{8.52}$$

The remaining linear combination at level $m = j - 1$ is given by

$$|j - 1, j - 1\rangle = \frac{1}{\sqrt{2j}} \left( \sqrt{2j_2} |j_1, j_1 - 1\rangle \otimes |j_2, j_2\rangle - \sqrt{2j_1} |j_1, j_1\rangle \otimes |j_2, j_2 - 1\rangle \right) \tag{8.53}$$

and is the highest $m$ value for the irreducible representation $j - 1$. One may pursue this process recursively, and find that

$$D^{(j_1)} \otimes D^{(j_2)} = \bigoplus_{j=k}^{j_1+j_2} D^{(j)} \tag{8.54}$$

It remains to determine the number $k$. One could do this directly. A convenient trick, however, is to determine $k$ by making sure that the dimensions work out correctly.

$$(2j_1 + 1)(2j_2 + 1) = \sum_{j=k}^{j_1+j_2} (2j + 1) \tag{8.55}$$

Using

$$\sum_{\ell=0}^{N} (2j + 1) = (N + 1)^2 \tag{8.56}$$

we readily find that

$$(2j_1 + 1)(2j_2 + 1) = (j_1 + j_2 + 1)^2 - k^2 \qquad \Rightarrow \qquad k^2 = (j_1 - j_2)^2 \tag{8.57}$$

so that $k = |j_1 - j_2|$. We recover easily the previous case where $j_2 = \frac{1}{2}$.

## 8.10   Systematics of Clebsch-Gordan coefficients

The above construction makes it clear that there are two ways of describing the states of a system in which two angular momenta are added. The first is as the eigenstates of $\mathbf{J}_1^2, J_1^3, \mathbf{J}_2^2, J_2^3$, and we label these eigenstates as

$$|j_1, m_1\rangle \otimes |j_2, m_2\rangle = |j_1, j_2; m_1, m_2\rangle \tag{8.58}$$

But, alternatively, the same states may be label by the eigenvalues of an equivalent set of commuting observables, $\mathbf{J}_1^2, \mathbf{J}_2^2, \mathbf{J}^2, J^3$, and we label these states as

$$|j_1, j_2; j, m\rangle \tag{8.59}$$

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Each group of states forms an orthogonal basis for the same Hilbert space. It is convenient to normalize the states as follows,

$$\begin{aligned}
\langle j_1, j_2; m_1', m_2' | j_1, j_2; m_1, m_2 \rangle &= \delta_{m_1', m_1} \delta_{m_2', m_2} \\
\langle j_1, j_2; j', m' | j_1, j_2; j, m \rangle &= \delta_{j', j} \delta_{m', m}
\end{aligned} \tag{8.60}$$

We have already show that

$$\begin{aligned}
|j_1, j_2; j, +j\rangle &= |j_1, j_2; +j_1, +j_2\rangle & j = j_1 + j_2 \\
|j_1, j_2; j, -j\rangle &= |j_1, j_2; -j_1, -j_2\rangle
\end{aligned} \tag{8.61}$$

More generally, the above orthonormality conditions imply that the passage from one basis to the other is by a unitary matrix,

$$|j_1, j_2; j, m\rangle = \sum_{m_1} \sum_{m_2} |j_1, j_2; m_1, m_2\rangle \langle |j_1, j_2; m_1, m_2| j_1, j_2; j, m\rangle \tag{8.62}$$

By choosing the phases of the states in both bases, all coefficients may in fact be chosen to be real.

By applying the angular momentum generators $J_a = J_{a1} + J_{2a}$ to both sides, we obtain recursion relations between the matrix elements. Applying $J_3$, we get

$$m | j_1, j_2; j, m\rangle = \sum_{m_1} \sum_{m_2} (m_1 + m_2) | j_1, j_2; m_1, m_2\rangle \langle |j_1, j_2; m_1, m_2| j_1, j_2; j, m\rangle \tag{8.63}$$

Taking the inner product with $\langle j_1, j_2; m_1', m_2' |$, we obtain,

$$(m - m_1 - m_2) \langle |j_1, j_2; m_1, m_2| j_1, j_2; j, m\rangle = 0 \tag{8.64}$$

Applying $J_\pm = J_{1\pm} + J_{2\pm}$, we get

$$\begin{aligned}
N_{j,m}^\pm | j_1, j_2; j, m \pm 1\rangle &= \sum_{m_1} \sum_{m_2} N_{j_1, m_1}^\pm | j_1, j_2; m_1 \pm 1, m_2\rangle \langle |j_1, j_2; m_1, m_2| j_1, j_2; j, m\rangle \\
&\quad + \sum_{m_1} \sum_{m_2} N_{j_2, m_2}^\pm | j_1, j_2; m_1, m_2 \pm 1\rangle \langle |j_1, j_2; m_1, m_2| j_1, j_2; j, m\rangle
\end{aligned}$$

where

$$N_{j,m}^\pm = \sqrt{j(j+1) - m(m \pm 1)} = \sqrt{(j \mp m)(j \pm m + 1)} \tag{8.65}$$

Taking the inner product with $\langle j_1, j_2; m_1', m_2' |$, we obtain,

$$\begin{aligned}
N_{j,m}^\pm \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \pm 1\rangle &= N_{j_1, m_1 \mp 1}^\pm \langle j_1, j_2; m_1 \mp 1, m_2 | j_1, j_2; j, m\rangle \\
&\quad + N_{j_2, m_2 \mp 1}^\pm \langle j_1, j_2; m_1, m_2 \mp 1 | j_1, j_2; j, m\rangle
\end{aligned} \tag{8.66}$$

Here, we have dropped the $'$ on $m_1$ and $m_2$. The initial condition on this recursion relation is the highest weight matrix element

$$\langle j_1, j_2; j, j | j_1, j_2; j_1, j_2 \rangle = 1 \qquad\qquad j = j_1 + j_2 \qquad\qquad (8.67)$$

A detailed discussion on how the above recursion relation fixes all the Clebsch Gordan coefficients may be found in Sakurai.

## 8.11 Spin Models

A spin model is a statistical mechanical lattice model for which each lattice site has a two-dimensional Hilbert space of states. (More generally, one could consider spin models with higher angular momentum representations, and thus with higher dimensional Hilbert spaces at each lattice point.) A natural way of realizing this two-dimensional Hilbert space is by a spin $1/2$ degree of freedom at each lattice site. The lattice $\Lambda$ is usually a square lattice in $d$ dimensions, and the interactions are usually limited to nearest neighbor interactions only. Spin often being responsible for the presence of a magnetic moment, one often also includes a uniform magnetic field $B$ which acts as an external source. Schematically, the general Hamiltonian is of the form,

$$H = -J \sum_{\langle i,j \rangle, i,j \in \Lambda} S_i S_j - B \sum_{i \in \Lambda} S_i \qquad\qquad (8.68)$$

Here the notation $\langle i, j \rangle$ stands for the inclusions of nearest neighbor pairs only, and $i$ and $j$ run over all points of a lattice $L$. One such Hamiltonian is given by the *Heisenberg model*, for which all three components of spin are retained,

$$H = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - B \sum_i S_{iz} \qquad\qquad (8.69)$$

where the $B$ field has been taken to be in the $z$ direction.

## 8.12 The Ising Model

Henceforth, we shall concentrate on the simplest Hamiltonian, namely that of the *Ising model*. Here, the spins $S_i$ are taken to be the $z$-component $S_i^z$ of the spin operator $\mathbf{S}$. The Ising model Hamiltonian is given by

$$H = -J \sum_{\langle i,j \rangle} S_{iz} S_{jz} - B \sum_i S_{iz} \qquad\qquad (8.70)$$

Since all operators in the Hamiltonian mutually commute, the quantum system actually behaves classically. Note that, for $B = 0$, the Hamiltonian is invariant under the unitary operation $R$ of simultaneous reversal of all spins

$$R S_{iz} R^\dagger = -S_{iz} \tag{8.71}$$

A basis for all the quantum states is given by the tensor product of the states $|i, \sigma_i\rangle$ where $i$ runs through the lattice $\Lambda$ and for each $i$, the variable $\sigma_i = \pm 1$, namely the eigenvalues of $S_i^z$. The eigenvalue of the Hamiltonian on such a state is

$$H|\sigma_i, i \in \Lambda\rangle = E_{\{\sigma_i\}}|\sigma_i, i \in \Lambda\rangle \qquad\qquad |\sigma_i, i \in \Lambda\rangle = \bigotimes_{i \in \Lambda} |i, \sigma_i\rangle \tag{8.72}$$

and the energy eigenvalue is

$$E_{\{\sigma_i\}} = -J \sum_{\langle i,j\rangle} \sigma_i \sigma_j - B \sum_i \sigma_i \tag{8.73}$$

Under the operation of spin reversal $R$, the eigenvalues behave as $R(\sigma_i) = -\sigma_i$.

There are two important cases to distinguish between depending on the sign of $J$. If $J > 0$ and $B = 0$, the ground (or minimum energy) state of the system is attained when all spins are lined up in the same direction, either all up $\sigma_i = +1$ or all down $\sigma_i = -1$. This interaction is referred to as *ferromagnetic*. If $J < 0$ and $B = 0$, the configuration with all spins aligned is actually maximum energy, so the minimum energy configuration will have alternation between spins up and down. This interaction is referred to as *anti-ferromagnetic*.

## 8.13   Solution of the 1-dimensional Ising Model

The simplest Ising model is in one dimension, in which case the Hamiltonian may be written down even more explicitly,

$$H = -J \sum_{i=1}^{N} S_{iz} S_{i+1\,z} - B \sum_{i=1}^{N} S_{iz} \tag{8.74}$$

and we use the periodicity convention $S_{N+1\,z} = S_{1z}$. To compute $Z$, we write it as a sequential product,

$$
\begin{aligned}
Z &= \mathrm{tr}\big(\mathcal{E}_1 \mathcal{E}_2 \cdots \mathcal{E}_{N-1} \mathcal{E}_N\big) \\
\mathcal{E}_i &= \exp\left\{\beta J S_{iz} S_{i+1\,z} + \frac{1}{2}\beta B \left(S_{iz} + S_{i+1\,z}\right)\right\}
\end{aligned}
\tag{8.75}
$$

We define the identity operator

$$I_i = \sum_{\sigma_i = \pm 1} |i, \sigma_i\rangle\langle i, \sigma_i| \tag{8.76}$$

and insert the product $I_1 \otimes I_2 \otimes \cdots \otimes I_N$ in between $\mathcal{E}_{i-1}$ and $\mathcal{E}_i$ for all $i$. The problem now becomes one of $2 \times 2$ matrix multiplication. To see this, we work out the matrix elements of $\mathcal{E}_i$ that enter here,

$$\mathbf{T}_{\sigma',\sigma} = \langle \sigma' | \mathcal{E}_i | \sigma \rangle = \exp \left\{ \beta J \sigma' \sigma + \frac{1}{2} \beta B (\sigma + \sigma') \right\} \tag{8.77}$$

The partition function is then given by

$$Z = \sum_{\{\sigma_i = \pm 1\}} T_{\sigma_1,\sigma_2} T_{\sigma_2,\sigma_3} \cdots T_{\sigma_N,\sigma_1} = \operatorname{tr} \mathbf{T}^N \tag{8.78}$$

Written out explicitly, the matrix $\mathbf{T}$ is given by

$$\mathbf{T} = \begin{pmatrix} e^{\beta J + \beta B} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J - \beta B} \end{pmatrix} \tag{8.79}$$

Its eigenvalues $\lambda_\pm$ satisfy the equation,

$$\lambda_\pm^2 - 2\lambda_\pm \, e^{\beta J} \operatorname{ch}(\beta B) + 2 \operatorname{sh}(2\beta J) = 0 \tag{8.80}$$

which is solved by

$$\lambda_\pm = e^{\beta J} \operatorname{ch}(\beta B) \pm \sqrt{e^{2\beta J} \operatorname{sh}^2(\beta B) + e^{-2\beta J}} \tag{8.81}$$

Therefore, the partition function is given by

$$Z = \lambda_+^N + \lambda_-^N \tag{8.82}$$

for all values of $N$, $\beta$, $J$, and $B$.

In statistical mechanics and thermodynamics, we are mostly interested in taking the thermodynamics limit of the system, which here corresponds to taking $N \to \infty$. The number of sites $N$ plays the role of volume, and it is then more appropriate to consider the large volume limit of intensive quantities, such as the free energy per unit volume etc. Thus, we shall be interested in the limit,

$$f = \lim_{N \to \infty} \frac{F}{N} = -\frac{1}{\beta} \lim_{N \to \infty} \frac{1}{N} \ln \left( \lambda_+^N + \lambda_-^N \right) \tag{8.83}$$

The value of the limit will depend on which of the eigenvalues $\lambda_\pm$ is the larger one. Clearly, we have

$$\begin{aligned} \lambda_+ > \lambda_- \quad &\text{when} \quad J > 0 \\ \lambda_+ < \lambda_- \quad &\text{when} \quad J < 0 \end{aligned} \tag{8.84}$$

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and thus,

$$f = -\frac{1}{\beta} \ln \lambda_+ \qquad \text{when} \qquad J > 0$$

$$f = -\frac{1}{\beta} \ln |\lambda_-| \qquad \text{when} \qquad J < 0 \tag{8.85}$$

In both cases, these functions are analytic functions of $\beta$, so there are no phase transitions for any finite value of $\beta$. In other words, the system is in the same thermodynamic phase for all temperatures.

## 8.14   Ordered versus disordered phases

An important qualitative characteristic of the dynamics of statistical magnetic systems is order versus disorder. For magnetic systems, this property may be understood systematically in terms of the magnetization, defined as the thermodynamic average of the spin,

$$S^z = \lim_{N \to \infty} \frac{1}{N} \sum_i S_i^z \tag{8.86}$$

The magnetization $M(B)$ per unit volume is then defined by

$$M(B) \quad = \quad \frac{\text{Tr}\left(S^z e^{-\beta H}\right)}{\text{Tr}\left(e^{-\beta H}\right)} = -\lim_{N \to \infty} \frac{1}{N} \frac{\partial \ln Z}{\partial(\beta B)} \tag{8.87}$$

In the case of the 1-dimensional Ising model, and for $B = 0$, this quantity is easily computed for both $J > 0$ or $J < 0$. The eigenvalues $\lambda_\pm$ both depend on $\beta B$ through an even function of $\beta B$, and thus, the magnetization $M(B)$ at zero external magnetic field always vanishes. This result is interpreted as the fact that the spins in the system, on average, point in all directions randomly, so that their total contribution to magnetization vanishes in the bulk.

When can a system be ordered then ? We have seen previously that for $J > 0$, the minimum energy states are

$$\begin{aligned}|+\rangle \qquad\qquad &\sigma_i = +1 \qquad i \in \Lambda \\ |-\rangle \qquad\qquad &\sigma_i = -1 \qquad i \in \Lambda \end{aligned} \tag{8.88}$$

Note that, these states are mapped into one another $R|\pm\rangle = |\mp\rangle$ by the spin reversal symmetry $R$ of the Hamiltonian for $B = 0$. At high temperatures, the spins are allowed to fluctuate away wildly from these minimum energy states, but one would expect that, as temperature is lowered, that fluctuations away from these ground states are suppressed.

If both ground states contribute to the partition function, then the total magnetization will get wiped out, and the system will remain in a disordered phase. When the volume, or $N$, is finite, this will always be the case. But when $N \to \infty$, it is possible for the system to get stuck in one ground state or the other. The reason this only happens for infinite $N$ is that it would then take an infinite number of spin flips to transition between the $|+\rangle$ and $|-\rangle$ states, and this may get energetically impossible. When the system gets stuck in one of its ground states, $M(0) \neq 0$ and we have spontaneous magnetization, familiar from ferromagnetism below the Curie temperature. The operation of spin reversal, which is a symmetry of the Hamiltonian for $B = 0$ is then NOT a symmetry of the physical system any more, as a definite non-zero value of $M(0)$ is not invariant under $R$. The symmetry $R$ is said to be *spontaneously broken*, and the system is then in an ordered phase, close to one of its ground states. We have already shown that, for the 1-dimensional Ising model, this phenomenon does not take place.

The 2-dimensional Ising model, however, does exhibit an ordered phase below a critical temperature $T_c$. This is known since the model was solved exactly by Lars Onsager in 1944, and the critical temperature is known analytically,

$$\text{sh}(2J\beta_c) = 1 \qquad\qquad \frac{1}{\beta_c} = k_B T_c = 2J \times 1.134542 \qquad (8.89)$$

The corresponding magnetization was computed by C.N. Yang,

$$
\begin{aligned}
M(0) &= \left(1 - \frac{1}{\text{sh}^4(2J\beta)}\right)^{1/8} & T < T_c \\
M(0) &= 0 & T > T_c \qquad (8.90)
\end{aligned}
$$

Note that as $T \nearrow T_c$, the expression $M(0)$ vanishes and joins continuously with the $T > T_c$ result. The phase transition at $T = T_c$ is actually second order.

Whether the 3-dimensional Ising model allows for an exact solution is one of the great outstanding problems of statistical mechanics. Proposals have been made that the model behaves as a theory of free fermionic random surfaces, but the details have never been conclusive. Numerical studies of the model have shown however that it also admits a phase transition between ordered (low temperature) and disordered (high temperature) phases.

# 9 Symmetries in Quantum Physics

> *Symmetry, as wide or as narrow as you may define its meaning,*
> *is one idea by which man through the ages has tried to*
> *comprehend and create order, beauty and perfection.*
> – Hermann Weyl –

Symmetries can manifest themselves in different ways.

• *A symmetries of an object* is the oldest of the two concepts. The circle, the regular hexagon, square, or triangle, for example, represent some of the deepest symbols of civilization, mainly because of their high degree of symmetry. The most elementary definition of symmetry then is that an object is symmetric if it will appear the same if viewed from a transformed perspective. For all the above planar figures, their shapes will appear unchanged after certain planar rotations about their centers.

• *A symmetry of the laws of Nature* is a more recent concept, which can be traced back to the Renaissance. Galileo realized that the laws governing classical mechanics do not change if we transform our observational frame in time or in space – in a uniform manner. This property is referred to as Galilean relativity; it includes the symmetries of time translation as well as space translation and rotations. Einstein considerably extended the range of applicability of the relativity principle to special and then general relativity. In the latter, the laws of physics are unchanged under any transformation of our observational frame.

## 9.1 Symmetries in classical mechanics

Recall that in classical mechanics we encountered two types of symmetries, following the model of the above discussion.

- Symmetries of the solutions of the Euler Lagrange equations
  (such as, for example, symmetries of shapes of orbits);

- Symmetries of the Euler Lagrange equations themselves
  (i.e. symmetries of the laws of Nature).

From the modern perspective on physics, the symmetries of the laws of Nature are considered to be primordial. For example, translation and rotation invariance are ingrained in the basic laws of Nature, and are associated with the conservation of energy, momentum and angular momentum. The symmetries of the solutions, such as the symmetries of orbits, are viewed to be less fundamental. In fact, while the orbits of most planets are roughly circular, closer inspection reveals that they are really closer to elliptical, with further deviations from the elliptical form. Thus the symmetries of the solutions are for the most only approximate and

not primordial. This lack of exact symmetry of orbits is what ultimately caused the downfall of the Ptolemy model of the planets.

By definition, *a symmetry of an equation* is a *transformation on the dynamical variables that maps any solution to the equation to a solution of the same equation.* Symmetry transformations may be

- discrete
  (such as parity, time reversal, translation and rotation in a crystal);

- continuous, i.e. parametrized by continuous parameters
  (such as translation and rotation invariance in the continuum).

It is well-known that time and space translation invariance imply conservation of energy and momentum respectively and that rotation invariance implies conservation of angular momentum. This connection between a continuous symmetry and an associated conserved quantity or *conserved charge* is a general one thanks to a theorem by Emmy Noether.

We consider a mechanical system described by a Lagrangian $L(q, \dot{q}; t)$ for positions $q_i(t)$ with $i = 1, \cdots, N$. Now consider a continuous symmetry acting on $q_i(t)$. A continuous symmetry (such as a translation or a rotation) will depend upon a continuous parameter $\alpha$, which we shall assume to be real. Thus, the new positions $\tilde{q}_i$ are given as a function of this parameter, in such a way that

$$
\begin{aligned}
\tilde{q}_i(t, \alpha) &= \text{differentiable function of } \alpha \\
\tilde{q}_i(t, 0) &= q_i(t)
\end{aligned}
\tag{9.1}
$$

*For any given $\alpha$, the transformation $q_i(t) \to \tilde{q}_i(t, \alpha)$ is a symmetry provided every solution $q_i(t)$ of the Euler-Lagrange equations is mapped into a solution $\tilde{q}_i(t, \alpha)$ of the same Euler-Lagrange equations.* In particular, this means that if $q_i(t)$ is a stationary trajectory of the action $S[q]$, then so is $\tilde{q}_i(t, \alpha)$. (Notice that the values of the end points $q_i(t_{1,2})$ will in general be transformed into different values $q_i(t_{1,2}, \alpha)$.) Since the symmetry is continuous, we may restrict to an infinitesimal version of the transformation, defined by

$$
\delta q_i(t) = \delta q_i(q, \dot{q}; t) = \lim_{\alpha \to 0} \frac{\tilde{q}_i(t, \alpha) - \tilde{q}_i(t, 0)}{\alpha} = \left. \frac{\partial \tilde{q}_i(t, \alpha)}{\partial \alpha} \right|_{\alpha = 0}
\tag{9.2}
$$

The infinitesimal transformation $\delta q_i$ is a symmetry provided

$$
\delta L = \sum_i \left( \frac{\partial L}{\partial q_i} \delta q_i + \frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i \right) = \frac{d}{dt} X(q, \dot{q}; t)
\tag{9.3}
$$

Here, the variation must be carried out <u>*without using the Euler-Lagrange equations*</u>, and the quantity $X(q, \dot{q}; t)$ must be a function of $q_i(t)$ and $\dot{q}_i(t)$ which is <u>*local in time*</u>.

## 9.2 Noether's Theorem

(1) If $\delta q_i(t)$ is a symmetry transformation, there exists a *conserved charge $C$*, given by

$$C = \sum_i p_i \delta q_i - X \qquad\qquad p_i = \frac{\partial L}{\partial \dot{q}_i} \qquad\qquad (9.4)$$

The charge $C$ is conserved, namely we have $\dot{C} = dC/dt = 0$, for any path $q_i(t)$ which obeys the Euler-Lagrange equations. The result is proven by straightforward calculation, and the use of the Euler-Lagrange equations.

(2) The conserved charge generates the infinitesimal transformation as follows,

$$\delta q_i = \{q_i, C\} \qquad\qquad (9.5)$$

This result is proven by starting from the $\delta L = \dot{X}$ (which holds without the use of the Euler-Lagrange equations), using it to compute $\partial X/\partial p_i$ and $\partial X/\partial q_i$, and then using those derivatives to evaluate $\{q_i, C\}$. Note that conservation means $\dot{C} = 0$,

$$\dot{C} = \frac{dC}{dt} = \frac{\partial C}{\partial t} + \{C, H\} = 0 \qquad\qquad (9.6)$$

even though $C$ may have *explicit time dependence*.

A first simple example is provided by translations of the dynamical variables $q_i$. The finite transformation is $\tilde{q}_i(t, \alpha) = q_i(t) + \alpha v_i$ where $v_i$ are constants. As a result, $\delta q_i(t) = v_i$, and $\delta \dot{q}_i = 0$. Variation of the Lagrangian gives,

$$\delta L = \sum_i \frac{\partial L}{\partial q_i} v_i \qquad\qquad (9.7)$$

which expresses the derivative of $L$ with respect to the combination $\sum_i q_i(t) v_i$. For this to be a symmetry, we need $\delta L$ to be a total time derivative of a local quantity $X$, without using the Euler-Lagrange equations. But this can happen only if $\delta L = X = 0$. in turn expressing the fact that the Lagrangian does not actually depend on the combination $\sum_i q_i(t) v_i$. As a result, the associated conserved charge is given by

$$C_v = \sum_i p_i \delta q_i = \sum_i p_i v_i \qquad\qquad (9.8)$$

expressing the fact that the associated momentum in that direction is conserved.

A second example is provided by time translations, whose finite transformation is $\tilde{q}_i(t, \alpha) = q_i(t + \alpha)$. The associated infinitesimal transformation is $\delta q_i(t) = \dot{q}_i(t)$, and we also have $\delta \dot{q}_i(t) = \ddot{q}_i(t)$. Now compute the variation of the Lagrangian,

$$\delta L = \sum_i \left( \frac{\partial L}{\partial q_i} \dot{q}_i + \frac{\partial L}{\partial \dot{q}_i} \ddot{q}_i \right) = \frac{dL}{dt} - \frac{\partial L}{\partial t} \qquad\qquad (9.9)$$

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The rhs is a total time derivative only if $\partial L/\partial t = 0$, namely the Lagrangian has *no explicit time dependence*. Assuming this to be the case, we see that $X = L$, the associated conserved charge is readily computed, and found to be the Hamiltonian,

$$H = \sum_i p_i \dot{q}_i - L \tag{9.10}$$

which is what we expect: energy conservation results from time translation invariance.

## 9.3   Group and Lie algebra structure of classical symmetries

Transformations that permute the elements of a set form a group, which is generally a subgroup of the full permutation group of the set in question. Generally, symmetry transformations act as permutations on the space of all solutions of an equation, and therefore also form a group. It is actually in this context that groups were first discovered by Galois in his study of the behavior of solutions to polynomial equations under permutations of these solutions.

Continuous symmetries depend differentiably on parameters and generally form Lie groups, while their infinitesimal versions form Lie algebras. This may be seen as follows. Suppose a given Lagrangian system has two infinitesimal transformations $\delta_1 q_k(t)$ and $\delta_2 q_k(t)$, both of which generate infinitesimal symmetries with associated conserved charges $C_1$ and $C_2$, both of which are conserved. The sum of the two infinitesimal transformations $\delta_1 q_k(t) + \delta_2 q_k(t)$ is then also a symmetry with associated conserved charge $C_1 + C_2$. But furthermore, as is characteristic of a Lie algebra, there is an antisymmetric *commutator* of transformations

$$\delta_1\Big(\delta_2 q_k(t)\Big) - \delta_2\Big(\delta_1 q_k(t)\Big) \tag{9.11}$$

which also produces a symmetry, with associated conserved charge $\{C_1, C_2\}$. To see this, we work out the composition rule in terms of Poisson brackets, using the fact that $\delta_a q_k(t) = \{q_k(t), C_a\}$, and we find,

$$
\begin{aligned}
\delta_1\Big(\delta_2 q_k(t)\Big) - \delta_2\Big(\delta_1 q_k(t)\Big) &= \Big\{C_1, \{C_2, q_k(t)\}\Big\} - \Big\{C_2, \{C_1, q_k(t)\}\Big\} \\
&= \Big\{\{C_1, C_2\}, q_k(t)\Big\}
\end{aligned}
\tag{9.12}
$$

The last line was obtained from the first by the use of the Jacobi identity which always holds for the Poisson bracket.

As a final remark, the charges $C$, discussed above always generate transformations of the system, even if these transformations are not necessarily symmetries. For example, in a mechanical system with degrees of freedom $q_k$ and $p_\ell$ for $k, \ell = 1, 2, 3$ and canonical Poisson brackets $\{q_k, p_\ell\} = \delta_{k\ell}$, the (orbital) angular momentum generator, defined by

$$L^a = \sum_{k,\ell} \varepsilon^{ak\ell} q_k p_\ell \tag{9.13}$$

will always generate rotations

$$\delta_a q_\ell = \{q_\ell, L_a\} = \sum_m \varepsilon^{a\ell m} q_m \tag{9.14}$$

whether or not rotations are actually a symmetry of a certain Lagrangian or not.

## 9.4  Symmetries in Quantum Physics

In quantum mechanics, the (only) quantities that can be measured are the eigenvalues of observables, and the probabilities for one state to overlap with another state. A transformation in quantum mechanics is a linear (or anti-linear for time reversal) map from the Hilbert space $\mathcal{H}$ into itself. A quantum mechanical symmetry must preserve the outcome of all observations, and hence must leave all probabilities unchanged. In the case of linear transformations, we must have the following transformation law on states,

$$
\begin{aligned}
|\varphi\rangle \to |\varphi'\rangle = g|\varphi\rangle & \qquad \langle \psi'|\varphi'\rangle = \langle \psi|g^\dagger g|\varphi\rangle = \langle \psi|\varphi\rangle \\
|\psi\rangle \to |\psi'\rangle = g|\psi\rangle & \qquad g^\dagger g = I
\end{aligned}
\tag{9.15}
$$

Thus, to be a symmetry, a linear transformation must be unitary. On observables, the action of $g$ is by conjugation,

$$A \to A' = g^\dagger A g \tag{9.16}$$

Since $g$ is unitary, the set of all eigenvalues (i.e. the spectrum) of $A'$ exactly coincides with the set of all eigenvalues of $A$.

From the above point of view, all unitary transformations are candidates to be symmetries, as they represent a general change of orthonormal basis in Hilbert space. Certain authors (see Weinberg, volume I) indeed leave the definition of a symmetry this general. Once the dynamics of the system is further determined by a Hamiltonian, however, it becomes more natural to have a more dynamics-related definition of symmetry. Dynamics may be formulated either in the Schrödinger or in the Heisenberg pictures, and a symmetry then operates as follows. In either case, we shall assume that we perform a unitary transformation $g$ which has *no explicit time dependence*.

In the Schrödinger picture, any state $|\varphi(t)\rangle$ satisfying the Schrödinger equation with the Hamiltonian $H$, is transformed to a state $g|\varphi(t)\rangle$ which must satisfy the Schrödinger equation for the same Hamiltonian. As a result, we must have for all states $|\varphi(t)\rangle$,

$$
\begin{aligned}
i\hbar \frac{\partial}{\partial t}|\varphi(t)\rangle &= H|\varphi(t)\rangle \\
i\hbar \frac{\partial}{\partial t}\Big(g|\varphi(t)\rangle\Big) &= H\Big(g|\varphi(t)\rangle\Big)
\end{aligned}
\tag{9.17}
$$

Since, by assumption, $g$ has no time dependence, this requires $[g, H]|\varphi(t)\rangle = 0$ for all states $|\varphi(t)\rangle$, which can only happen is

$$[g, H] = 0 \qquad \Rightarrow \qquad \frac{dg}{dt} = 0 \tag{9.18}$$

in other words, $g$ must be conserved in time.

The derivation in the Heisenberg picture is analogous. Any observable $A(t)$ satisfying the Heisenberg equation is transformed into an observable $g^\dagger A(t) g$ which must also satisfy the Heisenberg equation, so that

$$
\begin{aligned}
i\hbar \frac{\partial}{\partial t} A(t) &= [A(t), H] \\
i\hbar \frac{\partial}{\partial t}\left(g^\dagger A(t) g\right) &= [g A(t) g^\dagger, H]
\end{aligned}
\tag{9.19}
$$

Since $g$ has no explicit time dependence, this requires

$$\left[A, g[g^\dagger, H]\right] = 0 \tag{9.20}$$

which in turn again requires that $[g, H] = 0$. It is possible to extend this result to the case where $g$ does have explicit time dependence as well; the correct equation is then that $\dot{g} = 0$.

Continuous symmetries allow us to consider infinitesimal symmetry transformations. Since $g$ is unitary and parametrized by a continuous parameter, we may expand the transformation around the identity,

$$g = I - i\varepsilon G + \mathcal{O}(\varepsilon^2) \tag{9.21}$$

where $G$ must be a self-adjoint operator, and thus an observable. The transformation rule on observables is deduced directly from the finite transformation law $A \to A' = g^\dagger A g$, and is given by

$$g^\dagger A g - A = i\varepsilon[G, A] + \mathcal{O}(\varepsilon^2) \tag{9.22}$$

One defines the infinitesimal transformation by

$$\delta A = i[G, A] \tag{9.23}$$

The composition of two infinitesimal symmetry transformations $\delta_1$ and $\delta_2$ is given by their associated conserved charges $G_1$ and $G_2$ by,

$$
\begin{aligned}
(\delta_1 \delta_2 - \delta_2 \delta_1) A &= -[G_1, [G_2, A]] + [G_2, [G_1, A]] \\
&= -i[G, A]
\end{aligned}
\tag{9.24}
$$

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where the composition is given by

$$G = -i[G_1, G_2] \tag{9.25}$$

using the Jacobi identity. Thus the infinitesimal symmetry transformations naturally form a Lie algebra.

## 9.5 Examples of quantum symmetries

Many of the most important examples have already been encountered in the special cases that we have studied. Here, we shall limit the enumeration to continuous symmetries. Important discrete symmetries will be studied later on.

- space translation invariance; charge = momentum;

- time translation invariance; charge = energy;

- space rotation symmetry; charge = angular momentum;

- boosts in (non) relativistic mechanics; charge = Lorentz generators;

- $U(1)$ phase rotations associated with gauge invariance; charge = electric charge;

- $SU(3)$ rotations of the strong interactions; charge = color;

- $SU(3)$ approximate symmetry between $u, d, s$ quarks; charge = isospin and strangeness.

The existence of symmetries has important consequences;

* The states at a given energy level transform under a unitary representation of the symmetry group or of the symmetry Lie algebra;

* Selection rules imply relations between certain probability amplitudes and imply the vanishing of other probability amplitudes and expectation values.

In the subsequent subsections, we shall discuss examples of these phenomena.

## 9.6 Symmetries of the multi-dimensional harmonic oscillator

The $N$-dimensional harmonic oscillator provides an excellent laboratory for learning about symmetries and their realizations. The dynamical variables are $q_i(t)$ and $p_i(t)$, and canonical commutation relations $[q_i, p_j] = i\hbar \delta_{ij}$, with $i, j = 1, \cdots, N$. The Hamiltonian is

$$H = \sum_{i=1}^{N} \left( \frac{1}{2m} p_i^2 + \frac{1}{2} m\omega^2 q_i^2 \right) \tag{9.26}$$

It is chosen to have maximal symmetry.[7]

### 9.6.1 The orthogonal group $SO(N)$

In the case of $N = 3$, we simply have the isotropic 3-dimensional harmonic oscillator,

$$N = 3 \qquad\qquad H = \frac{1}{2m}\mathbf{p}^2 + \frac{1}{2}m\omega^2\mathbf{x}^2 \qquad\qquad (9.27)$$

It is of course well-known that this Hamiltonian is invariant under simultaneous rotations of $\mathbf{x}$ and $\mathbf{p}$, given by $\delta\mathbf{x} = \vec{\omega} \times \mathbf{x}$ and $\delta\mathbf{p} = \vec{\omega} \times \mathbf{p}$. The associated conserved charges are the three components of angular momentum $\mathbf{L} = \mathbf{x} \times \mathbf{p}$.

For general dimension $N$, the harmonic oscillator is invariant under orthogonal transformations in $N$-dimensional space. A convenient way to see this is by organizing the degrees of freedom in column matrices,

$$Q = \begin{pmatrix} q_1 \\ q_2 \\ . \\ q_N \end{pmatrix} \qquad\qquad P = \begin{pmatrix} p_1 \\ p_2 \\ . \\ p_N \end{pmatrix} \qquad\qquad (9.28)$$

The Hamiltonian then takes the form,

$$H = \frac{1}{2m}P^t P + \frac{1}{2}m\omega^2 Q^t Q \qquad\qquad (9.29)$$

Orthogonal transformations in $N$-dim space are defined as *linear transformations which leave the $N$-dimensional Euclidean norm $Q^t Q$ invariant*. On $Q$, we have,

$$Q \to Q' = MQ \qquad\qquad \text{such that} \qquad\qquad (Q')^t Q' = Q^t Q \qquad\qquad (9.30)$$

for a real $N \times N$ matrix $M$, and for all $Q$. This requires that $M^t M = I$. The set of all real matrices satisfying $M^t M = I$ forms a group under matrix multiplication, referred to as the orthogonal group $O(N)$. Indeed, if we have $M_1^t M_1 = M_2^t M_2 = I$ then $(M_1 M_2)^t(M_1 M_2) = M_2^t M_1^t M_1 M_2 = I$. The identity element is the unit matrix $I$ and the inverse is the transpose $M^{-1} = M^t$. Clearly, if we let $Q \to MQ$ and $P \to MP$, then both the Hamiltonian and the canonical commutation relations are invariant, and thus all orthogonal transformations, which belong to $O(N)$ are symmetries of the harmonic oscillator quantum system.

Rotations in $N$ dimensional space are all orthogonal transformations, but all orthogonal transformations are not rotations. A rotation is continuously connected to the identity orthogonal transformation, since one may think of a rotation as obtained by making a sequence

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[7]A more general form of the $N$-dimensional harmonic oscillator would be obtained by replacing the potential term by $\frac{1}{2}m\sum_{i,j=1}^{N}\omega_{ij}^2 q_i q_j$ for some positive real matrix $\omega^2$.

of small incremental rotations starting from the identity. But the relation $M^t M = I$ implies that $\det M = \pm 1$. These two cases are not continuously connected to one another, and only the set $\det M = +1$ contains the identity matrix $M = I$. Hence, the matrices for which $\det M = -1$ are not rotations. One example of such a matrix is

$$(M_0)_{ij} = \delta_{ij} - 2\delta_{iN}\delta_{jN} \tag{9.31}$$

Its effect on $Q$ is to reverse the sign of $q_N$, leaving all other $q_i$ unchanged. This transformation is a *space parity transformation* in the direction $N$, and is clearly not a rotation. Any matrix $M$ with $\det M = -1$ may be written as $M = M_0 M'$ where now $\det M' = 1$. Thus, any orthogonal transformation is either a rotation in $N$ dimensions or the product of a rotation by a parity transformation. The group of rotations consists of matrices $M$ such that we have both $M^t M = I$ and $\det M = +1$, and is denoted by $SO(N)$, the prefix $S$ standing for the condition of unit determinant.

It is also very useful to examine the infinitesimal rotations in $N$-dim space. To do so, we expand $M$ around the identity $I$ to linear order,

$$M = I + \varpi + \mathcal{O}(\varpi^2) \tag{9.32}$$

and insist on the relation $M^t M = I$ to this order. This requires that the matrix $B$ be anti-symmetric, i.e. $\varpi^t = -\varpi$. A real anti-symmetric $N \times N$ matrix has $N(N-1)/2$ independent entries, and this yields the dimension of the orthogonal groups,

$$\dim SO(N) = \dim O(N) = \frac{1}{2} N(N-1) \tag{9.33}$$

Finally, infinitesimal rotations are generated by the angular momentum operators,

$$L_{ij} = q_i p_j - q_j p_i \qquad\qquad i, j = 1, \cdots, N \tag{9.34}$$

Since we have

$$[L_{ij}, q_k] = i\hbar(\delta_{ik} q_j - \delta_{jk} q_i) \tag{9.35}$$

the rotations are generated by the unitary operator

$$U = \exp\left\{ -\frac{i}{2\hbar} \sum_{i,j=1}^{N} \varpi_{ij} L_{ij} \right\} \tag{9.36}$$

It is then easy to verify that

$$U q_i U^\dagger = q_i + \sum_{j=1}^{N} \varpi_{ij} q_j + \mathcal{O}(\varpi^2) \tag{9.37}$$

so that $U$ indeed correctly generates a rotation by $\varpi$. The rotation generators $L_{ij}$ have the following commutation relations,

$$[L_{ij}, L_{kl}] = i\hbar(\delta_{ik}L_{jl} - \delta_{jk}L_{il} - \delta_{il}L_{jk} + \delta_{jl}L_{ik}) \tag{9.38}$$

Antisymmetry of $\varpi_{ij}$ and $L_{ij}$ under $i \leftrightarrow j$ guarantees that the number of independent rotations is $N(N-1)/2$.

### 9.6.2 The unitary groups $U(N)$ and $SU(N)$

The $N$-dimensional harmonic oscillator actually has a symmetry larger than $SO(N)$. This is not so easy to see directly in $q_i, p_i$ coordinates, but becomes apparent when we recast the problem in terms of raising and lowering operators, defined by

$$
\begin{aligned}
a_i &= \frac{1}{\sqrt{2m\hbar\omega}}\left( + ip_i + m\omega q_i\right) \\
a_i^\dagger &= \frac{1}{\sqrt{2m\hbar\omega}}\left( - ip_i + m\omega q_i\right)
\end{aligned}
\tag{9.39}
$$

for $i = 1, \cdots, N$. The Hamiltonian is then

$$H = \sum_{i=1}^{N} \hbar\omega\left(a_i^\dagger a_i + \frac{1}{2}\right) = \frac{1}{2}\hbar\omega N + \hbar\omega \sum_{i=1}^{N} a_i^\dagger a_i \tag{9.40}$$

while the canonical commutation relations are $[a_i, a_j^\dagger] = \delta_{ij}$. Again, it is convenient to arrange the $a_i$ and $a_i^\dagger$ into matrices,

$$A = \begin{pmatrix} a_1 \\ a_2 \\ . \\ a_N \end{pmatrix} \qquad\qquad A^\dagger = ( a_1^\dagger \quad a_2^\dagger \quad \cdot \quad a_N^\dagger ) \tag{9.41}$$

The Hamiltonian then takes the form

$$H = \frac{1}{2}\hbar\omega N + \hbar\omega A^\dagger A \tag{9.42}$$

Since the observables $a_i$ are not self-adjoint, they are inherently complex variables, and linear transformations between them should be allowed to take on complex values. Thus, we shall now consider making linear transformations on $A$ but with complex coefficients,

$$A \to A' = MA \qquad\qquad A^\dagger \to (A')^\dagger = A^\dagger M^\dagger \tag{9.43}$$

Here, $M$ is now an $N \times N$ matrix with complex matrix elements. The hamiltonian will be invariant provided the quadratic form $A^\dagger A$ is invariant for all $A$, which requires $A^\dagger A \to (A')^\dagger A' = A^\dagger M^\dagger M A = A^\dagger A$, so that we must have

$$M^\dagger M = I \tag{9.44}$$

The set of complex matrices satisfying this relation forms the group of unitary $N \times N$ matrices, usually referred to as $U(N)$. The identity of the group is simply the identity matrix, while the inverse is given by the dagger : $M^{-1} = M^\dagger$. Note that when $M$ is restricted to have real coefficients, we recover the orthogonal transformations discussed in the preceding subsection, and we thus find that $SO(N)$ is a subgroup of $U(N)$.

The corresponding infinitesimal transformations are obtained by linearizing $M$ around the identity matrix,

$$M = I + i\varpi + \mathcal{O}(\varpi^2) \qquad\qquad \varpi^\dagger = \varpi \tag{9.45}$$

The infinitesimal transformations are thus parametrized by general $N \times N$ Hermitian matrices $\varpi$. The number of free (real) parameters of these Hermitian matrices is $N^2$, so that

$$\dim U(N) = N^2 \tag{9.46}$$

The corresponding conserved charges are as follows,

$$T^i{}_j = a_i^\dagger a_j \tag{9.47}$$

with commutation relations for the Lie algebra of $U(N)$,

$$[T^i{}_j, T^k{}_\ell] = \delta_j{}^k T^i{}_\ell - \delta_\ell{}^i T^k{}_j \tag{9.48}$$

The generators $T^i{}_j$ are actually not Hermitian, but suitable linear combinations may be constructed which are Hermitian,

$$\begin{aligned} T_{ij}^+ &= a_i^\dagger a_j + a_j^\dagger a_i \\ T_{ij}^- &= -i\left(a_i^\dagger a_j - a_j^\dagger a_i\right) \end{aligned} \tag{9.49}$$

The $N(N-1)/2$ combinations $T_{ij}^-$ satisfy the commutation relations of the subalgebra $SO(N) \subset U(N)$, and we have the relation $\hbar T_{ij}^- = L_{ij}$.

Finally, note that the group $U(N)$ is actually the product of two groups. Any unitary matrix $M_C$ in $U(N)$ which is proportional to the identity $M_C = \varepsilon I$ for $|\varepsilon| = 1$, commutes with all elements in $U(N)$. The elements $M_C$ themselves form a group, namely $U(1)$, and we thus have

$$U(N) = U(1) \times SU(N) \qquad\qquad SU(N) \equiv \{M \in U(N),\ \det M = 1\} \tag{9.50}$$

This immediately gives the real dimension $\dim SU(N) = N^2 - 1$. [Note that $SU(N)$ itself still contains non-trivial elements $M_C$ which are proportional to the identity $M_C = \varepsilon I$ as long as $\varepsilon^N = 1$. The set of all such elements forms a finite group, $Z_N$ which is referred to as the *center of $SU(N)$* since they commute with all elements of $SU(N)$.]

### 9.6.3 The group $Sp(2N)$

Is $U(N)$ the most general symmetry group leaving the Hamiltonian invariant ? In general, it is a difficult question to answer whether one has found the most general symmetry of a given system. In particular, for the harmonic oscillator Hamiltonian, it would seem that we can have a symmetry still larger than $U(N)$. Introduce the following $2N$-dimensional column matrix $X$,

$$H = \frac{1}{2m} X^t X \qquad\qquad X = \begin{pmatrix} m\omega Q \\ P \end{pmatrix} \tag{9.51}$$

The Hamiltonian $H$ is now clearly invariant under arbitrary orthogonal transformations $X \to X' = MX$, where $M \in SO(2N)$. This group is larger than $U(N)$, since we have

$$SO(N) \subset U(N) \subset SO(2N) \tag{9.52}$$

Actually, even though $SO(2N)$ leaves the Hamiltonian invariant, it is not a symmetry of the full quantum system, because the canonical commutation relations are not invariant. Expressed on the components $x_\alpha$ with $\alpha = 1, \cdots, 2N$ of the matrix $X$, the commutation relations $[q_i, p_j] = i\hbar\delta_{ij}$ become,

$$[x_\alpha, x_\beta] = i\hbar m\omega J_{\alpha\beta} \qquad\qquad J = \begin{pmatrix} 0 & +I \\ -I & 0 \end{pmatrix} \tag{9.53}$$

Real linear transformations $X \to X' = MX$ which leave these canonical commutation relations invariant must obey

$$M^t J M = J \tag{9.54}$$

The set of all real matrices $M$ satisfying $M^t J M = J$ forms the *symplectic group $Sp(2N)$*, for which the inverse is given by $M^{-1} = -J M^t J$.

The Hamiltonian is invariant under $SO(2N)$ while the canonical commutation relations are invariant under $Sp(2N)$. The entire system will thus be invariant under the largest common subgroup of $SO(2N)$ and $Sp(2N)$. This is the set of real $2N \times 2N$ matrices $M$ which satisfy both $M^t M = 1$ and $M^t J M = J$, which requires that $[M, J] = 0$. As a result, $M$ must be of the form

$$M = \begin{pmatrix} A & B \\ -B & A \end{pmatrix} \qquad\qquad M^t M = I \tag{9.55}$$

The $N \times N$ matrix $U = A + iB$ is then automatically unitary and belongs to $U(N)$. We conclude that $U(N)$ was indeed the largest symmetry group of the $N$-dimensional harmonic oscillator, confirming our earlier study from a different point of view.

## 9.7  Selection rules

In interpreting the strengths of various physical transitions, it is often striking how different the rates for various processes turn out to be. The most important ones are that unless energy and momentum are conserved in a process, the corresponding transition amplitude must vanish. Such a condition is often referred to as a *selection rule*. In the case of energy momentum conservation, the selection rule is exact and results from the exact symmetry of the invariance of the laws of nature under translations in time and in space. Another exact selection rule is the conservation of total angular momentum, associated with the invariance of the laws of Nature under space rotations. Yet another exact selection rule is the conservation of electric charge, which is the result of an exact gauge invariance of electro-dynamics.

The conservation of energy, momentum, angular momentum and electric charge are by now so well-established selection rules that they their validity is used to detect new forms of matter. One of the oldest such examples was the discovery of the neutrino by Pauli. By the 1930's the neutron was known to decay into a proton and an electron. If these were the only decay products, however, then angular momentum could not be conserved during the process, since the spin of the neutron, proton and electron are all $\hbar/2$, and a $\hbar/2$ unit of angular momentum is missing in the balance. An integer unit $\hbar$ could be carried off by orbital angular momentum, but a half integer unit cannot. This lack of balance led Pauli to conjecture the existence of a new particle, the neutrino, with spin $\hbar/2$.

Some selection rules are only approximate and result not in the vanishing of certain transition probabilities but in their suppression instead.

In particle physics, a number of such approximate selection rules are associated with symmetries of the strong and electro-magnetic interactions which, however, fail to be symmetries of the weak interactions. For example, the lightest strongly interacting particles are the three *pions* $\pi^0$ and $\pi^\pm$. Their quark composition, mass and life-times are given by

$$
\begin{aligned}
\pi^0 &= (\bar{u}u - \bar{d}d)/\sqrt{2} & m_{\pi^0} &= 135\,MeV & \tau_{\pi^0} &= 10^{-17}s \\
\pi^+ &= \bar{d}u & m_{\pi^+} &= 140\,MeV & \tau_{\pi^+} &= 10^{-8}s \\
\pi^- &= \bar{u}d & m_{\pi^-} &= 140\,MeV & \tau_{\pi^-} &= 10^{-8}s
\end{aligned}
\tag{9.56}
$$

The reason for the vast difference in life-times is that strong and electro-magnetic interactions preserve individual quark number, while the weak interactions do not. The $\pi^0$ can decay via

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electro-magnetic interactions, which occurs fast, while the $\pi^\pm$ cannot, resulting in typical weak scale life-times. Other approximate selection rules resulting from the effects of the weak interactions are as follows,

- individual quark number (up, down, charm, strange, top, bottom)

- individual lepton number (electron, $\mu$, $\tau$)

- parity

- CP (charge conjugation combined with parity)

In the remainder of this section, we shall explore the implications of the exact selection rule of the conservation of angular momentum. The techniques developed here will be applicable, however, also to selection rules that are only approximate.

## 9.8  Vector Observables

In practice, selection rules will often manifest their effect through the vanishing of certain probability amplitudes, which may emerge as the matrix elements of certain observables. Here, we shall be interested in selection rules associated with rotation invariance. The states of the system may be organized as combinations of angular momentum eigenstates $|j, m\rangle$. It readily follows from the action of the angular momentum generators $J_a$, $a = 1, 2, 3$ on these states that

$$
\begin{array}{llll}
(1) & \langle j', m'|J_a|j, m\rangle = 0 & \text{if} & j' \neq j \\
(2) & \langle j,\, m'|J_a|j, m\rangle = 0 & \text{if} & |m' - m| > 1
\end{array}
\tag{9.57}
$$

These results may be viewed as a simple form of angular momentum selection rules.

Analogous selection rules may be derived for operators other than $J_a$. The simplest case is for *vector observables*. A vector observable is actually a triplet $\mathbf{V} = (V_1, V_2, V_3)$ of observables which under rotations transform exactly as angular momentum itself does. Let $\mathcal{R} = \exp\{-i\vec{\omega} \cdot \mathbf{J}\}$ be any finite rotation, then a vector observable is defined to obey the transformation rule,

$$
\mathcal{R} V_a \mathcal{R}^\dagger = \sum_{b=1}^{3} R_a{}^b V_b
\tag{9.58}
$$

with $R$ a real $3 \times 3$ orthogonal matrix, i.e. satisfying $R^t R = I$. It is more convenient to use the infinitesimal version of this equation, given by

$$
[J_a, V_b] = i\hbar \sum_{c=1}^{3} \varepsilon_{abc} V_c
\tag{9.59}
$$

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Examples of vector observables include the angular momentum generators $\mathbf{J}$ themselves, the position operators $\mathbf{x}$, and the momentum generators $\mathbf{p}$. We shall now establish selection rules for *all* vector observables.

We begin by decomposing $\mathbf{V}$ in the raising and lowering basis that we also use for $\mathbf{J}$ itself.

$$V_0 = V_3 \qquad\qquad V_\pm = \frac{1}{\sqrt{2}}\left(V_1 \pm iV_2\right) \qquad\qquad (9.60)$$

so that the commutator relations become,

$$
\begin{aligned}
[J_3, V_q] &= q\hbar V_q & q = -, 0, + \\
[J_\pm, V_0] &= \mp\sqrt{2}\hbar V_\pm \\
[J_\pm, V_\pm] &= 0 \\
[J_\pm, V_\mp] &= \pm\sqrt{2}\hbar V_0 & (9.61)
\end{aligned}
$$

In fact, we can write this set of commutation relations in a way that will easily generalize to tensor observables later,

$$[J_a, V_q] = \sum_{q'}\left(D^{(1)}(J_a)\right)_{q,q'} V_{q'} \qquad\qquad (9.62)$$

where $q'$ ranges over the values $-, 0, +$.

## 9.9    Selection rules for vector observables

We shall study relations between various matrix elements of $V^q$, and obtain the following results, which are often referred to as the *Wigner-Eckardt theorem*,

(1)      $(m' - m - q)\langle j', m', \alpha'|V_q|j, m, \alpha\rangle = 0$ $\qquad\qquad$ (9.63)

(2)      $\langle j', m', \alpha'|V_q|j, m, \alpha\rangle = 0$   whenever   $|j' - j| \geq 2$

(3)      matrix elements with $j' - j = 0, \pm 1$ are all related to one another;

Here, $\alpha$ and $\alpha'$ represent all the quantum numbers other than $j$ and $m$. In the Coulomb problem, for example, $\alpha$ would be the principal quantum number, which fixes the energy of the state. For the special vector observable $J_q = V_q$, the matrix elements $\langle j', m', \alpha'|V_q|j, m, \alpha\rangle$ will vanish unless we also have $\alpha' = \alpha$, but for general vector observables, this need not be the case.

• To prove (1), we take the matrix elements of $[J_3, V_q] = \hbar q V_q$, or

$$\langle j', m', \alpha'|J_3 V_q - V_q J_3|j, m, \alpha\rangle - \hbar q\langle j', m', \alpha'|V_q|j, m, \alpha\rangle = 0 \qquad (9.64)$$

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Applying $J_3$ on either side gives (1).

• To prove (2), we shall assume without loss of generality that $j' - j \geq 2$. Now consider the matrix element of the vanishing operator $[J_+, V_+] = 0$,

$$\langle j', j + 2, \alpha'|[J_+, V_+]|j, j, \alpha\rangle = 0 \tag{9.65}$$

In the commutator, the term with $J_+$ on the right of $V_+$ vanishes, so we are left with

$$\sqrt{j'(j' + 1) - (j + 1)(j + 2)}\, \langle j', j + 1, \alpha'|V_+|j, j, \alpha\rangle = 0 \tag{9.66}$$

Since $j'(j' + 1) - (j + 1)(j + 2) \neq 0$ for $j' - j \geq 2$, it follows that

$$\langle j', j + 1, \alpha'|V_+|j, j, \alpha\rangle = 0 \tag{9.67}$$

Next, using $[J_+, V_0] = -\hbar\sqrt{2}V_+$, and then $[J_+, V_-] = \sqrt{2}\hbar V_0$, we also find that

$$\langle j', j, \alpha'|V_0|j, j, \alpha\rangle = \langle j', j - 1, \alpha'|V_-|j, j, \alpha\rangle = 0 \tag{9.68}$$

As a result, we then have

$$\langle j', m, \alpha'|V_q|j, j, \alpha\rangle = 0 \tag{9.69}$$

for all $q$ and all $m$. Next, we evaluate

$$
\begin{aligned}
\sqrt{2j}\langle j', m, \alpha'|V_q|j, j - 1, \alpha\rangle &= \langle j', m, \alpha'|V_q J_-|j, j, \alpha\rangle \\
&= \langle j', m, \alpha'|J_- V_q|j, j, \alpha\rangle \\
&\quad - \sum_{q'} D^{(1)}(J^-)_{qq'}\langle j', m, \alpha'|V_{q'}|j, j, \alpha\rangle
\end{aligned}
\tag{9.70}
$$

The second term on the right hand side vanishes in view of (9.69). The first term may be re-expressed in terms of $\langle j', m + 1, \alpha'|V_q|j, j, \alpha\rangle$ which vanishes in view of (9.69). Thus, we also have $\langle j', m, \alpha'|V_q|j, j - 1, \alpha\rangle = 0$ for all $m, q$. It is now clear that this argument may be recursively repeated and leads to

$$\langle j', m', \alpha'|V_q|j, m, \alpha\rangle = 0 \tag{9.71}$$

for all $m, m', q$ as long as $j' - j \geq 2$, which proves assertion (2).

• To prove (3), we first show that the matrix elements of $V_\pm$ are related to those of $V_0$, by using the commutator relations $[J_\pm, V_0] = \mp\sqrt{2}\hbar V_\pm$, and we find,

$$
\begin{aligned}
\sqrt{2}\langle j', m', \alpha'|V_\pm|j, m, \alpha\rangle &= \pm N_{j,m}^\pm \langle j', m', \alpha'|V_0|j, m \pm 1, \alpha\rangle \\
&\quad \mp N_{j',m'}^\mp \langle j', m' \mp 1, \alpha'|V_0|j, m, \alpha\rangle
\end{aligned}
\tag{9.72}
$$

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Thus, it remains to relate the different matrix elements of $V^0$ to one another. This is done using the double commutator relation,

$$[J_+, [J_-, V_0]] = 2\hbar^2 V_0 \tag{9.73}$$

Taking the matrix elements of this relation,

$$\langle j', m', \alpha' | [J_+, [J_-, V_0]] | j, m, \alpha \rangle = 2\hbar^2 \langle j', m', \alpha' | V_0 | j, m, \alpha \rangle \tag{9.74}$$

In view of (1), we know that only the matrix elements with $m' = m$ can be non-vanishing, and we now specialize to this case without loss of generality. Working out the commutators and applying the operators $J_\pm$ to the states, we obtain,

$$\left( N_{j',m}^- N_{j',m-1}^+ + N_{j,m}^+ N_{j,m+1}^- - 2 \right) \langle j', m, \alpha' | V_0 | j, m, \alpha \rangle \tag{9.75}$$
$$= N_{j',m}^- N_{j,m}^- \langle j', m-1, \alpha' | V_0 | j, m-1, \alpha \rangle + N_{j',m}^+ N_{j,m}^+ \langle j', m+1, \alpha' | V_0 | j, m+1, \alpha \rangle$$

This is a second order recursion relation. Without loss of generality we shall assume that $j' \geq j$. Taking $m = j$, we get

$$\left( N_{j',j}^- N_{j',j-1}^+ - 2 \right) \langle j', j, \alpha' | V_0 | j, j, \alpha \rangle = N_{j',j}^- N_{j,j}^- \langle j', j-1, \alpha' | V_0 | j, j-1, \alpha \rangle \tag{9.76}$$

Given that we now have two initial data for the second order recursion relation, it follows that all matrix elements $\langle j', m, \alpha' | V_0 | j, m, \alpha \rangle$ are known as a function of the single one $\langle j', j, \alpha' | V_0 | j, j, \alpha \rangle$, which proves (3).

## 9.10 Tensor Observables

Higher rank tensor observables sometimes occur as well, but it is rare that tensors of rank higher than 2 are needed, and we restrict here to tensors of rank 2. Quadrupole moments produce a tensor of rank 2 for example, $x_i x_j$ which is manifestly symmetric. Generally, tensor of rank 2 arise as sums of tensor products of vector observables, as is the case in the quadrupole moments. Consider a single one of these tensor products,

$$T_{ij} = U_i V_j \qquad\qquad i, j = 1, 2, 3 \tag{9.77}$$

where $U_i$ and $V_j$ are vector observables. Here we shall generally take the observables $U$ and $V$ to be different quantities, but they could be the same.

The tensor $T^{ij}$ admits a unique decomposition into its trace part $T_0$, its anti-symmetric part $T_1$ and its symmetric traceless part $T_2$, according to the following formula,

$$T_{ij} = \frac{1}{3} \delta_{ij} T^0 + \sum_{k=1}^{3} \varepsilon_{ijk} T_k^1 + T_{ij}^2 \tag{9.78}$$

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where

$$T^0 = \sum_{k=1}^{3} T_{kk}$$

$$T_k^1 = \sum_{i,j=1}^{3} \frac{1}{2}\varepsilon_{kij}T_{ij}$$

$$T_{ij}^2 = \frac{1}{2}T_{ij} + \frac{1}{2}T_{ji} - \frac{1}{3}\delta_{ij}T^0 \tag{9.79}$$

The component $T^0$ is a scalar and transforms in the $j = 0$ representation of the rotation algebra; $T_i^1$ is a vector observable and transforms in the $j = 1$ representation of the rotation algebra. Finally, the symmetric traceless tensor $T_{ij}^2$ has 5 linearly independent components $T_{++}^2, T_{+0}^2, T_{+-}^2 - T_{00}^2, T_{0-}^2, T_{--}^2$, and form an irreducible representation $j = 2$.

The Wigner-Eckardt theorem may be generalized to tensor observables. Let us illustrate this by discussion point (2) of this theorem. Since we have

$$\langle j', m', \alpha'|U_k|j'', m'', \alpha''\rangle = 0 \qquad\qquad |j' - j''| \geq 2$$
$$\langle j'', m'', \alpha''|V_\ell|j, m, \alpha\rangle = 0 \qquad\qquad |j - j''| \geq 2 \tag{9.80}$$

it follows that

$$\langle j', m', \alpha'|T_{k\ell}|j, m, \alpha\rangle = 0 \qquad\qquad |j' - j| \geq 3 \tag{9.81}$$

This result follows by inserting the identity between $U_k$ and $V_\ell$ and representing the identity by the completeness relation $I = \sum_{j'', m'', \alpha''} |j'', m'', \alpha''\rangle\langle j'', m'', \alpha''|$.

## 9.11    $P$, $C$, and $T$

The operations of reversal of space, $P$, reversal of time, $T$, and reversal of charges, $C$, are discrete transformations which are all symmetries of quantum electrodynamics (QED), but not necessarily of the other interactions. It is a very general result that, in any quantum theory invariant under special relativity (as QED and the Standard Model of Particle Physics are), the combined transformation $CPT$ is a symmetry. This result is often referred to as the $CPT$ theorem, and goes back to Pauli, who gave a first proof of the theorem. Of course, it is ultimately an experimental question as to whether $CPT$ is a symmetry of Nature, and so far, no violations have been observed.

Parity is a symmetry of the strong interactions, but is violated ("maximally") by the weak interactions. The combined operation $CP$ (equivalent to $T$ in a theory with $CPT$ invariance) is also violated by the weak interactions. $CP$ also appears to be a symmetry

of the strong interactions, though it is not well-understood why, as it would be natural to violate $CP$ also'in the strong interactions. This is often referred to as the *strong CP problem*, and remains an active area of investigation in particle physics.

*Parity* is the operation which reverses an odd number of space-like direction. In 3 space dimensions, it is convenient to take it to act by $\mathbf{x} \to -\mathbf{x}$, a transformation which commutes with rotations. On Hilbert space, the transformation acts by a linear operator $P$, which is self-adjoint and has unit square $P^2 = I$. On states and operators, $P$ acts as follows,

$$
\begin{aligned}
P \mathbf{x} P^\dagger &= -\mathbf{x} & P|\mathbf{x}\rangle &= |-\mathbf{x}\rangle \\
P \mathbf{p} P^\dagger &= -\mathbf{p} & P|\mathbf{p}\rangle &= |-\mathbf{p}\rangle \\
P \mathbf{L} P^\dagger &= +\mathbf{L} & P|\ell, m\rangle &= (-)^\ell |\ell, m\rangle
\end{aligned}
\tag{9.82}
$$

Because of the last equation, a state may be characterized by both its angular momentum quantum numbers $\ell, m$ or $j, m$ and its behavior under parity. It is important to note that a state of any given integer spin may be even or odd under parity. For example, spin zero states $|\alpha\rangle$ fall into two categories,

$$
\begin{aligned}
\pi|\alpha_+\rangle &= +|\alpha_+\rangle & |\alpha_+\rangle &= \text{ scalar} \\
\pi|\alpha_-\rangle &= -|\alpha_-\rangle & |\alpha_-\rangle &= \text{ pseudo-scalar}
\end{aligned}
\tag{9.83}
$$

The need for both kinds of states may be seen direct from the existence of spin zero operators which have, however, odd parity. For example,

$$
[\mathbf{J}, (\mathbf{x} \cdot \mathbf{S})] = 0 \qquad\qquad P(\mathbf{x} \cdot \mathbf{S}) P^\dagger = -(\mathbf{x} \cdot \mathbf{S})
\tag{9.84}
$$

Therefore, if $|\alpha_+\rangle$ is a scalar state with even parity, and spin 0, then the state $(\mathbf{x} \cdot \mathbf{S})|\alpha_+\rangle$ must also be spin zero, but have odd parity, and is thus a pseudo-scalar. Similarly, spin 1 states that are odd under parity are referred to as *vector* states, while spin 1 states that are even under parity are referred to as pseudo-vectors or more commonly as *axial vectors*. Parity provides with a single selection rule, given by

$$
(1 - \pi_{\mathcal{O}} \pi_\alpha \pi_\beta) \langle \beta | \mathcal{O} | \alpha \rangle = 0 \qquad\qquad
\begin{aligned}
P|\alpha\rangle &= \pi_\alpha |\alpha\rangle \\
P|\beta\rangle &= \pi_\beta |\beta\rangle \\
P\mathcal{O}P^\dagger &= \pi_{\mathcal{O}} \mathcal{O}
\end{aligned}
\tag{9.85}
$$

where $\pi_\alpha^2 = \pi_\beta^2 = \pi_{\mathcal{O}}^2 = 1$.

*Charge conjugation*, $C$, maps the electron into a state with the same mass and momentum, but with opposite electric charge; this state is the positron. Similarly, $C$ maps any particle into its anti-particle. The existence of anti-particles is required by special relativity,

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and may be viewed as a relativistic effect. For this reason, this operation is not normally encountered in non-relativistic quantum mechanics, and we shall introduce it only later when we discuss the Dirac equation.

*Time-reversal* reverses the direction of time $t \to -t$. In classical mechanics, time reversal leaves position and energy unchanged, but reverses the sign of momentum and angular momentum. In electrodynamics, the electric field and the electric charge density are unchanged, but the sign of the magnetic field and the electric current are reversed. Under these transformations, the laws of mechanics and electrodynamics are then invariant under time reversal. On the other hand, the fundamental laws of quantum mechanics are expressed via operators acting on Hilbert space and the Schrödinger equation. For example,

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \psi + V \psi \tag{9.86}$$

This equation is *not invariant* under $\psi(t, \mathbf{x}) \to \psi(-t, \mathbf{x})$. What is needed in addition is the operation of complex conjugation. The Schrödinger equation is indeed invariant under

$$T \; : \; \psi(t, \mathbf{x}) \to \psi(-t, \mathbf{x})^* \tag{9.87}$$

Therefore, the operation of time reversal acts not by a linear transformation, but rather by an *anti-linear transformation*, which involves an extra complex conjugation. We have instead,

$$
\begin{aligned}
T|\alpha\rangle &= |\alpha'\rangle & \langle\beta'|\alpha'\rangle &= \langle\beta|\alpha\rangle^* \\
T|\beta\rangle &= |\beta'\rangle & |\langle\beta'|\alpha'\rangle|^2 &= |\langle\beta|\alpha\rangle|^2
\end{aligned}
\tag{9.88}
$$

Thus, probability is unchanged under time reversal, though the probability amplitude is changed. As a result, we have

$$T(a|\alpha\rangle) = a^* T|\alpha\rangle \tag{9.89}$$

for any complex number $a$.

# 10    Bound State Perturbation Theory

We have now solved exactly a number of quantum mechanical problems. Systems of physical interest in Nature, however, are often more complex than these problems, and cannot be solved exactly. Perturbation theory is the approximation technique that allows one to study systems that may be viewed as small deviations (i.e. perturbations) away from exactly solved ones. In principle, successively higher orders in perturbation theory will yield results closer and closer to the solution of the full system. In practice, however, perturbation theory has many limitations that we shall illustrate below.

One distinguishes the following broad classes of perturbation theory, in order of generally increasing difficulty,

1. time independent perturbation theory

    - bound state spectrum
    - continuous spectrum (scattering theory)

2. time dependent perturbation theory

These distinctions are mostly of a technical nature, with bound state perturbation theory resembling most closely the perturbation theory of finite systems.

The general problem may be posed as follows. Let the Hamiltonian $H_0$ be solvable and denote its energy eigenvalues by $E_n^0$ and its eigenstates by $|E_n^0\rangle$. For any given $E_n^0$, there may be just a single state (regular perturbation theory) or several states (degenerate perturbation theory). The question now is how to calculate the energy eigenvalues $E_n(\lambda)$ and the eigenstates $|E_n(\lambda)\rangle$ for the family of Hamiltonians

$$H = H_0 + \lambda H_1 \tag{10.1}$$

where $\lambda$ is a real parameter, $H_0$ and $H_1$ are independent of $\lambda$, and we assume that $H_1^\dagger = H_1$. The parameter $\lambda$ may correspond to an adjustable quantity in an experiment, such as an external electric field (such as in the Stark effect) or a magnetic field (such as in the Zeeman effect). It may also be a fixed quantity in which we decide to expand, such as for example the coupling of a certain interaction. Thus, we have

$$
\begin{aligned}
H_0|E_n^0\rangle &= E_n^0|E_n^0\rangle \\
(H_0 + \lambda H_1)|E_n(\lambda)\rangle &= E_n(\lambda)|E_n(\lambda)\rangle
\end{aligned}
\tag{10.2}
$$

We seek a solution of the type

$$
\begin{aligned}
E_n(\lambda) &= E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \mathcal{O}(\lambda^3) \\
|E_n(\lambda)\rangle &= |E_n^0\rangle + \lambda|E_n^1\rangle + \lambda^2|E_n^2\rangle + \mathcal{O}(\lambda^3)
\end{aligned}
\tag{10.3}
$$

## 10.1 The validity of perturbation theory

We shall address two questions here. First, in which physical problems can we expect to have a small parameter naturally available in which to expand. Second, in what sense is the perturbative expansion convergent.

### 10.1.1 Smallness of the coupling

There are four fundamental forces of Nature.

1. Electro-Magnetism and electrodynamics

2. Weak interactions

3. Strong interactions

4. Gravity

Compared to all the other forces, gravity is always weak at the quantum level, and we shall ignore its effects throughout. Electrodynamics is the foremost example of a system in which there is a small dimensionless parameter, namely the fine structure constant, $\alpha \sim 1/137.036$. As a result, perturbation theory in electrodynamics can be carried out successfully in many situations. One of the oldest and most famous ones is the calculation of the quantum corrections to the electron and muon magnetic moments. The lowest order value results directly from the Dirac equation, and the first correction was evaluated by Tomonaga, Schwinger and Feynman, a result for which they were awarded the Nobel prize. Since then higher order corrections have been included as well, and certain relevant effects due to the weak and strong interactions, and the best value known to date is as follows,

$$\mu = g \left( \frac{e}{2mc} \right) \qquad\qquad g_\mu(\text{exp}'\text{nt}) = 2 \times 1.001159652410(200)$$

$$g_\mu(\text{theory}) = 2 \times 1.001159652359(282) \qquad (10.4)$$

In view of the unification of electro-magnetism and weak interactions in the Standard Model of particle physics, the weak interactions also have roughly the coupling constant $\alpha$, though at energies well below the mass of the $W^\pm$ (about 80 GeV), their strength is further suppressed. Thus, the weak interactions may also be treated perturbatively.

The situation is different for the strong interactions, as their name suggests. At low energies, such as in nuclear physics, the strong force dominates all other forces, including electromagnetic. Because of this, two protons can actually bind in a Helium nucleus. Remarkably, however, the strong interactions decrease in strength at high energies, phenomenon referred to as *asymptotic freedom*. Experimentally, this property was discovered in 1968 in

a famous MIT/SLAC experiment. Theoretically, asymptotic freedom was found to be a generic property of non-Abelian gauge theories (with not too many fermions), in a famous calculation by Gross, Wilczek and Politzer (1973). Thus, perturbation theory can be used also for the strong interactions, provided the energies involved are large.

### 10.1.2 Convergence of the expansion for finite-dimensional systems

One would hope, ideally, that the perturbative expansions of energy and state in (10.3) form a convergent Taylor series. Is this really the case ? When the corresponding quantum problem has a finite-dimensional Hilbert space, and $H_0$, $H_1$ may be represented by $N \times N$ matrices (and $|E_n\rangle$ by an $N$-dimensional column matrix), the perturbative expansion of (10.3) will in fact be convergent, with some finite radius of convergence. This is because the energy eigenvalues are solutions to the characteristic equation,

$$\det (E_n - H_0 - \lambda H_1) = 0 \qquad\qquad n = 1, \cdots, N \qquad\qquad (10.5)$$

and the eigenvalues depend analytically on the parameter $\lambda$. On the other hand, for quantum systems with infinite-dimensional Hilbert spaces, the situation is more complicated, and the $\lambda$-dependence may not be analytic.

### 10.1.3 The asymptotic nature of the expansion for infinite dimensional systems

It is instructive to consider how perturbation theory is carried out in the path integral in order to shed light on the convergence issues. For a simple one-dimension quantum mechanical system given by the following Hamiltonian or, equivalently, Lagrangian

$$
\begin{aligned}
H &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 + \lambda V(q) \\
L &= \frac{1}{2}m\dot{q}^2 - \frac{1}{2}m\omega^2 q^2 - \lambda V(q)
\end{aligned}
\qquad\qquad (10.6)
$$

with $V(q)$ given, for example, by $q^4$, the path integral for the partition function assumes the form,

$$\int \mathcal{D}q \, \exp\left\{ \frac{1}{\hbar} \int_0^{\beta\hbar} dt \, L(q, \dot{q}) \right\} \qquad\qquad (10.7)$$

This path integral is complicated, but for the sake of understanding the perturbative expansion, we shall truncate it to the contributions of just the $t$-independent functions $q(t)$, i.e. constant $q$. This gives an ordinary integral, which is of the general form,

$$I(\omega, \lambda) = \int_{-\infty}^{+\infty} dq \, \exp\{-\omega^2 q^2 - \lambda q^4\} \qquad\qquad (10.8)$$

Here we have absorbed various constants (such as $\hbar$, $m$) into $\omega$ and $\lambda$. The integral $I(\omega, \lambda)$ retains just the basic structure of the path integral. Expanding the integrand in powers of $\lambda$ for fixed $\omega$ gives,

$$I(\omega, \lambda) = \sum_{n=0}^{\infty} \frac{(-\lambda)^n}{n!} \int_{-\infty}^{+\infty} dq \, q^{4n} \, \exp\{-\omega^2 q^2\} \tag{10.9}$$

The calculation of the individual integrals for given $n$ are carried out by setting $x = q^2$, which reduces the integral to a $\Gamma$-function. These functions are defined by the integral representation

$$\Gamma(z) = \int_{0}^{\infty} dx \, x^{z-1} \, e^{-x} \tag{10.10}$$

for all complex $z$ such that $\mathrm{Re}(z) > 0$. There, the function obeys

$$\Gamma(z+1) = z\Gamma(z) \tag{10.11}$$

Using this relation throughout the plane allows one to analytically continue $\Gamma(z)$ throughout the complex plane. The resulting function is holomorphic throughout the complex plane, except for simple poles at all negative integers, and at zero. On positive integers $n$, the $\Gamma$ function reduces to the factorial, $\Gamma(n+1) = n!$. Just as for the factorial, the large $z$ behavior of the $\Gamma$-function is given by Sterling's formula,

$$\Gamma(z) = e^{z \ln z - z} \sqrt{\frac{2\pi}{z}} \left\{ 1 + \frac{1}{12z} + \frac{1}{288z^2} + \cdots \right\} \qquad |\arg(z)| < \pi \tag{10.12}$$

For curiosity's sake, we also expand $I(\omega, \lambda)$ for fixed $\lambda$ and small $\omega$, and using the same techniques as above, we find,

$$
\begin{aligned}
I(\omega, \lambda) &= \frac{1}{\omega} \sum_{n=0}^{\infty} \frac{\Gamma\left(2n + \frac{1}{2}\right)}{n!} \left(\frac{-\lambda}{\omega^4}\right)^n & \text{small } \lambda \\
I(\omega, \lambda) &= \frac{1}{4\lambda^{1/4}} \sum_{n=0}^{\infty} \frac{\Gamma\left(\frac{2n+1}{4}\right)}{n!} \left(\frac{-\omega^2}{\sqrt{\lambda}}\right)^n & \text{small } \omega
\end{aligned} \tag{10.13}
$$

Using Sterling's formula one may determine the radii of convergence of each of the above series expansions. The expansion for fixed $\lambda > 0$ and small $\omega$ has infinite radius of convergence. The series for fixed $\omega$ and small $\lambda$, however, has zero radius of convergence !

The interpretation of this result is very illuminating. Suppose we changed the sign of $\lambda$ and made $\lambda < 0$. The integral is then clearly divergent (at $q \to \infty$). If the integral admitted a Taylor series expansion around $\lambda = 0$ with *finite* radius of convergence, then

the integral for negative but small $\lambda$ would be well-defined and finite. So, the fact that the integral is divergent for any negative value of $\lambda$, no matter how small, forces us to have a series expansion that must have zero radius of convergence.

On the other hand, changing the sign of $\omega^2$ in the integral may change its value, but not its convergence properties, no matter how large $\omega^2$ is. This explains why the series expansion on power of $\omega^2$ can have infinite radius of convergence.

Another way of looking at this problem is that the non-convergence of the small $\lambda$ expansion comes from the behavior of the integral at $q \to \pm\infty$. There, it is the $q^4$ term that dominates, and so expanding in its strength is a singular thing to do. Generally, expanding in the dominant behavior will lead to non-convergent expansions.

Finally, note that the integral $I(\omega, \lambda)$ is a perfectly fine function. In fact, it is given by a modified Bessel function as follows,

$$I(\omega, \lambda) = \frac{\omega}{\sqrt{\lambda}} \, e^{\frac{\omega^4}{4\lambda}} \, K_{\frac{1}{4}}\left(\frac{\omega^4}{4\lambda}\right) \tag{10.14}$$

Looking up the asymptotics of this function in a standard reference (Bateman Vol II, page 86, formula (7)), we recover the asymptotic expansion derived above.

## 10.2    Non-degenerate perturbation theory

The basic assumption is that the energy level which we want to study of the unperturbed Hamiltonian $H_0$ is non-degenerate (other energy levels may or may not be degenerate). We also assume that the energy and the state have an expansion of the type (10.3). Thus, we need to solve the following problem,

$$(H_0 + \lambda H_1)|E_n\rangle = (E_n^0 + \Delta_n)|E_n\rangle \tag{10.15}$$

where we use the abbreviation $\Delta_n = E_n - E_n^0 = \lambda E_n^1 + \lambda^2 E_n^2 + \mathcal{O}(\lambda^3)$. Contracting both sides of the first equation with the unperturbed state $\langle E_n^0|$, we find,

$$\langle E_n^0|(H_0 + \lambda H_1)|E_n\rangle = \langle E_n^0|(E_n^0 + \Delta_n)|E_n\rangle \tag{10.16}$$

Using now the self-adjointness of $H_0$, we see that the first term on the left of the equations cancels with the first term on the right. The remaining terms give us an expression for $\Delta_n$,

$$\Delta_n = \lambda \frac{\langle E_n^0|H_1|E_n\rangle}{\langle E_n^0|E_n\rangle} \tag{10.17}$$

We learn immediately from this that the calculation of the energy correction to a given order requires the correction to the state to one lesser order. In fact, it is immediate to find the first order energy correction,

$$E_n^1 = \langle E_n^0|H_1|E_n^0\rangle \tag{10.18}$$

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assuming that the state $|E_n^0\rangle$ is normalized. The equation determining the first order correction to the state are obtained by expanding (10.15) to order $\lambda$, and are given as follows,

$$(H_0 - E_n^0)|E_n^1\rangle = (E_n^1 - H_1)|E_n^0\rangle \tag{10.19}$$

The operator $H_0 - E_n^0$ is not invertible, however, since it has a zero eigenvalue with eigenvector $|E_n^0\rangle$. To solve this equation, we now contract with an arbitrary state $\langle E_m^0|$, and again use the self-adjointness of $H_0$,

$$(E_m^0 - E_n^0)\langle E_m^0|E_n^1\rangle = \langle E_m^0|(E_n^1 - H_1)|E_n^0\rangle \tag{10.20}$$

When $m = n$, this equation is automatically satisfied, and thus yields no information on the quantity $\langle E_n^0|E_n^1\rangle$. But all other matrix elements are uniquely determined and we have

$$\langle E_m^0|E_n^1\rangle = -\frac{\langle E_m^0|H_1|E_n^0\rangle}{E_m^0 - E_n^0} \qquad\qquad m \neq n \tag{10.21}$$

This result allows us to write down the solution, using the completeness relation on all the states $|E_m^0\rangle$, and we have

$$|E_n^1\rangle = c|E_n^0\rangle - \sum_{m\neq n} |E_m^0\rangle\frac{\langle E_m^0|H_1|E_n^0\rangle}{E_m^0 - E_n^0} \tag{10.22}$$

The coefficient $c$ is, at this time arbitrary and not determined by the equation. The correction to the energy of second order in $\lambda$ may be derived from by expanding (10.17) to second order in $\lambda$, and we obtain,

$$E_n^2 = \langle E_n^0|H_1|E_n^1\rangle - cE_n^1 \tag{10.23}$$

Substituting in here the first order correction to the state, we obtain,

$$E_n^2 = -\sum_{m\neq n} \frac{|\langle E_m^0|H_1|E_n^0\rangle|^2}{E_m^0 - E_n^0} \tag{10.24}$$

Here, we have used the self-adjointness of $H_1$ to relate $\langle E_m^0|H_1|E_n^0\rangle = \langle E_n^0|H_1|E_m^0\rangle^*$.

An important consequence of this formula is that *the second order correction to the ground state energy is always negative*, since for the ground state we have $E_m^0 - E_n^0 > 0$ for all $m \neq n$, and numerator is manifestly positive.

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A). A qualitative description of the various situations: time indep.
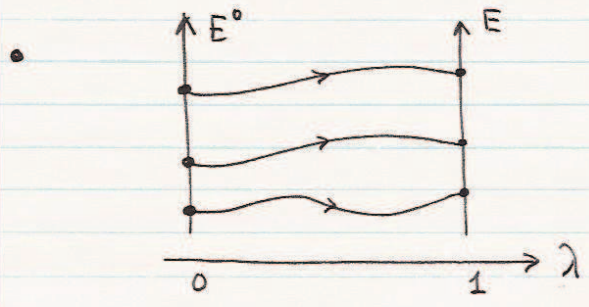


bound state,
regular perturbation theory
(or non-degenerate)



degenerate states with the same energy.

degenerate perturbation thy.



level crossing



not differentiable at $\lambda = 0$
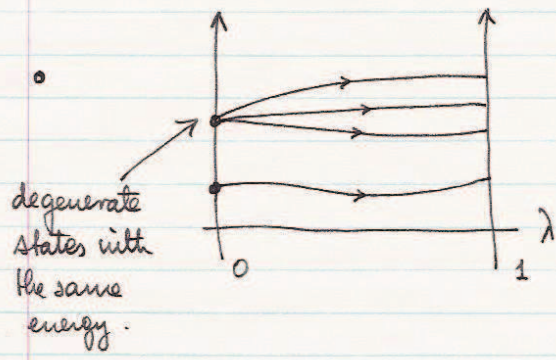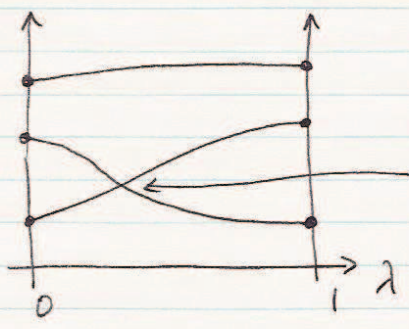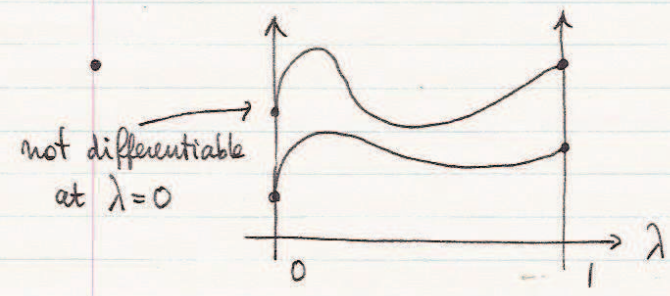
singular perturbation theory.

Figure 10: Different possible behaviors of bound state perturbation theory

## 10.3   Some linear algebra

It will be useful to analyze in a little more detail the procedure for solving equation (10.19) above, as the generalization of this method will enter when we deal with degenerate perturbation theory. It is best to illustrate the issues for an $N$-dimensional Hilbert space $\mathcal{H}$, whose vectors are represented by column vectors, and whose inner product is given by $(u, v) = u^\dagger v$ for all $u, v \in \mathcal{H}$. In this case, we have a Hermitian linear operator $A$, represented by an $N \times N$ Hermitean matrix, and a vector $b$ in Hilbert space. The relevant linear equation, analogous to (10.19) is then,

$$Ax = b \tag{10.25}$$

where $x \in \mathcal{H}$ is the unknown vector. When $A$ is invertible, we have simply $x = A^{-1}b$. When $A$ is not invertible, the above equation may still admit solution, under certain conditions. When $A$ is not invertible, it has a non-trivial null-space or *kernel*, and a non-trivial *range*, defined by

$$\begin{aligned}
\text{Ker}\, A &= \{v \in \mathcal{H} \text{ such that } Av = 0\} \\
\text{Range}\, A &= A\mathcal{H}
\end{aligned} \tag{10.26}$$

Equation (10.25) has at least one solution if and only if $b \in \text{Range}\, A$. This rather abstract condition may be translated into a simple concrete criterion. To test whether a given $b$ belongs to Range $A$, we proceed as follows. If $b$ belongs to Range $A$, then it follows that $(v, b) = (v, Ax) = (Av, x) = 0$ for all $v \in \text{Ker}\, A$. For any vector subspace $\mathcal{V}$ of $\mathcal{H}$, we define it orthogonal complement as follows,

$$\mathcal{V}^\perp = \{v \in \mathcal{H} \text{ such that } (u, v) = 0 \text{ for all } u \in \mathcal{V}\} \tag{10.27}$$

For any vector space we clearly have

$$\mathcal{V} \oplus \mathcal{V}^\perp = \mathcal{H} \tag{10.28}$$

The sum is direct since a vector belonging to both $\mathcal{V}$ and $\mathcal{V}^\perp$ must necessarily vanish. From this definition, we conclude that $\text{Range}\, A \subset (\text{Ker}\, A)^\perp$. Conversely, if $v \in (\text{Range}\, A)^\perp$, then we have $(v, Ax) = (Av, x) = 0$ for all $x \in \mathcal{H}$, so that $v \in \text{Ker}\, A$, and we also have $(\text{Range}\, A)^\perp \subset \text{Ker}\, A$. As a result, we must have[8]

$$\text{Range}\, A = (\text{Ker}\, A)^\perp \tag{10.29}$$

---

[8]For non-selfadjoint operators, the corresponding equation is analogously given by $\text{Range}\, A^\dagger = (\text{Ker}\, A)^\perp$, where $A^\dagger$ is the adjoint operator to $A$.

Thus, we conclude that $b \in \operatorname{Range} A$ if and only if

$$(v, b) = 0 \qquad \text{for all} \qquad v \in \operatorname{Ker} A \qquad (10.30)$$

If this condition is satisfied, equation (10.25) admits at least one solution which we denote by $x_0$. The general solution is then

$$x = x_0 + u \qquad \text{for any} \qquad u \in \operatorname{Ker} A \qquad (10.31)$$

The above discussion readily extends to infinite-dimensional Hilbert spaces, as long as the operator $A$ is bounded. In general, if $A$ is unbounded, subtle new issues may arise.

## 10.4    The Stark effect for the ground state of the Hydrogen atom

Faraday investigated the effect of electric and magnetic fields on light, in particular on its polarization and wavelength (color). He discovered that polarization is influenced by magnetic fields, but he found no change in color. Actually, both electric and magnetic fields change the energy levels of atoms and molecules, and will thus change the frequencies of radiation emitted and absorbed. The effects are so small, however, that more refined experimentation than Faraday disposed of in the mid 1800's to observe the effects. The effect of electric fields was established by Stark. We shall study it here as an example of how to use perturbation theory, both non-degenerate and degenerate.

The correction to the Hamiltonian of an electron in the presence of an electric field $\mathcal{E}$ along the $z$ axis is given by

$$H_1(\mathbf{x}) = e\mathcal{E}z \qquad (10.32)$$

where $z$ is the coordinate along the $z$-axis, and $-e$ is the charge of the electron. The electric field also interacts with the electrically positive nucleus, but since the mass of the nucleus is much larger than that of the electron, this effect may be safely neglected. Spin will similarly be neglected. We shall concentrate on atoms with only a single electron, whose states are labeled by the quantum numbers $n, \ell, m$ of the Coulomb problem, so the states are denoted by $|n, \ell, m\rangle$ with $n \geq \ell + 1$, and $|m| \leq \ell$.

For $n \geq 2$, each energy level is degenerate, so we shall have to develop degenerate perturbation theory to handle this reliably. For the ground state, first order perturbation theory gives

$$E^1_{|1,0,0\rangle} = \langle 1, 0, 0 | H_1 | 1, 0, 0 \rangle = e\mathcal{E} \langle 1, 0, 0 | z | 1, 0, 0 \rangle = 0 \qquad (10.33)$$

The above matrix element vanishes by rotation invariance of the ground state. Second order perturbation theory of the ground state always lowers the energy on general principles. We cannot quite calculate this effect here, though, because the summation over all states, which enters second order perturbation theory, will involve here the bound state part, but also the continuous spectrum part.

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## 10.5 Excited states and degenerate perturbation theory

The energy of a state $|n, \ell, m\rangle$ is

$$E_n^0 = -\frac{1}{2n^2} m_e c^2 \alpha^2 \tag{10.34}$$

and is independent of the angular momentum quantum numbers $\ell, m$. To investigate the Stark effect on excited states, we begin by evaluating the matrix elements of $H_1$ in the basis $|n, \ell, m\rangle$. For simplicity, we shall concentrate on the first excited states with $n = 2$. There are 4 states, and we have the following matrix elements,

$$H_1 = e\mathcal{E} \begin{pmatrix} 0 & \mathcal{M} & 0 & 0 \\ \mathcal{M}^* & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad \begin{matrix} |2,0,0\rangle \\ |2,1,0\rangle \\ |2,1,+1\rangle \\ |2,1,-1\rangle \end{matrix} \tag{10.35}$$

Here, all diagonal matrix elements vanish because $z$ has odd parity while the states $|2, \ell, m\rangle$ all have definite parity. The following 5 matrix elements vanish because of the Wigner-Eckard theorem,

$$\langle 2,0,0|z|2,1,\pm1\rangle = \langle 2,1,0|z|2,1,\pm1\rangle = \langle 2,1,1|z|2,1,-1\rangle = 0 \tag{10.36}$$

The only remaining matrix elements are non-vanishing, and we set

$$\begin{aligned} \langle 2,0,0|z|2,1,0\rangle &= \mathcal{M} \\ \langle 2,1,0|z|2,0,0\rangle &= \mathcal{M}^* \end{aligned} \tag{10.37}$$

This completes the calculation of the matrix elements of $H_1$. The full Hamiltonian in this basis is now given by putting together the contribution from the unperturbed Hamiltonian, which gives $E_2^0$ for all 4 states, with $H_1$, and we get

$$H = \begin{pmatrix} E_2^0 & e\mathcal{E}\mathcal{M} & 0 & 0 \\ e\mathcal{E}\mathcal{M}^* & E_2^0 & 0 & 0 \\ 0 & 0 & E_2^0 & 0 \\ 0 & 0 & 0 & E_2^0 \end{pmatrix} \qquad \begin{matrix} |2,0,0\rangle \\ |2,1,0\rangle \\ |2,1,+1\rangle \\ |2,1,-1\rangle \end{matrix} \tag{10.38}$$

Diagonalizing this matrix, we obtain the 4 energy eigenvalues,

$$\begin{aligned} E_{2,1} &= E_2^0 + e\mathcal{E}|\mathcal{M}| \\ E_{2,2} &= E_2^0 - e\mathcal{E}|\mathcal{M}| \\ E_{2,3} = E_{2,4} &= E_2^0 \end{aligned} \tag{10.39}$$

Note that a two-fold degeneracy remains on the last two states.

## 10.6   The Zeeman effect

A magnetic field on a (Hydrogen like) atom interacts with both the electron spin as well as its orbital angular momentum generated magnetic moment. To first order in a constant magnetic field $B$ along the $z$ axis, the perturbing Hamiltonian is given by

$$H_1 = -\frac{eB}{2m_e c}(L^z + 2S^z) \tag{10.40}$$

The factor of 2 in front of spin is due to the fact that the gyro-magnetic ratio for the electron is 2 (up to order $\alpha$ corrections). This time, spin needs to be taken into account, so we shall label the states by $|n, \ell, m_\ell, m_s\rangle$ where $m_\ell$ is the orbital magnetic quantum number, satisfying $|m_\ell| \leq \ell$, while $m_s$ is the spin magnetic quantum number given by $m_s = \pm 1/2$.

Conveniently, $H_1$ is diagonal in this basis. So, although in excited states this is degenerate perturbation theory, it is straightforward to evaluate the corrections. The diagonal matrix elements of $H_1$ are given by

$$
\begin{aligned}
E^1_{|n,\ell,m_\ell,m_s\rangle} &= -\frac{eB}{2m_e c}\langle n, \ell, m_\ell, m_s|(L^z + 2S^z)|n, \ell, m_\ell, m_s\rangle \\
&= -\frac{eB}{2m_e c}(m_\ell + 2m_s) \tag{10.41}
\end{aligned}
$$

This same correction may of course also be evaluated in the basis $|j, \ell, m\rangle$ but the formula is slightly more involved,

$$
\begin{aligned}
E^1_{|n,j,\ell,m\rangle} &= -\frac{eB}{2m_e c}\langle n, j, \ell, m|(J^z + S^z)|n, j, \ell, m\rangle \\
&= -\frac{eB}{2m_e c} m \left(1 \pm \frac{1}{2\ell + 1}\right) \tag{10.42}
\end{aligned}
$$

where the above $\pm$ refers to the two cases $j = \ell \pm 1/2$, and $m = m_\ell + m_s$ is the total magnetic quantum number.

## 10.7   Spin orbit coupling

Alkali atoms, such as Li, Na, K, etc, show many of the properties of single electron atoms and ions, because only one electron occurs on top of a completely filled shell (characteristic of the noble gases). But the cloud of inner electrons does interact with the outer electron via spin orbit coupling. The magnetic moment of the outer electron couples to the orbital magnetic moment, via a perturbing Hamiltonian of the type

$$H_1 = \phi(r)\mathbf{L} \cdot \mathbf{S} \tag{10.43}$$

In the basis of states given by the tensor product of the spin and orbital quantum numbers, this Hamiltonian is not diagonal. One could evaluate the matrix elements of $H_1$ in this basis and

then diagonalize that matrix for each level of degeneracy $n$. Actually, it is much more convenient to change basis and use the methods of addition of angular momentum. We shall use instead the following maximal set of commuting observables (in addition to the Hamiltonian), $\mathbf{J}^2, \mathbf{L}^2, J^z$, where $\mathbf{J} = \mathbf{L} + \mathbf{S}$. The operator $\mathbf{S}^2$ need not be included since its value is fixed at $3\hbar^2/4$.

In the basis of these commuting observables, the states are labeled again by $|n, j, \ell, m\rangle$, and $H_1$ is diagonal in this basis, since we have the following well-known formula,

$$2\mathbf{L} \cdot \mathbf{S} = \mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2 \tag{10.44}$$

so that we may evaluate the first order perturbations in a straightforward manner, and we obtain,

$$E^1_{|n,j,\ell,m\rangle} = \frac{1}{2}\left(j(j+1) - \ell(\ell+1) - \frac{3}{4}\right)\hbar^2 \langle n, j, \ell, m|\phi(r)|n, j, \ell, m\rangle \tag{10.45}$$

The last matrix element must be evaluated using the radial wave-functions of the Coulomb problem.

## 10.8   General development of degenerate perturbation theory

We now develop the general perturbation theory of an energy level $E^0_d$ of $H_0$ which admits an $N$-fold degeneracy. We shall denote the unperturbed states by $|E^0_d; i\rangle$ where $i = 1, \cdots, N$, and $E^0_d$ is the common unperturbed energy,

$$H_0|E^0_d; i\rangle = E^0_d|E^0_d; i\rangle \qquad i = 1, \cdots, N \tag{10.46}$$

Under the perturbation by $\lambda H_1$, the $N$ degenerate levels will generally split and these energies will be denoted by $E_{d,i} = E_{d,i}(\lambda)$. The equation of interest is

$$(E_{d,i} - H_0 - \lambda H_1)|E_{d,i}\rangle = 0 \tag{10.47}$$

Both the energy and the state admit an expansion in powers of $\lambda$,

$$\begin{aligned} E_{d,i} &= E^0_d + \lambda E^1_{d,i} + \lambda^2 E^2_{d,i} + \mathcal{O}(\lambda^3) \\ |E_{d,i}\rangle &= |E^0_d; i\rangle + \lambda|E^1_{d,i}\rangle + \lambda^2|E^2_{d,i}\rangle + \mathcal{O}(\lambda^3) \end{aligned} \tag{10.48}$$

The key idea is to rearrange the energy eigenvalue before starting to expand in powers of $\lambda$.

Let $\mathcal{H}_0$ denote the $N$-dimensional subspace of the full Hilbert space $\mathcal{H}$ generated by the degenerate states $|E^0_D, i\rangle$, and denote by $P_0$ the projection operator onto $\mathcal{H}_0$. The orthogonal complement of $\mathcal{H}_0$ is denoted $\mathcal{H}_1$ and consists of all the eigenstates of $H_0$ with eigenvalue different from $E^0_D$. Since $H_0$ is self-adjoint, the spaces $\mathcal{H}_0$ and $\mathcal{H}_1$ are guaranteed to be orthogonal and their sum to equal $\mathcal{H}$. Let $P_1$ denote the projection operator onto $\mathcal{H}_1$. We then have

$$\begin{aligned} \mathcal{H}_0 \oplus \mathcal{H}_1 &= \mathcal{H} & P_0 P_1 = P_1 P_0 = 0 \\ P_0 + P_1 &= I & P_0^2 = P_0, \ P_1^2 = P_1 \end{aligned} \tag{10.49}$$

The operators $P_0$ and $P_1$ commute with $H_0$, by construction.

We will now use these projectors to decompose the eigenvalue equation (10.47). Inserting the identity in front of the state gives,

$$(E_{d,i} - E_d^0 - \lambda H_1)P_0|E_{d,i}\rangle + (E_{d,i} - H_0 - \lambda H_1)P_1|E_{d,i}\rangle = 0 \tag{10.50}$$

Here, we have used the fact that all states in $P_0|E_{d,i}\rangle$ have eigenvalue $E_d^0$ under $H_0$. Our next step is to project this equation with $P_0$ and $P_1$, and we obtain,

$$P_0 \qquad \left(E_{d,i} - E_d^0 - \lambda P_0 H_1\right)P_0|E_{d,i}\rangle = \lambda P_0 H_1 P_1|E_{d,i}\rangle$$

$$P_1 \qquad \left(E_{d,i} - H_0 - \lambda P_1 H_1\right)P_1|E_{d,i}\rangle = \lambda P_1 H_1 P_0|E_{d,i}\rangle \tag{10.51}$$

We shall deduce from these the equations that yield $P_0|E_{d,i}\rangle$ and $P_1|E_{d,i}\rangle$.

The operator $P_1(E_{d,i} - H_0 - \lambda H_1)P_1$ is invertible on $\mathcal{H}_1$ provided $\lambda$ is sufficiently small. The reason is that for $\lambda = 0$, it reduces to the operator $P_1(E_d^0 - H_0)P_1$ which is by construction invertible on $\mathcal{H}_1$. Invertibility is an *open condition*, which means that in the space of all self-adjoint operators, any operator in a sufficiently small neighborhood of the invertible operator will also be invertible. Concretely, a finite-dimensional matrix $A$ is invertible if $\det A \neq 0$. But this means that if we consider a family of operators $A + \lambda B$ for sufficiently small $\lambda$, we will still have $\det(A + \lambda B) \neq 0$. Thus, perturbatively speaking, the operator $P_1(E_{d,i} - H_0 - \lambda H_1)P_1$ will be invertible on $\mathcal{H}_1$. As a result, we have

$$P_1|E_{d,i}\rangle = \lambda \left(\frac{1}{E_{d,i} - H_0 - \lambda P_1 H_1}\right)_{\mathcal{H}_1} P_1 H_1 P_0|E_{d,i}\rangle \tag{10.52}$$

Here the subscript $\mathcal{H}_1$ stands for the inverse operator restricted to the subspace $\mathcal{H}_1$. It remains to determine $P_0|E_{d,i}\rangle$ and the corresponding energies $E_{d,i}$. To do so, we substitute the expression for $P_0|E_{d,i}\rangle$, found above, into equation $P_0$, and we find,

$$\left(E_{d,i} - E_d^0 - \lambda P_0 H_1\right)P_0|E_{d,i}\rangle = \lambda^2 P_0 H_1 P_1 \left(\frac{1}{E_{d,i} - H_0 - \lambda P_1 H_1}\right)_{\mathcal{H}_1} P_1 H_1 P_0|E_{d,i}\rangle \tag{10.53}$$

To order $\mathcal{O}(\lambda^0)$, this equation is satisfied trivially.

### 10.8.1 Solution to first order

To order $\mathcal{O}(\lambda)$, the right hand side may be dropped, and the energy may be approximated by $E_{d,i} - E_d^0 = \lambda E_{d,i}^1 + \mathcal{O}(\lambda^2)$. The resulting equation becomes,

$$\left(E_{d,i}^1 - P_0 H_1 P_0\right)|E_d^0; i\rangle = 0 \tag{10.54}$$

The energy eigenvalues are determined by the eigenvalues of the operator $P_0 H_1 P_0$ restricted to $\mathcal{H}_0$, and are solutions of the characteristic equation,

$$\det\left(E_{d,i}^1 - P_0 H_1 P_0\right)_{\mathcal{H}_0} = 0 \tag{10.55}$$

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Note that the eigenstates that are being determined by this eigenvalue equation are the ones to lowest order. They must be eigenvectors of the Hamiltonian $P_0 H_1 P_0$. This is precisely the setting that we had encountered already when dealing with the Stark effect to this order.

Next, we derive the corrections to the states to order $\lambda$. The simplest part is given by (10.52), and to order $\mathcal{O}(\lambda)$ results in,

$$P_1\left(|E_d^0; i\rangle + \lambda |E_{d,i}^1\rangle\right) = \lambda \left(\frac{1}{E_d^0 - H_0}\right)_{\mathcal{H}_1} P_1 H_1 P_0 |E_d^0; i\rangle \tag{10.56}$$

By construction, $P_1 |E_d^0; i\rangle = 0$, so that the remaining equation gives,

$$P_1 |E_{d,i}^1\rangle = \left(\frac{1}{E_d^0 - H_0}\right)_{\mathcal{H}_1} P_1 H_1 P_0 |E_d^0; i\rangle \tag{10.57}$$

The solution for $P_0 |E_{d,i}^1\rangle$ needs to be handled at the same time as the second order correction to the energy, which we proceed to do now.

## 10.8.2   Solution to second order

Determining $P_0 |E_{d,i}^1\rangle$ proceeds analogously from (10.58), which we approximate up to order $\lambda^2$ included. Retaining only $\mathcal{O}(\lambda^2)$ contributions on the right hand side gives,

$$\left(E_{d,i} - E_d^0 - \lambda P_0 H_1\right) P_0 |E_{d,i}\rangle = \lambda^2 P_0 H_1 P_1 \left(\frac{1}{E_d^0 - H_0}\right)_{\mathcal{H}_1} P_1 H_1 P_0 |E_d^0; i\rangle \tag{10.58}$$

Expanding the left hand side to this order gives,

$$\begin{aligned}\left(E_{d,i} - E_d^0 - \lambda P_0 H_1\right) P_0 |E_{d,i}\rangle &= \lambda (E_{d,i}^1 - P_0 H_1) P_0 |E_d^0; i\rangle + \lambda^2 E_{d,i}^2 |E_d^0; i\rangle \\ &\quad + \lambda^2 \left(E_{d,i}^1 - P_0 H_1\right) P_0 |E_{d,i}^1\rangle\end{aligned} \tag{10.59}$$

The first term on the right hand side vanishes in view of our results for $E_{d,i}^1$ and $|E_d^0; i\rangle$. The other terms are now all of the same order, $\lambda^2$, as were the terms on the right hand side of (10.58). This gives the final equation,

$$E_{d,i}^2 |E_d^0; i\rangle + \left(E_{d,i}^1 - P_0 H_1\right) P_0 |E_{d,i}^1\rangle = P_0 H_1 P_1 \left(\frac{1}{E_d^0 - H_0}\right)_{\mathcal{H}_1} P_1 H_1 P_0 |E_d^0; i\rangle \tag{10.60}$$

We first determine $E_{d,i}^2$ by taking the product of the above equation with $\langle E_d^0; i|$. The second term on the right hand side cancels out in this process in view of (10.54), and we have

$$E_{d,i}^2 = \langle E_d^0; i| P_0 H_1 P_1 \left(\frac{1}{E_d^0 - H_0}\right)_{\mathcal{H}_1} P_1 H_1 P_0 |E_d^0; i\rangle \tag{10.61}$$

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This formula may be rendered more explicit by introducing a complete set of orthonormalized eigenstates of $H_0$ belonging to $\mathcal{H}_1$, which we denote by $|E_k^0\rangle$, and we have

$$E_{d,i}^2 = -\sum_k \frac{|\langle E_d^0; i|H_1|E_k^0\rangle|^2}{E_k - E_d^0} \tag{10.62}$$

Once $E_{d,i}^2$ is known, the equation for $P_0|E_{d,i}^1\rangle$ may be written as,

$$\left(E_{d,i}^1 - P_0 H_1\right) P_0 |E_{d,i}^1\rangle = E_{d,i}^2 |E_d^0; i\rangle + P_0 H_1 P_1 \left(\frac{1}{E_d^0 - H_0}\right)_{\mathcal{H}_1} P_1 H_1 P_0 |E_d^0; i\rangle \tag{10.63}$$

By construction, this equation is now orthogonal to $\langle E_{d,i}^1|$.

If the eigenvalue $E_{d,i}^2$ is *non-degenerate* with any of the other eigenvalues $E_{d,j}^1$, for $j \neq i$, then the operator on the left hand side may be inverted on the subspace of $\mathcal{H}_0$ which is orthogonal to $|E_{d,i}^1\rangle$, and we get

$$P_0|E_{d,i}^1\rangle = \sum_{j \neq i}^N |E_{d,j}^1\rangle \frac{1}{E_{d,i}^1 - E_{d,j}^1} \langle E_{d,j}^1|P_0 H_1 P_1 \left(\frac{1}{E_d^0 - H_0}\right)_{\mathcal{H}_1} P_1 H_1 P_0 |E_d^0; i\rangle \tag{10.64}$$

Introducing again a complete set of states $|E_k\rangle$ for $\mathcal{H}_1$, we may recast this formula as follows,

$$P_0|E_{d,i}^1\rangle = \sum_{j \neq i}^N |E_{d,j}^1\rangle \frac{1}{E_{d,i}^1 - E_{d,j}^1} \sum_k \frac{\langle E_{d,j}^1|H_1|E_k\rangle \langle E_k|H_1|E_d^0; i\rangle}{E_d^0 - E_k} \tag{10.65}$$

If, on the other hand, the energy level $E_{d,i}^1$ remains degenerate, then the above formula cannot be applied, since some of the denominators in $E_{d,i}^1 - E_{d,j}^1$. When this happens, one needs to rearrange the corresponding degenerate *order* $\lambda^0$ states so as to be eigenstates of the second order perturbation

$$P_0 H_1 P_1 \left(\frac{1}{E_d^0 - H_0}\right)_{\mathcal{H}_1} P_1 H_1 P_0 \tag{10.66}$$

as well. We shall not work out this case explicitly here.

## 10.9    Periodic potentials and the formation of band structure

The electronic structure in crystals is organized in bands. Empty or completely filled bands are electronically inactive, while partially filled band allow for electronic conductivity, providing a quantitative explanation for the fundamental distinction between insulators and conductors. Here, we shall derive the basic mechanism responsible for the formation of bands.

For simplicity, we concentrate on one-dimensional systems. The crystalline structure translates into a periodic potential for the electron, giving rise to a Hamiltonian of the form,

$$H = \frac{p^2}{2m} + V(x) \qquad\qquad V(x+a) = V(x) \tag{10.67}$$

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Here, $a$ is the lattice spacing of the crystal. As a result, the translation operator by a finite shift $a$, denoted by $T(a)$, and given by

$$T(a) = \exp\{iap/\hbar\} \tag{10.68}$$

must commute with $H$. We choose a basis of eigenstates for $H$ which also diagonalizes $T(a)$. The eigenvalues of $T(a)$ are phases specified by a wave-number $k$, so that

$$
\begin{aligned}
T(a)|k,n\rangle &= e^{-ika}|k,n\rangle \\
H|k,n\rangle &= E_{k,n}|k,n\rangle
\end{aligned}
\tag{10.69}
$$

By construction, for given $a$, the wave-number is periodic with period $k \to k + 2\pi/a$, so states are labeled uniquely when $k$ runs over and interval of length $2\pi/a$, called a Brillouin zone, for example the first Brillouin zone is specified by

$$-\frac{\pi}{a} \le k \le \frac{\pi}{a} \tag{10.70}$$

The additional index $n$ is a further quantum number needed to describe all the states.

It is useful to view the problem in a Schrödinger equation picture, for wave functions $\psi_{k,n}(x) = \langle x|k,n\rangle$, so that $\psi_{k,n}(x+a) = e^{ika}\psi_{k,n}(x)$. Alternatively, the wave function may be expressed in terms of a periodic wave function $\varphi_{k,n}(x)$ and a phase factor,

$$
\begin{aligned}
\psi_{k,n}(x) &= e^{ikx}\varphi_{k,n}(x) \\
\varphi_{k,n}(x+a) &= \varphi_{k,n}(x)
\end{aligned}
\tag{10.71}
$$

where the periodic wave function now obeys a $k$-dependent Schrödinger equations,

$$\left(\frac{(p+\hbar k)^2}{2m} + V(x)\right)\varphi_{k,n}(x) = E_{k,n}\varphi_{k,n}(x) \tag{10.72}$$

The quantum number $n$ now labels the discrete spectrum of this periodic equation.

For vanishing potential, $V = 0$, it is straightforward to solve this problem, and we have the energy levels of a periodic free system,

$$p\varphi_{k,n} = \frac{2\pi n\hbar}{a}\varphi_{k,n} \qquad\qquad n = 0, \pm 1, \pm 2, \cdots \tag{10.73}$$

so that the energies are

$$E_{k,n} = \frac{\hbar^2}{2m}\left(k + \frac{2\pi n}{a}\right)^2 \tag{10.74}$$

For certain values of $k$ within the Brillouin zone, energy levels are be degenerate, namely

$$E_{k,n'} = E_{k,n} \qquad\qquad n' \ne n \tag{10.75}$$

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This occurs when

$$2k = -\frac{2\pi}{a}(n' + n) \tag{10.76}$$

Within the first Brillouin zone, this occurs precisely when

$$
\begin{aligned}
k &= 0 & n' &= -n \neq 0 \\
k &= \pm\frac{\pi}{a} & n' + n &= \mp 1
\end{aligned}
\tag{10.77}
$$

At each of those points, the spectrum of the free Hamiltonian is degenerate, since two states occur with the same energy.

We concentrate on the degeneracies at the edge of the Brillouin zone, $k = k +_= \pi/a$, where the levels $n' = -n - 1$ and $n$ are degenerate. We now turn on *any perturbation which mixes the degenerate levels*. We introduce the notation,

$$
\begin{aligned}
\langle k_+, -n-1|V|k_+, n\rangle &= V_{-+} & \langle k_+, n|V|k_+, n\rangle &= V_{++} \\
\langle k_+, n|V|k_+, n'\rangle &= V_{+-} & \langle k_+, -n-1|V|k_+, -n-1\rangle &= V_{--} \quad (10.78)
\end{aligned}
$$

Self-adjointness of $V$ implies $V_{-+} = V_{+-}^*$, and we require that this mixing matrix element be non-zero. The energy levels in the presence of the potential $V$ for sufficiently small $V$ are then determined by the equation

$$\det \begin{pmatrix} E - E_0 - V_{++} & -V_{+-} \\ -V_{-+} & E - E_0 - V_{--} \end{pmatrix} = 0 \tag{10.79}$$

where $E_0 = E_{k_+,n} = E_{k,-n-1}$. This gives the following quadratic equation for the two energy levels,

$$\left(E - E_0 - \frac{1}{2}(V_{++} + V_{--})\right)^2 = |V_{+-}|^2 + \frac{1}{4}(V_{++} - V_{--})^2 \tag{10.80}$$

with solutions,

$$E = E_0 + \frac{1}{2}(V_{++} + V_{--}) \pm \frac{1}{2}\sqrt{(V_{++} - V_{--})^2 + 4|V_{+-}|^2} \tag{10.81}$$

This effect opens an energy gap in the spectrum, and creates a band structure.

## 10.10   Level Crossing

The problem of electronic band formation, discussed in the preceding section, is fundamentally a problem of level crossing. In fact, the conclusion obtained above indicates that, as soon as interactions are turned on, levels do not cross one another. This effect is quite general, and we shall now also prove it more generally.

We shall assume that two levels, with energies $E_n^0$ and $E_{n'}^0$, are very close to one another, so that $E_{n'}^0 - E_n^0$ is small compared to the gaps between either $E_n^0$ or $E_{n'}^0$ and any other energies in

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the spectrum. We do not assume, however, that $E_{n'}^0 = E_n^0$, so that we can apply *non-degenerate perturbation theory*. First order perturbation theory will split the levels significantly and lift the approximate degeneracy unless we have $E_n^1 = E_{n'}^1$, namely when $\langle E_n^0|H_1|E_n\rangle = \langle E_{n'}^0|H_1|E_{n'}\rangle$. In this case, we need to go to second order perturbation theory.

At second order perturbation theory, we may continue to use *non-degenerate perturbation theory* to deduce those second order corrections, and they are given by

$$
E_n^2 = -\sum_{m\neq n} \frac{|\langle E_m^0|H_1|E_n^0\rangle|^2}{E_m^0 - E_n^0}
$$

$$
E_{n'}^2 = -\sum_{m\neq n'} \frac{|\langle E_m^0|H_1|E_{n'}^0\rangle|^2}{E_m^0 - E_{n'}^0} \tag{10.82}
$$

This is a complicated sum, in general with an infinite number of terms. The assumption that $|E_{n'}^0 - E_n^0| \ll |E_m^0 - E_n^0|$ for all $m \neq n, n'$, which we made above, however, allows us to retain the essential contributions of these sums only. The smallness of $E_{n'}^0 - E_n^0$ allows us to approximate each sum by just a single term, and we get

$$
E_n^2 = -\frac{|\langle E_{n'}^0|H_1|E_n^0\rangle|^2}{E_{n'}^0 - E_n^0} + \mathcal{O}(1)
$$

$$
E_{n'}^2 = -\frac{|\langle E_n^0|H_1|E_{n'}^0\rangle|^2}{E_n^0 - E_{n'}^0} + \mathcal{O}(1) \tag{10.83}
$$

where we neglected terms that have finite limits as $E_{n'}^0 - E_n^0 \to 0$. We now read off the second order behavior,

$$
E_{n'}^0 > E_n^0 \quad \Rightarrow \quad E_{n'}^2 > 0, \quad E_n^2 < 0
$$

$$
E_{n'}^0 < E_n^0 \quad \Rightarrow \quad E_{n'}^2 < 0, \quad E_n^2 > 0 \tag{10.84}
$$

In either case, the levels repel one another. This effect is sometimes referred to as the *no-level crossing Theorem*.

There is, however, one very important exception to this effect. We tacitly assumed that the matrix element $\langle E_{n'}^0|H_1|E_n^0\rangle$ does not vanish in deriving the non-level crossing theorem. Naturally, if this matrix element vanishes, then the degeneracy is not lifted, and levels can actually cross. Putting together the conditions from first and second order perturbation theory for levels to cross, we have

$$
\langle E_n^0|H_1|E_n\rangle = \langle E_{n'}^0|H_1|E_{n'}\rangle
$$

$$
\langle E_{n'}^0|H_1|E_n^0\rangle = 0 \tag{10.85}
$$

which means that $H_1$ restricted to the two-dimensional subspace of states $|E_n\rangle$ and $|E_{n'}\rangle$ is actually proportional to the identity operator. The full Hamiltonian then necessarily has an $SU(2)$ symmetry which rotates these two states into one another.

Thus, we have discovered an important amendment to the *no level crossing theorem*, namely that levels can cross if and only if the Hamiltonian $H$ has a symmetry at the point where the levels are to cross.

# 11 External Magnetic Field Problems

In the chapter on perturbation theory, we have studied the effect of small magnetic fields on atoms and ions via the Zeeman effect. The application of strong magnetic fields produces further, and remarkable effects, such as the Quantized Hall Effect. In this chapter, we shall solve (anew) the general problem of charged particles in the presence of a strong magnetic field, and then apply the methods and results to the case of the quantized Hall Effect.

## 11.1 Landau levels

In problem set 8 of 221A, we studied the problem of a 2-dimensional particle with electric charge $2e$ in the presence of a uniform magnetic field, given by the following classical Lagrangian,

$$L(x, y, \dot{x}, \dot{y}) = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) - \frac{1}{2}m\omega^2(x^2 + y^2) + \frac{1}{2}eB(x\dot{y} - y\dot{x}) \tag{11.1}$$

This Lagrangian essentially also applies to a 3-dimensional charged particle in a magnetic field, since the direction along the magnetic field will be decoupled from the dynamics of the other directions. The corresponding canonical momenta are

$$p_x = m\dot{x} - \frac{1}{2}eBy$$

$$p_y = m\dot{y} + \frac{1}{2}eBx \tag{11.2}$$

The Hamiltonian is then given by

$$H(x, y, p_x, p_y) = \frac{1}{2m}(p_x + \frac{1}{2}eBy)^2 + \frac{1}{2m}(p_y - \frac{1}{2}eBx)^2 + \frac{1}{2}m\omega^2(x^2 + y^2) \tag{11.3}$$

Note that since we are not assuming the magnetic field to be small, we keep the term of order $B^2$. In problem set 8, functional methods were used to derive the partition function, and it was found to be given by

$$Z = \text{Tr} \, e^{-\beta H} = \frac{e^{-\frac{1}{2}\beta\hbar\omega_+}}{1 - e^{-\beta\hbar\omega_+}} \times \frac{e^{-\frac{1}{2}\beta\hbar\omega_-}}{1 - e^{-\beta\hbar\omega_-}} \tag{11.4}$$

where the frequencies $\omega_\pm \geq 0$ are given by

$$\omega_\pm = \omega_B \pm \left|\frac{eB}{2m}\right| \qquad\qquad \omega_B^2 = \omega^2 + \frac{e^2B^2}{4m^2} \tag{11.5}$$

The full spectrum is deduced by expanding the denominators in a Taylor series and we find,

$$E(n_+, n_-) = \frac{1}{2}\hbar\omega_+(1 + 2n_+) + \frac{1}{2}\hbar\omega_-(1 + 2n_-) \tag{11.6}$$

for $n_\pm \geq 0$. Effectively, the system decomposes into two independent harmonic oscillators, with frequencies $\omega_+$ and $\omega_-$. Clearly, something interesting happens when $\omega \to 0$, since then $\omega_- \to 0$,

and the partition function will diverge in this limit. Below, we investigate in the operator language, the phenomenon that drives this divergence.

It is straightforward to recover this result in the operator formulation. We set $\omega = 0$, so that $\omega_B = |eB/2m|$, and introduce the following harmonic oscillator combinations,

$$
\begin{aligned}
a_1 &= \frac{1}{\sqrt{2m\hbar\omega_B}}(ip_x + m\omega_B x) \\
a_2 &= \frac{1}{\sqrt{2m\hbar\omega_B}}(ip_y + m\omega_B y)
\end{aligned}
\tag{11.7}
$$

and their Hermitian conjugates. By construction they obey canonical commutation relations $[a_i, a_j^\dagger] = \delta_{ij}$ for $i, j = 1, 2$. Re-expressing the Hamiltonian in terms of these oscillators,

$$
H = \hbar\omega_B \left( a_1^\dagger a_1 + a_2^\dagger a_2 + 1 \right) + i\frac{eB\hbar}{2m} \left( a_1^\dagger a_2 - a_2^\dagger a_1 \right)
\tag{11.8}
$$

Finally, we make the following orthonormal change of variables,

$$
\begin{aligned}
a &\equiv \frac{1}{\sqrt{2}}(a_1 + ia_2) \\
b &\equiv \frac{1}{\sqrt{2}}(a_1 - ia_2)
\end{aligned}
\tag{11.9}
$$

and their conjugates. These oscillators still obey canonical commutation relations,

$$
\begin{aligned}
[a, b] = [a, b^\dagger] &= 0 \\
[a^\dagger, b] = [a^\dagger, b^\dagger] &= 0 \\
[a, a^\dagger] = [b, b^\dagger] &= 1
\end{aligned}
\tag{11.10}
$$

Using the following relations

$$
\begin{aligned}
2a^\dagger a &= a_1^\dagger a_1 + a_2^\dagger a_2 + i\left( a_1^\dagger a_2 - a_2^\dagger a_1 \right) \\
2b^\dagger b &= a_1^\dagger a_1 + a_2^\dagger a_2 - i\left( a_1^\dagger a_2 - a_2^\dagger a_1 \right)
\end{aligned}
\tag{11.11}
$$

the Hamiltonian may be recast as follows,

$$
H = \frac{1}{2}\hbar\omega_+ (1 + 2a^\dagger a) + \frac{1}{2}\hbar\omega_- (1 + 2b^\dagger b)
\tag{11.12}
$$

The above spectrum then follows at once.

As $\omega \to 0$, the problem is reduced to that of a charged particle in a magnetic field, and the frequency $\omega_- \to 0$. Remarkably, as a result, the spectrum becomes infinitely degenerate, since the energies do not depend upon $n_-$ any more. Alternatively, as $\omega = 0$, we have

$$
[H, b] = [H, b^\dagger] = 0
\tag{11.13}
$$

For each value of $n_+$, there is a *Landau level* with an infinite degeneracy. The algebra of $b$ and $b^\dagger$ represent the symmetry algebra of this degeneracy. Of course, in any physical system, space is not truly of infinite extent and the magnetic field is not quite uniform. Nonetheless, this infinite degeneracy makes the Landau levels an incredibly interesting phenomenon.

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## 11.2   Complex variables

The $x, y$ parts of the combinations $a$ and $b$ correspond to forming the complex variables

$$z = \frac{1}{\sqrt{2}}(x + iy) \qquad\qquad p_z = \frac{1}{\sqrt{2}}(p_x - ip_y)$$

$$\bar{z} = \frac{1}{\sqrt{2}}(x - iy) \qquad\qquad p_{\bar{z}} = \frac{1}{\sqrt{2}}(p_x + ip_y) \qquad (11.14)$$

which satisfy the canonical commutation relations,

$$\begin{aligned}
[z, p_z] = [\bar{z}, p_{\bar{z}}] &= i\hbar \\
[z, p_{\bar{z}}] = [\bar{z}, p_z] &= 0
\end{aligned} \qquad (11.15)$$

and as a result,

$$p_z = -i\hbar\frac{\partial}{\partial z} \qquad\qquad p_{\bar{z}} = -i\hbar\frac{\partial}{\partial \bar{z}} \qquad (11.16)$$

The oscillators now become,

$$a = \frac{1}{\sqrt{2m\hbar\omega_B}}\Big(ip_{\bar{z}} + m\omega_B z\Big) \qquad\qquad a^\dagger = \frac{1}{\sqrt{2m\hbar\omega_B}}\Big(-ip_z + m\omega_B \bar{z}\Big)$$

$$b = \frac{1}{\sqrt{2m\hbar\omega_B}}\Big(ip_z + m\omega_B \bar{z}\Big) \qquad\qquad b^\dagger = \frac{1}{\sqrt{2m\hbar\omega_B}}\Big(-ip_{\bar{z}} + m\omega_B z\Big) \qquad (11.17)$$

Since we are assuming $\omega = 0$, the Hamiltonian depends only on $a$ and $a^\dagger$, $H = \hbar\omega_B(2a^\dagger a + 1)$. The lowest Landau level $|0, n_-\rangle$ is characterized by $a|0, n_-\rangle = 0$. The wave functions of the lowest Landau level satisfy the differential equation

$$\left(\frac{\partial}{\partial \bar{z}} + \frac{m\omega_B}{\hbar}z\right)\psi(z, \bar{z}) = 0 \qquad (11.18)$$

Its general solution is straightforward (since as a differential equation in $\bar{z}$, you may think of $z$ as a constant coefficient), and we get

$$\psi(z, \bar{z}) = \varphi(z)\psi^{(0)}(z, \bar{z}) \qquad\qquad \psi^{(0)}(z, \bar{z}) = \exp\left\{-\frac{m\omega_B}{\hbar}|z|^2\right\} \qquad (11.19)$$

where $\varphi(z)$ is an arbitrary complex analytic function of $z$. Actually, $\varphi(z)$ cannot has poles since they would lead to non-square integrable wave functions. Also, assuming that $\psi(z, \bar{z})$ is single-valued, it follows that $\varphi(z)$ must be single-valued, and thus cannot have branch cuts. Therefore, $\varphi(z)$ must be single-valued and holomorphic throughout the complex plane. A basis for such functions is obtained by polynomials (and square integrable Taylor expandable functions by completeness). Notice that all such polynomial functions are obtained by applying $b^\dagger$ repeatedly to the ground state $\psi^{(0)}$ of both $a$ and $b$, since we have

$$\psi_{n_-}^{(0)} \sim (b^\dagger)^{n_-}\psi_0(z, \bar{z}) \sim z^{n_-}\psi_0(z, \bar{z}) \qquad (11.20)$$

This agrees with general principles that the group theory of $b, b^\dagger$ must precisely reproduce the normalizable spectrum.

## 11.3 Calculation of the density of states in each Landau level

An important characterization of the Landau levels is the number of quantum states that are available. This is easy to compute as we have the explicit wave-functions available. Consider the lowest Landau level first. All states in this level are obtained by applying powers of $b^\dagger$ to the ground state with wave function $\psi_0(z, \bar{z})$. The result is (the overall normalization will be immaterial),

$$\psi_n^{(0)}(z, \bar{z}) \sim z^n \exp\left\{-\left|\frac{eB}{2\hbar}\right| \times |z|^2\right\} \tag{11.21}$$

In terms of radial coordinates, $x + iy = r\, e^{i\theta}$, we have

$$\psi_n^{(0)}(r, \theta) \sim r^n e^{in\theta} \times \exp\left\{-\left|\frac{eB}{4\hbar}\right| \times r^2\right\} \tag{11.22}$$

Clearly, because of the $\theta$-dependence, states for different $n$ are orthogonal to one another. The maximum of the probability density $\psi_n^{(0)}(r, \theta)$ is attained at radius

$$r_n^2 = 2n\left|\frac{\hbar}{eB}\right| \tag{11.23}$$

But this means that a given area $\pi R^2 \gg |\hbar/eB|$ will contain a number of states $N$ given by

$$N = \pi R^2 \left|\frac{eB}{2\pi\hbar}\right| \tag{11.24}$$

Hence the density of states of the first Landau level for magnetic field $B > 0$ is given by

$$n_B = \frac{N}{\pi R^2} = \frac{eB}{2\pi\hbar} \tag{11.25}$$

This is a classic result, you may find in Landau and Lifschitz. In a higher Landau level, the wave function will have an extra factor of $\bar{z}^{n_+}$. But for given, finite $n_+$, this extra factor will not modify the asymptotic behavior of the density of states found in the lowest Landau level, so that the formula (11.25) is valid for any Landau level.

## 11.4 The classical Hall effect

The set-up of the Hall effect (classical or quantum) is a conductor subject to an electric field $\mathbf{E}$ and a perpendicular magnetic field $\mathbf{B}$. For zero magnetic field, the electric field creates an electric current $\mathbf{j}$ which is parallel to $\mathbf{E}$. The zero magnetic field conductivity is denotes $\sigma_0$ and relates $\mathbf{j} = \sigma_0\mathbf{E}$. If the current is produced by individual charge carriers such as electrons, then the current is given by the density of carriers $n$ and their electric charge $e$ by $\mathbf{j} = ne\mathbf{v}$.

When the magnetic field is turned on, charge carriers are deviated and produce an electric current, or *Hall current*, transverse to the electric field. The strength of this current may be obtained from the Lorentz force formula,

$$m_e \frac{d\mathbf{v}}{dt} = e\mathbf{E} + e\mathbf{v} \times \mathbf{B} - \frac{ne^2}{m_e\sigma_0}\mathbf{v} \tag{11.26}$$

Here, $m_e$ is the electron mass and $\mathbf{v}$ its velocity. The last term account for the dissipative processes which lead to Ohm's law, and we have defined the relevant dissipation constant such that $\sigma_0$ is the conductivity in the absence of magnetic fields. In the stationary regime, we have a flow of charge carriers with constant velocity, so that $d\mathbf{v}/dt = 0$, and we thus obtain,

$$ne\mathbf{v} = \mathbf{j} = \sigma_0 \left( \mathbf{E} + \mathbf{v} \times \mathbf{B} \right) \tag{11.27}$$

Eliminating $\mathbf{v}$ in favor of $\mathbf{j}$ gives,

$$\mathbf{j} = \sigma_0 \left( \mathbf{E} + \frac{1}{ne} \mathbf{j} \times \mathbf{B} \right) \tag{11.28}$$

Choosing the $z$-axis along $\mathbf{B}$ with $\mathbf{E}$ in the $xy$-plane, the equation becomes,

$$\begin{aligned} j_x &= \sigma_0 E_x + \frac{\sigma_0 B}{ne} j_y \\ j_y &= \sigma_0 E_y - \frac{\sigma_0 B}{ne} j_x \end{aligned} \tag{11.29}$$

Inverting this relation to get the resistivity as a function of the magnetic field,

$$\begin{pmatrix} E_x \\ E_y \end{pmatrix} = \begin{pmatrix} \rho_{xx} & \rho_{xy} \\ \rho_{yx} & \rho_{yy} \end{pmatrix} \begin{pmatrix} j_x \\ j_y \end{pmatrix}$$

$$R_L = \rho_{xx} = \rho_{yy} = \frac{1}{\sigma_0}$$

$$R_H = \rho_{xy} = -\rho_{yx} = \frac{B}{ne} \tag{11.30}$$

Remarkably, the off-diagonal resistivity is independent of the normal conductivity and involves only the density of carriers, besides fundamental constants and the magnetic field itself.

## 11.5  The quantum Hall effect

Although the above picture of the Hall effect is applicable in the regime at room temperature and for a large class of materials, there are special experimental settings where the Hall resistivity $\rho_{xy}$ is not just a linear function of $B$, but exhibits remarkable structure.[9]

The experimental conditions for the Quantum Hall Effect (QHE) are as follows,

- A layer of electrons is trapped at the interface of two semi-conductors (a hetero-junction);

- The system is cooled to temperatures in the milli-Kelvin range;

- The system is very pure.

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[9]There is extensive literature on both the integer and fractional quantum Hall effects; a good source with both experimental and theoretical contributions is in *The Quantum Hall Effect*, R.E. Prange and S.M. Girvin, Eds, Springer 1990.
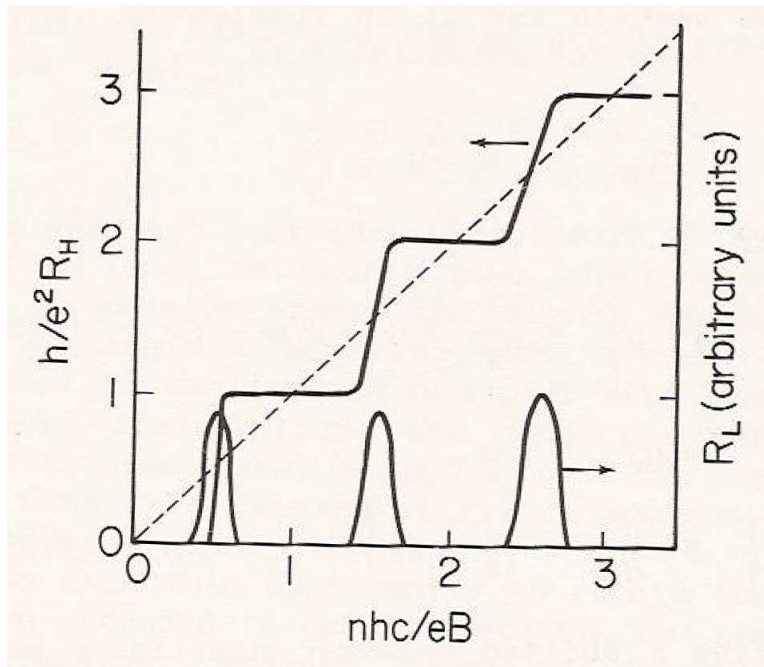
Figure 11: Schematic representation of the Hall and regular conductivity in the integer quantum Hall effect. (from R.E. Prange in *The quantum Hall effect*, Springer 1990).

A schematic rendition of the experimental observations characteristic of the (integer) Quantum Hall Effect (or QHE) is given in Figure 11. As the magnetic field $B$ is varied, it is observed that the Hall resistivity $R_H = \rho_{xy}$ does not follow a linear law, as would be expected from the discussion of the classical Hall effect, but instead exhibits *plateaux* on which the resistivity stays constant for a range of variations of $B$. Moreover, the values of the resistivity at the plateaux is observed to be

$$\rho_{xy} = \frac{2\pi\hbar}{e^2} \times \text{integer} \tag{11.31}$$

How can this phenomenon be explained ?

The key is to recall the density of carriers in a Landau level, given by

$$n_B = \frac{eB}{2\pi\hbar} \tag{11.32}$$

The contribution to the conductivity of one Landau level is then obtained by including only the density of states of one Landau level $n = n_B$, for which we get

$$(\rho_{xy})^{-1}\Big|_{1 \text{ Landau Level}} = \frac{n_B e}{B} = \frac{e^2}{2\pi\hbar} \tag{11.33}$$

Thus, the effect may be attributed to the contribution of filled Landau Levels, in which electrons behave effectively independently. Exactly why an entire Landau Level contributes, and not say 1.5 Landau Levels would require a more detailed discussion of which states are localized and which states are extended, and would require analysis of band structure and so on.

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The fundamental unit of 2-dimensional resistivity may be readily evaluated, using $\hbar = 1.05457 \times 10^{-34} Js$ and $e = 1.60218 \times 10^{-19} C$, and we find,

$$\frac{2\pi\hbar}{e^2} = 25,812.63 \ \Omega \tag{11.34}$$

The units work out as follows, $Js/C^2 = (J/C)(s/C) = V/A = \Omega$. Note that, by comparison, the expression for the fine structure constant is

$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} = \frac{1}{137.04} \tag{11.35}$$

Thus, we have, alternatively,

$$\frac{2\pi\hbar}{e^2} = \frac{1}{2\epsilon_0 c\alpha} \tag{11.36}$$

Measurement of the Hall resistivity now gives the most accurate determination of this combination of the fundamental constants $e$ and $\hbar$.

The actual experimental results are more complicated, and also even more interesting. In Figure 12, it is the Hall resistivity $\rho_{xy}$ which is shown as a function of $B$ directly. The resistivity is expressed as a dimensionless coefficient $1/\nu$ times the fundamental unit of 2-dimensonal resistivity $2\pi\hbar/e^2$, as follows,

$$\rho_{xy} = \frac{1}{\nu} \times \frac{2\pi\hbar}{e^2} \tag{11.37}$$

In the vicinity of the $\nu = 1$ plateau, more plateaux are discovered. It turns out (as you can see from Figure 12) that $\nu$ appears to always be a rational number whose denominator is an odd integer. This is the Fractionally Quantum Hall Effect (FQHE). The dynamics responsible for the FQHE is no longer that of independent electrons, but now results from collective effects, which are fascinating, but into which we cannot go here.

It is nonetheless possible to make direct contact with the structure of Landau levels as follows. We now consider the system to be governed by $N$ electrons, subject to the external magnetic field $B$ and to their mutual repulsive Coulomb interactions. It is impossible to solve such a system exactly, but Robert Laughlin proposed an educated guess for the wave function of such a system of $N$ electrons. We denote the planar coordinates of each electron by the complex numbers $z_i$, $i = 1, \cdots, N$. First of all, all of these electrons are assumed to be in the lowest Landau level, so their wave function must be of the form, (we take $eB > 0$),

$$f(z_1, \cdots, z_N) \exp\left\{-\frac{eB}{2\hbar} \sum_{i=1}^{N} |z_i|^2\right\} \tag{11.38}$$

where $f$ is a holomorphic function of all the $z_i$. Now in a strong magnetic field, spins up and down of the electron will be split, so the lowest energy states will have all the spins aligned. This makes the states symmetric in the spin quantum numbers, and Fermi-Dirac statistics then requires that the

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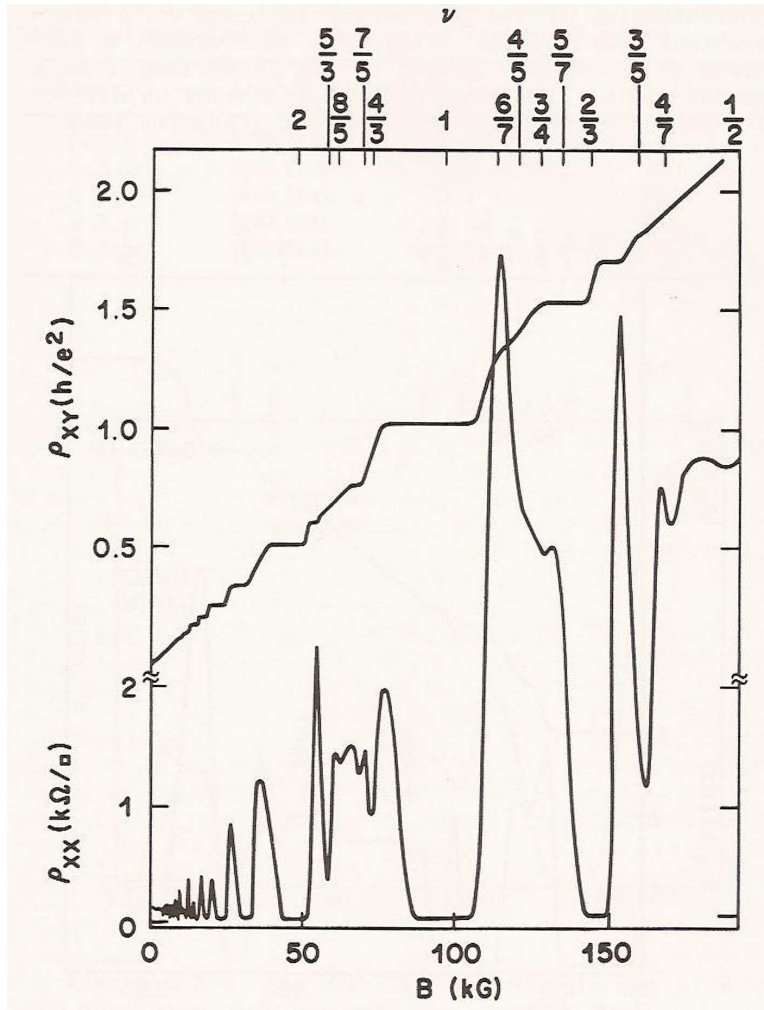
Figure 12: Actual experimental results exhibiting integer and fractional quantum Hall effects. (from A.M. Chang in *The quantum Hall effect*, Springer 1990).

wave function of the $N$ electrons be anti-symmetric under the interchange of any two coordinates $z_i$ and $z_j$ for $j \neq i$. The following wave functions will always be anti-symmetric in this way,

$$\prod_{i<j}(z_i - z_j)^m \times \exp\left\{-\frac{eB}{2\hbar}\sum_{i=1}^{N}|z_i|^2\right\} \tag{11.39}$$

whenever $m$ is an odd positive integer. The density of states is reduced to $\nu = 1/m$ which gives an explanation why only odd denominators occur.

# 12 Scattering Theory

Bound state perturbation theory, discussed in the preceding chapter, has allowed us to understand the energy shifts and modifications to quantum states as corrections to the Hamiltonian are successively taken into account. Various outcomes of calculations may be compared with the outcomes of various experiments, and used to check the theory. But, the parameters of the bound state problem are essentially fixed: we studied various discrete energy levels of various systems. The one way in which we can bring in external parameters is by applying external electric and/or magnetic fields.

Perturbation theory of the continuous spectrum is physically even more important. The reason is that in the continuous spectrum, the momentum or the energy of the incoming "probe" can always be adjusted at will, and thus automatically provides us with a tunable free parameter. This is called *scattering theory*. External electric and/or magnetic fields may also be present and will then allow us to probe the system with even more parameters and thus with even more detail. The free momentum of the incoming probe allows us to compare the outcome of theoretical calculations with the outcome of experiments for entire ranges of momentum and energy values. We can now compare entire functions of momentum as instead of isolated data points in the case of the discrete spectrum. Furthermore, scattering allows us to introduce supplementary energy into the system, and thus to access a range of excitations of the system beyond its ground state.

A large class of scattering problems may be approximated by scattering in the presence of a time-independent or static source. In two body problems, this may be done by going to the center of mass frame, and reducing the problem to a one-body problem in a potential, using translation invariance.

*Fixed-target experiments* are one example of such scattering processes. They are the oldest experimental set-ups for the systematic study of scattering. Here, a light probe (usually an electron, proton, neutron or neutrino) is used and scattered off a heavy target which is considered fixed, in as much as recoil effects of the target are negligible. An alternative experimental set-up is provided by *particle colliders*. In a collider experiment, two beams traveling in opposite directions are made to interact in a localized interaction region. Most frequently, the beams are symmetric, in the sense that they are composed of particle of the same mass and adjusted to have the same energy. The most popular set-ups are $e^+e^-$ colliders (SLAC), and $p^+p_-$ colliders (CERN). The resulting scattering products will then be evenly distributed in a $4\pi$ solid angle.[10]

At high energies $E$ (much larger than the mass $M$ of the target), (symmetric) collider experiments are much more efficient, due to relativistic effects. This is because what really matters for the strength of the interaction is the center of mass energy of the process. In a collider experiment, two beams of opposite momenta and equal energy $E$ produce a center of mass energy $E_{cm} = 2E$. But in a fixed target experiment, with a beam of particles of mass $m$ and energy $E$ incident on a target of particles of mass $M$, the center of mass energy is given by $E_{cm}^2 = 2EMc^2 + (M^2 - m^2)c^4$,

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[10]For certain experiments, there is actually an advantage to having an asymmetric set-up, with particle of unequal masses and/or unequal energies. This set-up will produce scattering products carrying a momentum peaked around a definite forward momentum which allows experimentalists to use a detector of less than $4\pi$ solid angle coverage.

or $E_{cm} \sim \sqrt{2EMc^2}$ for high energy. The linear energy dependence for a collider wins over the square root dependence of the fixed target experiment.

Again due to relativistic effects, the number of particles in a scattering process need not be conserved. Any interaction causes an acceleration, and if the probe particle carries electric charge, acceleration will read to electro-magnetic radiation. Quantum mechanically, the interacting charged particle emits a photon. The photon was not part of either the incoming probe or of the target, and it as not hidden inside these bodies either: the photon is genuinely a newly created particle, which did not exist in the system prior to interaction. Generally the number of particles may be changed during the course of interactions, and this effect is not limited to photons. For example, in $e^+e^-$ colliders, an interaction may cause the $e^+e^-$ to annihilate and be transformed purely into energy out of which new particles may be created, such as quarks, proton and anti-protons, $W^\pm$ or $Z$'s or even again $e^+e^-$ pairs. These effects are all relativistic, and their quantum description will properly require the formalism and tools of quantum field theory.

In this chapter, we shall limit attention to the non-relativistic case where the number of particles is conserved. In this set-up, the incoming probe will merely be deflected. This case is often referred to as *potential scattering*.

## 12.1   Potential Scattering

The fundamental problem of potential scattering is the resolution of the continuous part of the spectrum of the Hamiltonian,

$$H = H_0 + \lambda H_1 \tag{12.1}$$

Here, $H_0$ is the *unperturbed Hamiltonian*, whose solutions are assumed to be known exactly, $H_1$ is the perturbing Hamiltonian, and $\lambda$ is a small parameter, in terms of which perturbation theory will be organized. The eigenstates of $H_0$ will be denoted by $|\phi_\mathbf{k}\rangle$, and obey

$$H_0|\phi_\mathbf{k}\rangle = E|\phi_\mathbf{k}\rangle \qquad\qquad E = \frac{\hbar^2\mathbf{k}^2}{2m} \tag{12.2}$$

Here and later, it will be convenient to parametrized the energy eigenvalue $E$ by the wave vector $\mathbf{k}$ and the mass $m$. We then seek to solve for the eigenstates of the full Hamiltonian $H$ *at the same energy eigenvalue $E$*,

$$(H_0 + \lambda H_1)|\psi_\mathbf{k}\rangle = E|\psi_\mathbf{k}\rangle \tag{12.3}$$

The rationale for using the same energy eigenvalue is that if $H_0$ has a continuous spectrum in the vicinity of energy $E$, then a small (regular) perturbation on the spectrum should produce a continuous functional dependence on $\lambda$ (see the discussion in bound state perturbation theory), so that also $H$ should admit a continuous spectrum in the vicinity of $E$. Possible exceptions would include the case where $E$ is an endpoint of the spectrum of $H_0$, such as in the endpoint of an energy band, in which case a more detailed study will be required.

To solve (12.3) perturbatively, we move the perturbative correction piece to the right hand side of the equation,

$$(H_0 - E)|\psi_{\mathbf{k}}\rangle = -\lambda H_1|\psi_{\mathbf{k}}\rangle \tag{12.4}$$

The operator $H_0 - E$ is not quite invertible, and precisely has the states $|\phi_{\mathbf{k}}\rangle$ for its null-space. In the case of bound state perturbation theory, we remedied this situation by *inverting $H_0 - E$ on the subspace of the Hilbert space orthogonal to the its null-space.* This was possible because the null-space consisted of discrete states. In the case of the continuous spectrum, the natural way of dealing with the null-space is as follows. We add a small imaginary part $i\varepsilon$ to the energy $E$. Since $H_0$ is self-adjoint, all its eigenvalues are real, and thus the modified operator $H_0 - E \pm i\varepsilon$ will now be invertible, although the eigenvalue corresponding to states $|\phi_{\mathbf{k}}\rangle$ in the null-space will be tiny. This procedure naturally produces two solutions to (12.3) and (12.4), given by

$$|\psi_{\mathbf{k}}^{\pm}\rangle = |\phi_{\mathbf{k}}\rangle - \frac{\lambda}{H_0 - E \mp i\varepsilon} H_1|\psi_{\mathbf{k}}^{\pm}\rangle \qquad\qquad \varepsilon > 0 \tag{12.5}$$

This equation is known as the *Lippmann-Schwinger equation*. (Later on, we shall use an even more drastic extension of this equation and let $z = E \pm i\varepsilon$ take arbitrary values in the complex plane.) Although $\varepsilon$ was introduced here as a finite real positive number, it is understood that one must take the limit $\varepsilon \to 0$. To understand this $i\varepsilon$ prescription in more detail, it will be helpful to study its mathematical properties in some detail.

## 12.2   The $i\varepsilon$ prescription

The $i\varepsilon$ prescription is given by the limit

$$\lim_{\varepsilon \to 0} \frac{1}{x - i\varepsilon} \qquad\qquad x \in \mathbf{R}, \ \varepsilon > 0 \tag{12.6}$$

should be understood as a generalized function (or *distribution*) similar to the Dirac $\delta$-function. In fact, it contains a $\delta$-function, as may be seen by separating its real and imaginary parts,

$$\frac{1}{x - i\varepsilon} = \frac{x}{x^2 + \varepsilon^2} + \frac{i\varepsilon}{x^2 + \varepsilon^2} \tag{12.7}$$

The limit of the first term is, by definition, the sl principal value prescription $\mathrm{PV}(1/x)$, while the limit of the second may be found by integrating it against a smooth test function $f(x)$,

$$\lim_{\varepsilon \to 0} \int_{\mathbf{R}} dx \, \frac{i\varepsilon}{x^2 + \varepsilon^2} f(x) = \lim_{\varepsilon \to 0} \int_{\mathbf{R}} dx \, \frac{i}{x^2 + 1} f(\varepsilon x) = i\pi f(0) \tag{12.8}$$

Hence the limit of the second term is given by $i\pi\delta(x)$. Putting all together, we obtain,

$$\lim_{\varepsilon \to 0} \frac{1}{x - i\varepsilon} = \mathrm{PV}\frac{1}{x} + i\pi\delta(x) \tag{12.9}$$

This clearly demonstrates that the limit is a generalized function. It is customary when writing the $i\varepsilon$ prescription to simply omit the $\lim_{\varepsilon \to 0}$ symbol in front.

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## 12.3   The free particle propagator

In almost all cases,[11] $H_0$ will be the Hamiltonian for a free probe of mass $m$,

$$H_0 = \frac{\mathbf{P}^2}{2m} \tag{12.10}$$

where $\mathbf{P}$ is the momentum operator. The eigenstates are $|\phi_{\mathbf{k}}\rangle = |\mathbf{k}\rangle$ with energy $E = \hbar^2 \mathbf{k}^2/2m$, with wave function,

$$\phi_{\mathbf{k}}(\mathbf{x}) = \langle \mathbf{x}|\mathbf{k}\rangle = \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{3/2}} \tag{12.11}$$

The normalization has been chosen so that $\langle \mathbf{k}'|\mathbf{k}\rangle = \delta^{(3)}(\mathbf{k}' - \mathbf{k})$, which may be verified by inserting a complete set of position eigenstates

$$\int d^3\mathbf{x} \langle \mathbf{k}'|\mathbf{x}\rangle \langle \mathbf{x}|\mathbf{k}\rangle = \delta^{(3)}(\mathbf{k}' - \mathbf{k}) \tag{12.12}$$

In the position basis the Lippmann-Schwinger equation becomes,

$$\langle \mathbf{x}|\psi_{\mathbf{k}}^{\pm}\rangle = \langle \mathbf{x}|\phi_{\mathbf{k}}\rangle + \lambda \int d^3\mathbf{y} \, \langle \mathbf{x}|\frac{1}{E - H_0 \pm i\varepsilon}|\mathbf{y}\rangle \, \langle \mathbf{y}|H_1|\psi_{\mathbf{k}}^{\pm}\rangle \tag{12.13}$$

One defined the *propagator* or Green functions for the free non-relativistic particle as follows,

$$G_{\pm}(\mathbf{x}, \mathbf{y}; \mathbf{k}^2) = \frac{\hbar^2}{2m}\langle \mathbf{x}|\frac{1}{E - H_0 \pm i\varepsilon}|\mathbf{y}\rangle \tag{12.14}$$

The factor of $\hbar^2/2m$ has been pulled out for later convenience and to make the propagator depend only on $\mathbf{k}^2$, but not on $m$. Since $H_0$ is diagonal in the momentum basis $|\ell\rangle$, the propagator may be computed by inserting a complete set of momentum eigenstates,

$$G_{\pm}(\mathbf{x}, \mathbf{y}; \mathbf{k}^2) = \int d^3\mathbf{l} \, \langle x|\frac{1}{\mathbf{k}^2 - \mathbf{l}^2 \pm i\varepsilon}|\mathbf{l}\rangle \, \langle \mathbf{l}|\mathbf{y}\rangle = \int \frac{d^3\mathbf{l}}{(2\pi)^3} \frac{e^{i\mathbf{l}\cdot(\mathbf{x}-\mathbf{y})}}{\mathbf{k}^2 - \mathbf{l}^2 \pm i\varepsilon} \tag{12.15}$$

One may either evaluate this Fourier integral directly, or use the fact that $G_{\pm}$ satsifies,

$$(\Delta + \mathbf{k}^2)G_{\pm}(\mathbf{x}, \mathbf{y}; \mathbf{k}^2) = \delta^{(3)}(\mathbf{x} - \mathbf{y}) \tag{12.16}$$

For $\mathbf{k} = 0$, $G_{\pm}$ is just the Coulomb equation for a $\delta$-function charge with solution

$$G_{\pm}(\mathbf{x}, \mathbf{y}; 0) = -\frac{1}{4\pi r} \qquad\qquad r = |\mathbf{x} - \mathbf{y}| \tag{12.17}$$

---

[11]One notable exception is the Coulomb problem for which the exact solution is known, abeit complicated.

The factor of $4\pi$ gives the correct normalization for the $\delta$-function. For $\mathbf{k}^2 \neq 0$, rotation invariance of the Fourier integral shows that $G_\pm$ depends only on the scalars $\mathbf{k}^2$ and $r$, so that, away from $\mathbf{x} = \mathbf{y}$, $G_\pm$ must satisfy the radial equation

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial G_\pm}{\partial r}\right) + k^2 G_\pm = 0 \tag{12.18}$$

where $k = |\mathbf{k}|$. Using dimensional analysis, we must have $G_\pm(\mathbf{x}, \mathbf{y}; \mathbf{k}^2) = G_\pm(\mathbf{x}, \mathbf{y}; 0)f(kr)$, where $f(kr)$ is a dimensionless function of the dimensionless combination $kr$. Substitution into the above radial differential equations shows that

$$f''(kr) + f(kr) = 0 \tag{12.19}$$

whose solutions are $f(kr) = e^{\pm ikr}$. Putting all together, we obtain,

$$G_\pm(\mathbf{x}, \mathbf{y}; \mathbf{k}^2) = -\frac{e^{\pm ik|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} \tag{12.20}$$

Note that, since the exponentials equal 1 when $\mathbf{x} = \mathbf{y}$, this result is automatically properly normalized with respect to the $\delta$-function source.

## 12.4    The Lippmann-Schwinger equation in position space

In many cases of interest, the perturbing Hamiltonian $H_1$ is *local in position space* and actually given by a potential $V(\mathbf{x})$,

$$\langle \mathbf{x}|H_1|\mathbf{y}\rangle = \delta^{(3)}(\mathbf{x} - \mathbf{y})V(\mathbf{x}) \tag{12.21}$$

In terms of the incoming wave function $\phi_\mathbf{k}(\mathbf{x})$ and the full wave function $\psi_\mathbf{k}(\mathbf{x})$, defined by

$$\langle \mathbf{x}|\phi_\mathbf{k}\rangle = \phi_\mathbf{k}(\mathbf{x}) \qquad\qquad \langle \mathbf{x}|\psi_\mathbf{k}^\pm\rangle = \psi_\mathbf{k}^\pm(\mathbf{x}) \tag{12.22}$$

the Lippmann-Schwinger equation takes the form,

$$\psi_\mathbf{k}^\pm(\mathbf{x}) = \phi_\mathbf{k}(\mathbf{x}) + \int d^3\mathbf{y}\, G_\pm(\mathbf{x}, \mathbf{y}; \mathbf{k}^2)U(\mathbf{y})\psi_\mathbf{k}^\pm(\mathbf{y}) \tag{12.23}$$

where we have used the abbreviation

$$U(\mathbf{y}) = \frac{2m\lambda}{\hbar^2}V(\mathbf{y}) \tag{12.24}$$

so that $U$ is automatically of order $\lambda$, and thus small. If we symbolically denote this notation by

$$\psi = \phi + GU\psi \tag{12.25}$$

then the solution may be obtained in a power series in $\lambda$ by iterating the equation, i.e. substituting the left hand side into the right hand side repeatedly. At the first iteration, we obtain,

$$\psi = \phi + GU\phi + GUGU\psi \tag{12.26}$$

and the solution to all orders is

$$
\begin{aligned}
\psi &= \phi + GU\phi + GUGU\phi + \cdots \\
&= \phi + \sum_{n=1}^{\infty} (GU)^n \phi
\end{aligned}
\tag{12.27}
$$

The interpretation of the first term is free propagation; of the second term is a single interaction with the potential; of the subsequent terms of higher order exchanges with the potential.

## 12.5 Short range versus long range $V$ and massless particles

The basic assumption in scattering theory is that the potential $V(\mathbf{x})$ tends to zero as $|\mathbf{x}| \to \infty$. It is under this condition that the above description of the scattering process off a target really makes sense. Namely, in the far past, we have a wave (or more physically, a wave packet) incoming from spatial infinity where its behavior is that of a free particle. At finite time, and a finite distance away from the target, the particle interacts with the target, and then again moves out to spatial infinity at far future times, again behaving as a free particle.

But even if $V(\mathbf{x}) \to 0$ as $r = |\mathbf{x}| \to \infty$, the potential $V$ may tend to zero at different possible rates. One distinguishes the following two behaviors,

- *Short ranged*: the potential $V$ vanishes at least exponentially $V(\mathbf{x}) \sim e^{-r/\xi}$ with distance $r$ outside a bounded region of space; this includes the case where $V$ vanishes identically outside a bounded region of space of linear size $\xi$. The smallest such $\xi > 0$ is called the *range of the potential*. One example is the Yukawa potential, given by $V(\mathbf{x}) \sim e^{-r/\xi}/r$.

- *Long Ranged*: the potential $V$ vanishes like a power $V(\mathbf{x}) \sim r^{-\alpha}$ of distance where $\alpha > 0$ is called the *exponent*. One example is the Coulomb potential $V(\mathbf{x}) \sim 1/r$, for which the exponent is $\alpha = 1$.

The reason for this distinction has a deep physical underpinning. In relativistic quantum theories, interactions cannot be instantaneous, and must be mediated by the exchange of signals that travel at the speed of light or slower. In fact, these signals are particles themselves. In relativistic quantum field theory, the interaction potential may be obtained from summing up the contributions of repeated exchanges of particles. If the mediator of the interaction is massless, then the resulting interaction potential in the non-relativistic limit will always be long-ranged, while if the particle is massive, the interaction potential will be short ranged. The range of the interaction is related to the mass via the formula

$$
\xi = \frac{\hbar}{mc}
\tag{12.28}
$$

namely, it is the Compton wave length.

The four forces of Nature behave as follows,

- Gravitational: long-ranged, since it also obeys the Coulomb potential; the mediator of the gravity is the massless graviton.

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- Electro-magnetic: long-ranged; the mediator is the massless photon.

- Weak interactions: short-ranged; the mediator are the massive $W^{\pm}$ and $Z$ bosons with masses on the order of 80 $GeV/c^2$ and 90 $GeV/c^2$ respectively.

- Strong interactions: short-ranged in the following sense. Although the mediator of the strong force in QCD is the massless gluon, confinement makes the range of the strong interactions short, the scale being set by the mass of the lightest strongly interacting particle, namely the $\pi^{\pm}$ and $\pi^0$, whose masses are approximately 135 $MeV/c^2$.

## 12.6 The wave-function solution far from the target

In practice, one is interested in observing the scattering products far from the target, i.e. far from the core of the potential. In this limit, the equations simplify considerably, and will yield physical insight into the scattering process. The starting point is the integral equation (12.23), in the limit of large $r = |\mathbf{x}| \gg |\mathbf{y}|$. We use the approximation,

$$|\mathbf{x} - \mathbf{y}| = \sqrt{(\mathbf{x} - \mathbf{y})^2} = r - \frac{\mathbf{x} \cdot \mathbf{y}}{r} + \mathcal{O}(\mathbf{y}^2) \tag{12.29}$$

The propagator the becomes (we retain only the propagator $G = G_+$),

$$G(\mathbf{x}, \mathbf{y}; \mathbf{k}^2) = -\frac{e^{ikr}}{4\pi r} \times e^{-i\mathbf{k}' \cdot \mathbf{y}} \qquad\qquad \mathbf{k}' = k\frac{\mathbf{x}}{r} \tag{12.30}$$

The Lippmann-Schwnger equation is then solved by the following form of the wave function,

$$\psi_{\mathbf{k}}(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \left\{ e^{i\mathbf{k} \cdot \mathbf{x}} - \frac{e^{ikr}}{r} f(\mathbf{k}', \mathbf{k}) \right\} \tag{12.31}$$

where the function $f$ is given by

$$f(\mathbf{k}', \mathbf{k}) = -\frac{(2\pi)^{3/2}}{4\pi} \int d^3\mathbf{y}\, e^{-i\mathbf{k}' \cdot \mathbf{y}} U(\mathbf{y}) \psi_{\mathbf{k}}(\mathbf{y}) \tag{12.32}$$

Note that from the definition of $f$, we may readily read off that its dimension is a length, a remark that will come in very useful later.

## 12.7 Calculation of the cross section

Clearly, one of the key quantities we are going to be interested in is the intensity of the outgoing flux of particles, as a function of $\mathbf{k}$ and $\mathbf{k}'$. The corresponding physical quantity is the *cross section*. To evaluate it, we begin by obtaining a formula for the probability density $\rho$ and for the probability current density $\mathbf{j}$,

$$\begin{aligned} \rho(t, \mathbf{x}) &= \psi^*(t, \mathbf{x})\psi(t, \mathbf{x}) \\ \mathbf{j}(t, x) &= -\frac{i}{2m}\Big(\psi^*(t, \mathbf{x})\nabla\psi(t, \mathbf{x}) - \psi(t, \mathbf{x})\nabla\psi^*(t, \mathbf{x})\Big) \end{aligned} \tag{12.33}$$

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Using the time-dependent Schrödinger equation,

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + V\psi \tag{12.34}$$

one shows conservation of this current,

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{j} = 0 \tag{12.35}$$

The global form of the conservation of probability equation is that the time variation of the total probability $p_v$ in some volume $v$ plus the flux $\phi_{\partial v}$ through the boundary $\partial v$ of volume $v$ vanishes,

$$\frac{dp_v}{dt} + \phi_v = 0 \tag{12.36}$$

where we have

$$p_v = \int_v d^3\mathbf{x}\,\rho(t,\mathbf{x}) \qquad\qquad \phi_{\partial v} = \oint_{\partial v} d^2\mathbf{S}\cdot\mathbf{j}(t,\mathbf{x}) \tag{12.37}$$

A scattering process is considered to be a steady state process in which some of the incoming flux due to the plane wave $e^{i\mathbf{k}\cdot\mathbf{x}}$ is scattered off into a spherical wave. The *differential cross section* gives a quantitative evaluation of the strength of this scattering process, as a function of angle of the outgoing beam.

Using the definition of the probability current, we readily find that the incoming probability current density is given by the velocity $\mathbf{v}$ of the particles in the incoming planar wave beam,

$$\mathbf{j}_{\text{incident}} = \frac{\mathbf{v}}{(2\pi)^3} \tag{12.38}$$

where $m\mathbf{v} = \hbar\mathbf{k}$. The *differential cross section* is obtained by analyzing the probability flow of the outgoing wave as a function of angle, far away from the interaction region. Thus, we consider the flux through an infinitesimal surface element $d^2\mathbf{S}$, at a point $\mathbf{x}$ which is a long distance $r = |\mathbf{x}|$ away from the target. Fixing the solid angle to be $d\Omega$, we have

$$d^2\mathbf{S} = r^2 d\Omega\frac{\mathbf{x}}{r} \tag{12.39}$$

The flux through the solid angle $d\Omega$ is then given by

$$\begin{aligned}
\frac{d\phi}{d\Omega} &= d^2\mathbf{S}\cdot\mathbf{j}_{\text{scattered}} \\
&= \lim_{r\to\infty} r^2\frac{\mathbf{x}}{r}\cdot\mathbf{j}_{\text{scattered}}(\mathbf{x}) \tag{12.40}
\end{aligned}$$

The current density is obtained by substituting (12.31) into the general expression, and is given by

$$\mathbf{j}_{\text{scattered}} = -\frac{i}{2m}\frac{f(\mathbf{k}',\mathbf{k})^*}{(2\pi)^3}\frac{e^{-ikr}}{r}\nabla\left(f(\mathbf{k}',\mathbf{k})\frac{e^{ikr}}{r}\right) + c.c. \tag{12.41}$$

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where *c.c.* stands for the complex conjugate of the preceding term. In carrying out the $\nabla$ derivative with respect to the variable $\mathbf{x}$, several terms emerge. In view of the derivatives

$$\nabla_i \left( \frac{1}{r} \right) = -\frac{x_i}{r^3} \qquad\qquad \nabla_i \left( \frac{x^j}{r} \right) = \frac{r^2 \delta_i^j - x^j x_i}{r^3} \qquad (12.42)$$

we see that the $\nabla$ derivatives of the $1/r$ factor and of the outgoing momentum $\mathbf{k}' = k\mathbf{x}/r$ will lead to terms behaving like $1/r^3$ in $\mathbf{j}$ which will not contribute to the differential flux $d\phi/d\Omega$ since this involves taking the large $r$ limit. The only term that contributes is thus obtained by differentiating the exponential factor, which gives,

$$\mathbf{j}_{\text{scattered}} \sim \frac{\mathbf{k}'}{mr^2} \frac{|f(\mathbf{k}',\mathbf{k})|^2}{(2\pi)^3} \qquad (12.43)$$

The scattered differential flux is then found to be

$$\frac{d\phi}{d\Omega} = \frac{|\mathbf{v}|}{(2\pi)^3} |f(\mathbf{k}',\mathbf{k})|^2 \qquad (12.44)$$

The differential cross section is defined as the ratio of the differential flux by the total current density. The factors of $\frac{|\mathbf{v}|}{(2\pi)^3}$ cancel in both quantities and we are left with

$$\frac{d\sigma}{d\Omega} = |f(\mathbf{k}',\mathbf{k})|^2 \qquad (12.45)$$

Note that, because $f$ has dimensions of length, the differential cross section has dimensions of length square. The physical interpretation is that the cross section represents an effective aspect area for the target. This interpretation will be borne out in some simple examples that we shall study. The total cross section of the process is the integral of the differential cross section over the full range $4\pi$ of solid angle,

$$\sigma = \int_{4\pi} d\Omega \, \frac{d\sigma}{d\Omega} \qquad (12.46)$$

It again has dimension of length square.

A final remark is in order. In evaluating the incoming and outgoing fluxes, we seem to have neglected the cross term between the incoming wave and the outgoing one. While this term would contribute to the current density at any finite distance $\mathbf{x}$, in the limit of large $r$, its oscillatory behavior, given by $e^{i\mathbf{k}\cdot x - ikr}$, is responsible for the vanishing of its contribution to the differential flux.

## 12.8   The Born approximation

The Born approximation consists in retaining only a finite number of terms in the expansion in powers of $\lambda$. The first Born term is the one linear in $\lambda$, i.e. linear in the potential $V$. It is obtained by setting $\psi_{\mathbf{k}}^{\pm}(\mathbf{x}) = \phi_{\mathbf{k}}(\mathbf{x})$ in the expression for $f(\mathbf{k}',\mathbf{k})$ in (12.31), which yields,

$$f^{(1)}(\mathbf{k}',\mathbf{k}) = -\frac{1}{4\pi} \int d^3\mathbf{y} \, e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{y}} \, U(\mathbf{y}) \qquad (12.47)$$

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Its form is very simple, since $f^{(1)}(\mathbf{k}', \mathbf{k})$ is proportional to the Fourier transform of the potential evaluated on $\mathbf{k}' - bk$ which is proportional to the *momentum transfer* $\mathbf{q} = \hbar(\mathbf{k}' - \mathbf{k})$ of the process.

The first Born term for any spherically symmetric potential $U(r)$ may be computed as follows. The starting point is the integral representation, which we express is spherical coordinates defined with respect to the incoming momentum direction $\mathbf{k}$. We find,

$$
\begin{aligned}
f^{(1)}(\mathbf{q}) &= -\frac{1}{4\pi} \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin\theta \int_0^\infty dr \, r^2 U(r) \, e^{-iqr\cos\theta} \\
&= -\frac{1}{q} \int_0^\infty dr \, r \, U(r) \sin(qr)
\end{aligned}
\tag{12.48}
$$

Here, we use the notation $q = |\mathbf{q}|$.

## 12.8.1   The case of the Coulomb potential

For the Coulomb potential, we have

$$
U(r) = \frac{2m}{\hbar^2} V(r) = -\frac{2mZe^2}{\hbar^2} \frac{1}{r}
\tag{12.49}
$$

The first Born term is given by

$$
f^{(1)}(\mathbf{k}', \mathbf{k}) = \frac{mZe^2}{2\pi\hbar^2} \int d^3\mathbf{y} \frac{e^{-i(\mathbf{k}'-bk)\cdot\mathbf{y}}}{|\mathbf{y}|}
\tag{12.50}
$$

It is a standard result that

$$
\int d^3\mathbf{y} \frac{e^{i\mathbf{k}\cdot\mathbf{y}}}{|\mathbf{y}|} = \frac{4\pi}{\mathbf{k}^2}
\tag{12.51}
$$

To derive it, note first that the integral depends only on $\mathbf{k}^2$ in view of rotation invariance of the factor $d^3\mathbf{y}/|\mathbf{y}|$, and that it manifestly scales as $1/\mathbf{k}^2$. Finally the constant factor may be determined by multiplying both sides by $\mathbf{q}^2$, using the fact that $\mathbf{q}^2 = -\Delta$ in the momentum space representation, and the fact that $\Delta(1/|\mathbf{y}|) = 4\pi\delta^{(3)}(\mathbf{y})$. Collecting all terms, we have,

$$
f^{(1)}(\mathbf{k}', \mathbf{k}) = \frac{2mZe^2}{\hbar^2(\mathbf{k}' - \mathbf{k})^2}
\tag{12.52}
$$

If we define the angle between $\mathbf{k}'$ and $\mathbf{k}$ to be $\theta$, and use the fact that $|\mathbf{k}'| = |\mathbf{k}|$, we obtain,

$$
(\mathbf{k}' - \mathbf{k})^2 = 4k^2 \sin^2 \frac{\theta}{2}
\tag{12.53}
$$

As a result, the cross section is given by

$$
\frac{d\sigma}{d\Omega} = \left| f^{(1)}(\mathbf{k}', \mathbf{k}) \right|^2 = \frac{m^2 Z^2 e^4}{4\mathbf{q}^4 \sin^4 \frac{\theta}{2}}
\tag{12.54}
$$

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Note that the scale of the cross section is set by the momentum transfer $\mathbf{q}$, and the mass.

This formula exhibits singular behavior for forward scattering when $\theta \sim 0$. In fact, if one tried to integrate this formula to get the total cross section, one would find that it diverges because of the singularity at $\theta = 0$. Since this divergence occurs for vanishing momentum transfer, it amounts to an infrared (IR) problem. The fundamental cause for this problem is the fact that the photon, which is the particle that mediates the Coulomb interaction, is massless. Massless particles can be produced with very little momentum and energy. Thus, it is really not possible to distinguish between a charged particle (say and electron) state and that state with an added very low energy photon. Thus, the problem of Coulomb scattering is not strictly speaking one in which the number of photons is conserved. A proper calculation would really include the effects of this photon production, but this requires quantum field theory, and is beyond the scope of this course.

In practice, one does not necessarily scatter a charged particle off a target that exhibits Coulomb potential behavior all the way out to spatial infinity. For example, if one scatters off an electrically neutral atom, then the cloud of electrons effectively shields the Coulomb potential of the nucleus. Beyond a distance on the scale of the size of the atom, the electric potential will in fact fall off exponentially, since the electron wave functions do so in the Coulomb problem.

Finally, since the first Born term was computed in perturbation theory, we cannot physically take seriously its effects if these become large. Thus, the Rutherford formula for differential cross section should be trusted only for angles $\theta$ away from being to close to 0.

### 12.8.2 The case of the Yukawa potential

The typical potential for a short ranged potential is the Yukawa potential, given by

$$U(r) = -U_0 \frac{e^{-\mu r}}{r} \tag{12.55}$$

where $1/\mu$ is the range of the potential. The first Born term is then found to be

$$f^{(1)}(\mathbf{q}) = \frac{2mU_0}{\mathbf{q}^2 + \mu^2} \tag{12.56}$$

The finite range of this potential now makes its differential cross section finite at $\theta = 0$, and this effect may be interpreted as the fact that the Yukawa potential arises fundamentally from massive particle exchange.

## 12.9 The optical Theorem

A particularly simple and useful relation holds between the total cross section and the *forward scattering amplitude*, which is referred to as the optical theorem (for historical reasons). The relation is expressed as follows,

$$\sigma_{\text{tot}} = \int_{4\pi} d\Omega \left(\frac{d\sigma}{d\Omega}\right) = \frac{4\pi}{k}\text{Im}f(\mathbf{k}, \mathbf{k}) \tag{12.57}$$

The fact that on the right hand side, the scattering amplitude is being evaluated for equal initial and final momenta is responsible for the name forward scattering.

To prove this result, we start from the form of the full wave function $\psi$ in terms of the incoming free wave function $\phi$, and the scattered wave function $\chi$, related by

$$\psi = \phi + \chi \tag{12.58}$$

The probability current, integrated across a large sphere $S$ must vanish for this stationary problem when we take the free part $\phi$ or the full wave function $\psi$, leading to the following equations,

$$\oint_S d^2\mathbf{S} \cdot \mathrm{Im}(\phi^*\nabla\phi) = \oint_S d^2\mathbf{S} \cdot \mathrm{Im}(\psi^*\nabla\psi) = 0 \tag{12.59}$$

The total cross section, on the other hand, is given by the integral of the probability current for the scattered wave function $\chi$, as follows,

$$\frac{m|\mathbf{v}|}{(2\pi)^3}\sigma_{\mathrm{tot}} = \mathrm{Im}\oint_S d^2\mathbf{S} \cdot \chi^*\nabla\chi \tag{12.60}$$

Finally, we use the identity

$$\mathrm{Im}(\psi^*\nabla\psi) = \mathrm{Im}(-\phi^*\nabla\phi + \psi^*\nabla\phi - \phi\nabla\psi^* + \chi^*\nabla\chi) \tag{12.61}$$

Putting all together, and using Stokes' theorem, we have,

$$\mathrm{Im}\oint_S d^2\mathbf{S} \cdot \chi^*\nabla\chi = \mathrm{Im}\int d^3\mathbf{x} \cdot (\psi\Delta\phi^* - \phi^*\Delta\psi) \tag{12.62}$$

We now use the Schrödinger equation for $\phi$ and $\psi$ respectively,

$$\begin{aligned}
\Delta\phi &= -2mE\phi \\
\Delta\psi &= -2mE\psi + 2mV
\end{aligned} \tag{12.63}$$

The terms involving $E$ cancel out, and we are left with

$$k\,\sigma_{\mathrm{tot}} = 2m(2\pi)^3\mathrm{Im}\int d^3\mathbf{x}\,\phi V\psi^* = 4\pi\mathrm{Im}f(\mathbf{k},\mathbf{k}) \tag{12.64}$$

The advantage of this formula is that the forward scattering amplitude is often easier to evaluate than the full amplitude which then requires squaring to get the cross section and integrating over all solid angles to get the total cross section.

## 12.10  Spherical potentials and partial wave expansion

Many potentials of interest, such as the Coulomb and Yukawa potentials, have spherical symmetry, and only depend on a radial coordinate $r$, but not on the spherical angles $\theta$ and $\phi$. The spherical

symmetry of the problem then allows one to decouple the system into partial waves, producing conceptual and practical simplifications.

We consider a Hamiltonian of the form, expressed in coordinate representation,

$$H = -\frac{\hbar^2}{2m}\Delta + V(r) \tag{12.65}$$

We assume that $V(r) \to 0$ as $r \to \infty$. In order to avoid trailing factors of $\hbar$ and $m$, we express the Schrödinger equation in terms of the following variables instead,

$$U(r) = \frac{2m}{\hbar^2}V(r) \qquad\qquad E = \frac{\hbar^2 k^2}{2m} \tag{12.66}$$

where $k$ is a real wave number variable. Spherical symmetry now implies that $\mathbf{L}^2$ and $L_z$ commute with $H$, so that a basis of eigenfunctions $\psi_{\ell m}(\mathbf{r})$ of $H$ may be chosen in a basis where $\mathbf{L}^2$ and $L_z$ are diagonal,

$$\psi_{\ell m}(\mathbf{r}) = R_\ell(r)\, Y_\ell^m(\theta,\phi) \tag{12.67}$$

The Schrödinger equation then becomes,

$$R_\ell''(r) + \frac{2}{r}R_\ell'(r) - \frac{\ell(\ell+1)}{r^2}R_\ell(r) + k^2 R_\ell(r) - U(r)R_\ell(r) = 0 \tag{12.68}$$

It is this equation that we seek to solve perturbatively in powers of $U$.

## 12.10.1 Bessel Functions

For $U = 0$, (12.68) is the differential equation that defined (spherical) Bessel functions. The two linearly independent solutions of this second order differential equation are denoted by[12]

$$\begin{aligned} R_\ell^{(1)}(r) &= j_\ell(kr) &\qquad \text{regular as } r \to 0 \\ R_\ell^{(2)}(r) &= h_\ell(kr) &\qquad \text{singular as } r \to 0 \end{aligned} \tag{12.69}$$

These functions admit convenient integral representations, and we have

$$\begin{aligned} j_\ell(\rho) &= \frac{\rho^\ell}{2^{\ell+1}\ell!}\int_{-1}^{1} dz\, e^{i\rho z}(1-z^2)^\ell \\ h_\ell(\rho) &= -\frac{\rho^\ell}{2^\ell \ell!}\int_{1}^{1+i\infty} dz\, e^{i\rho z}(1-z^2)^\ell \end{aligned} \tag{12.70}$$

---

[12]Note that if $j_\ell$ is a solution, then so is $j_{-1-\ell}$. For $\ell$ not an integer, these solutions are linearly independent, but for integer $\ell$ these two solutions are proportional to one another, however, and cannot be used as a basis for both linearly independent solutions.

For real values of $\rho$, the function $j_\ell(\rho)$ is real, but $h_\ell(\rho)$ is complex. The asymptotic values of these functions are as follows. As $\rho \to 0$, we have,

$$
\begin{aligned}
j_\ell(\rho) &\sim \frac{\rho^\ell}{(2\ell+1)!!} \\
h_\ell(\rho) &\sim -i\frac{(2\ell-1)!!}{\rho^{\ell+1}}
\end{aligned}
\tag{12.71}
$$

while for $\rho \to \infty$, we have,

$$
\begin{aligned}
j_\ell(\rho) &\sim \frac{1}{\rho} \cos\left(\rho - \frac{\pi}{2}(\ell+1)\right) \\
h_\ell(\rho) &\sim -\frac{i}{\rho} e^{i\rho - i\pi\ell/2}
\end{aligned}
\tag{12.72}
$$

Note that the function $h_\ell(\rho)$ is sometimes denoted as $h_\ell^{(1)}(\rho)$, while $h^{(2)}(\rho) = (h^{(1)}(\rho^*))^*$.

## 12.10.2 Partial wave expansion of wave functions

The free wave solution $\phi(\mathbf{x})$ admits an expansion in terms of $j_\ell$, given as follows,

$$
e^{i\mathbf{k}\cdot\mathbf{r}} = e^{ikr\cos\theta} = \sum_{\ell=0}^{\infty} (i)^\ell (2\ell+1) j_\ell(kr) P_\ell(\cos\theta)
\tag{12.73}
$$

where $P_\ell(\cos\theta)$ are the Legendre polynomials, familiar from the structure of spherical harmonics. More generally now, we can express any wave function for the spherical potential problem in such an expansion in terms of spherical harmonics,

$$
\begin{aligned}
\phi_{\mathbf{k}}(\mathbf{r}) &= \frac{1}{(2\pi)^{3/2}} \sum_{\ell=0}^{\infty} (i)^\ell (2\ell+1) j_\ell(kr) P_\ell(\cos\theta) \\
\psi_{\mathbf{k}}(\mathbf{r}) &= \frac{1}{(2\pi)^{3/2}} \sum_{\ell=0}^{\infty} (i)^\ell (2\ell+1) R_\ell(kr) P_\ell(\cos\theta)
\end{aligned}
\tag{12.74}
$$

Note that the expansion involves only the spherical harmonics $Y_\ell^0$. The reason is that while the Schrödinger equation is invariant under all rotations, the initial conditions (namely given by the incoming plane wave) break this symmetry to rotations around the incoming wave vector $\mathbf{k}$ only. Thus, the wave functions can have no dependence on $\phi$ by symmetry, which prevents the occurrence of $Y_\ell^m$ for $m \neq 0$.

Instead of substituting these expressions into the integral equation we had derived earlier, it turns out to be much more convenient to work from the initial Schrödinger equation, which we express as follows,

$$
\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{\ell(\ell+1)}{r^2} + k^2\right) R_\ell(r) = U(r) R_\ell(r)
\tag{12.75}
$$

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Now, we know the solution $j_\ell(kr)$ for $U = 0$, and consider the full solution in a perturbative expansion in $U$. We set

$$R_\ell(r) = j_\ell(kr) + \chi_\ell(r) \tag{12.76}$$

To solve this problem, we define the Green function for the 1-dimensional differential operator as follows,

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{\ell(\ell+1)}{r^2} + k^2\right)G_\ell(r, r') = \frac{1}{r^2}\delta(r - r') \tag{12.77}$$

The reason for the factor of $1/r^2$ on the rhs is that the integration measure is $d^3\mathbf{r} = r^2 dr \, \sin\theta d\theta \, d\phi$, and the $\delta$-function in spherical coordinates thus inherits a compensating $1/r^2$ factor. In terms of this Green function, the integral equation for $R_\ell$ becomes,

$$R_\ell(r) = j_\ell(kr) + \int_0^\infty dr' \, (r')^2 G_\ell(r, r')U(r')R_\ell(r') \tag{12.78}$$

This integral equation may again be solved recursively.

## 12.10.3  Calculating the radial Green function

There is a standard, and very powerful, method for calculating the Green function for linear differential equations of second order in one variable. The method proceeds a s follows. When $r \neq r'$, the equation is just the homogeneous one, for which we know the two linearly independent solutions $j_\ell(kr)$ and $h_\ell(kr)$. At $r = r'$, the presence of a $\delta$-function requires the derivative in $r$ of $G_\ell(r, r')$ to be discontinuous, and thus the function $G_\ell(r, r')$ itself to be continuous. This may be achieved by using different linear combinations of the functions $j_\ell$ and $h_\ell$ for $r < r'$ and for $r > r'$.

We shall choose these linear combinations such that $G_\ell(r, r')$ is automatically regular at $r = 0$, and has the correct $e^{ikr}$ behavior as $r \to \infty$. The function $j_\ell(kr)$ is regular at $r = 0$, while the function $h_\ell(kr)$ behaves like $e^{ikr}$ as $r \to \infty$. Therefore, we use the following form for $G_\ell(r, r')$,

$$G_\ell(r, r') = \begin{cases} C_\ell j_\ell(kr)h_\ell(kr') & r < r' \\ C_\ell h_\ell(kr)j_\ell(kr') & r' < r \end{cases} \tag{12.79}$$

This expression guarantees continuity across $r = r'$ from the outset. We shall now recast this form in a more helpful form using the Heaviside step function $\theta(x)$. It is defined by

$$\theta(x) = \begin{cases} 1 & x > 0 \\ 0 & x < 0 \end{cases} \tag{12.80}$$

Its derivative is the $\delta$-function, $\theta'(x) = \delta(x)$. Using the Heaviside function, we now have

$$G_\ell(r, r') = C_\ell\theta(r' - r)j_\ell(kr)h_\ell(kr') + C_\ell\theta(r - r')h_\ell(kr)j_\ell(kr') \tag{12.81}$$

In differentiating once, continuity of $G_\ell(r, r')$ across $r = r'$ guarantees that the resulting $\delta$-functions will cancel, and we obtain,

$$\frac{d}{dr}G_\ell(r, r') = kC_\ell\theta(r' - r)j'_\ell(kr)h_\ell(kr') + kC_\ell\theta(r - r')h'_\ell(kr)j_\ell(kr') \tag{12.82}$$

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Differentiating a second time, and substituting the result into the defining equation (12.77) for $G_\ell(r, r')$, we obtain,

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{\ell(\ell+1)}{r^2} + k^2\right)G_\ell(r, r') = 2kC_\ell\delta(r - r')W(kr) \tag{12.83}$$

where

$$W(x) = j_\ell(x)h'_\ell(x) - j'_\ell(x)h_\ell(x) \tag{12.84}$$

This quantity is the Wronskian for the Bessel equation. The key property of the Wronskian is that it satisfies a first order linear differential equation which may always be integrated. This differential equation may be deduced directly from the second order equation, namely,

$$W'(x) = j_\ell(x)h''_\ell(x) - j''_\ell(x)h_\ell(x) = -\frac{2}{x}W(x) \tag{12.85}$$

and solved by

$$W(x) = \frac{W_0}{x^2} \tag{12.86}$$

where $W_0$ is a constant. Actually, even this constant may be calculated, using the asymptotic behavior of $j_\ell$ and of $h_\ell$, and we find $W_0 = i/2$. Putting all together, we find that

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{\ell(\ell+1)}{r^2} + k^2\right)G_\ell(r, r') = kC_\ell\delta(r - r')\frac{i}{k^2r^2} \tag{12.87}$$

Hence, the desired normalization for $G_\ell$ is recovered by setting $C_\ell = -ik$, and we have,

$$G_\ell(r, r') = -ik\left(\theta(r' - r)j_\ell(kr)h_\ell(kr') + \theta(r - r')h_\ell(kr)j_\ell(kr')\right) \tag{12.88}$$

## 12.11  Phase shifts

For asymptotically large distance $r$, and a potential that vanishes at infinity $V(r) \to 0$ as $r \to \infty$, it is only the second term in the Green function $G_\ell(r, r')$ of (12.88) that will contribute. This may be seen by decomposing the integration region over $r'$ into two pieces,

$$\begin{aligned}
R_\ell(r) &= j_\ell(kr) - ikh_\ell(kr)\int_0^r dr'\,(r')^2 j_\ell(kr')U(r')R_\ell(r') \\
&\quad -ikj_\ell(kr)\int_r^\infty dr'\,(r')^2 h_\ell(kr')U(r')R_\ell(r')
\end{aligned} \tag{12.89}$$

Since $h_\ell(kr')$ and $R_\ell(kr')$ fall off as $1/r'$ as $r' \to \infty$, we see that $U(r')$ should go to zero faster than $1/r'$. Under this assumption, the second term may be neglected as $r \to \infty$, and we may use the asymptotic behaviors of the Bessel functions to obtain, as $r \to \infty$,

$$\begin{aligned}
R_\ell(r) &\sim \frac{1}{kr}\sin\left(kr - \frac{\ell\pi}{2}\right) - \frac{e^{ikr-i\pi\ell/2}}{r}\int_0^\infty dr'\,(r')^2 j_\ell(kr')U(r')R_\ell(r') \\
&\sim \frac{1}{2ikr}\left\{-e^{-ikr+i\pi\ell/2} + e^{ikr-i\pi\ell/2}\left(1 - 2ik\int_0^\infty dr'\,(r')^2 j_\ell(kr')U(r')R_\ell(r')\right)\right\}
\end{aligned} \tag{12.90}$$

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The first term represents a radially incoming wave, while the second represents a radially outgoing wave. Because the potential $V(r)$ is spherically symmetric, the probability in each of the partial waves separately is conserved. Thus, the probability currents of the incoming and outgoing radial waves have to be equal. This requires that the moduli of the incoming and outgoing waves coincide. Therefore, the composite factor of the second term must in fact be a phase,

$$1 - 2ik \int_0^\infty dr' \, (r')^2 j_\ell(kr') U(r') R_\ell(r') = e^{2i\delta_\ell(k)} \tag{12.91}$$

for $\delta_\ell(k)$ a real function of $k$, for each $\ell$. The asymptotic form of the wave function thus becomes,

$$
\begin{aligned}
R_\ell(r) \quad &\sim \quad \frac{1}{2ikr} \left\{ -e^{-ikr + i\pi\ell/2} + e^{ikr - i\pi\ell/2 + 2i\delta_\ell(k)} \right\} \\
&\sim \quad \frac{e^{i\delta_\ell(k)}}{kr} \sin\left( kr - \frac{\pi\ell}{2} + \delta_\ell(k) \right)
\end{aligned}
\tag{12.92}
$$

The angles $\delta_\ell(k)$ are referred to as the *phase shift for angular momentum $\ell$*.

Alternatively, we may expose in $R_\ell(r)$ the contribution from the incoming plane wave, by isolating the function $j_\ell(kr)$. As a result, we have, as $r \to \infty$,

$$R_\ell(r) \sim j_\ell(kr) + \frac{e^{ikr - i\pi\ell/2}}{r} \times \frac{e^{2i\delta_\ell(k)} - 1}{2ik} \tag{12.93}$$

Therefore, we may now derive a partial wave expansion for the scattering amplitude $f(\mathbf{k}', \mathbf{k})$, by comparing the general definition of $f(\mathbf{k}', \mathbf{k})$ with the partial wave expansion obtained here. The definition is given by the behavior of the wave function $\psi_\mathbf{k}(\mathbf{r})$ for large $r$,

$$\psi_\mathbf{k}(\mathbf{r}) \sim \frac{1}{(2\pi)^{3/2}} \left\{ e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{e^{ikr}}{r} f(\mathbf{k}', \mathbf{k}) \right\} \tag{12.94}$$

The partial wave result in the same limit obtained here is given by,

$$\psi_\mathbf{k}(\mathbf{r}) - \phi_\mathbf{k}(\mathbf{r}) = \frac{e^{ikr}}{(2\pi)^{3/2} \, 2ikr} \sum_{\ell=0}^\infty (2\ell + 1) \left( e^{2i\delta_\ell(k)} - 1 \right) P_\ell(\cos\theta) \tag{12.95}$$

As a result, we obtain the partial wave expansion of $f(\mathbf{k}', \mathbf{k})$,

$$f(\mathbf{k}', \mathbf{k}) = \frac{1}{2ik} \sum_{\ell=0}^\infty (2\ell + 1) \left( e^{2i\delta_\ell(k)} - 1 \right) P_\ell(\cos\theta) \tag{12.96}$$

The total cross section may be computed by performing the angular integrations of $|f(\mathbf{k}', \mathbf{k})|^2$. To do so, we use the orthogonality of the Legendre polynomials as well as their normalizations,

$$\int_{4\pi} d\Omega \, P_\ell(\cos\theta) P_{\ell'}(\cos\theta) = \frac{4\pi \delta_{\ell,\ell'}}{2\ell + 1} \tag{12.97}$$

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The result is given by

$$\sigma_{\text{tot}} = \int_{4\pi} d\Omega |f(\mathbf{k}', \mathbf{k})|^2 = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell + 1) \sin^2 \delta_\ell \tag{12.98}$$

It is readily checked that the optical theorem is obeyed for this cross section. This may be seen by computing

$$\text{Im} f(\mathbf{k}, \mathbf{k}) = \frac{1}{2k} \sum_{\ell=0}^{\infty} (2\ell + 1) \left( 1 - \cos 2\delta_\ell(k) \right) P_\ell(1) \tag{12.99}$$

Using now the fact $P_\ell(1) = 1$ and that $1 - \cos 2\delta_\ell(k) = 2 \sin^2 \delta_\ell(k)$, it is easily seen that the relation of the optical theorem holds.

## 12.12  The example of a hard sphere

Assume we scatter off a spherical body with potential

$$V(r) = V_0 \theta(b - r) \qquad\qquad V_0 > 0 \tag{12.100}$$

for some radius $b$ and let $V_0 \to \infty$. This is a *hard sphere* of radius $b$. In this limit, clearly all the partial waves $R_\ell(kr)$ must vanish at $r \leq b$. Outside the hard sphere, for $r > b$, the solution is a linear combination of the spherical Bessel functions $j_\ell(kr)$ and $h_\ell(kr)$,

$$R_\ell(r) = j_\ell(kr) + c_\ell(k) h_\ell(kr) \tag{12.101}$$

where $c_\ell(k)$ is generally a complex function of $k$. Vanishing of $R_\ell(b)$ provides $c_\ell(k)$,

$$c_\ell(k) = -\frac{j_\ell(kb)}{h_\ell(kb)} \tag{12.102}$$

From the limit of $h_\ell(kr)$ as $r \to \infty$ and the result for the phase shift (12.93), we find that

$$e^{ikr - i\pi\ell/2} \times \frac{e^{2i\delta_\ell(k)} - 1}{2ik} = -\frac{j_\ell(kb)}{h_\ell(kb)} \frac{1}{k} e^{ikr - i(\ell+1)\pi/2} \tag{12.103}$$

we find that

$$e^{2i\delta_\ell(k)} - 1 = -2 \frac{j_\ell(kb)}{h_\ell(kb)} \tag{12.104}$$

Using the relation

$$j_\ell(kb) = \frac{1}{2} \left( h_\ell(kb) + h_\ell^*(kb) \right) \tag{12.105}$$

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the above relation becomes,

$$e^{2i\delta_\ell(k)} = -\frac{h_\ell^*(kb)}{h_\ell(kb)} \tag{12.106}$$

The phase shifts for the lowest values of $\ell$ may be computed explicitly, using the expressions for the corresponding Hankel functions,

$$
\begin{aligned}
h_0(\rho) &= -i\frac{e^{i\rho}}{\rho} \\
h_1(\rho) &= -i\frac{e^{i\rho}}{\rho^2}(1 - i\rho) \\
h_2(\rho) &= -i\frac{e^{i\rho}}{\rho^3}\left(-3 + 3i\rho + \rho^2\right)
\end{aligned} \tag{12.107}
$$

As a result, we have

$$
\begin{aligned}
e^{2i\delta_0(k)} &= e^{-2ikb} \\
e^{2i\delta_1(k)} &= e^{-2ikb} \times \frac{1 + ikb}{1 - ikb} \\
e^{2i\delta_2(k)} &= e^{-2ikb} \times \frac{-3 - 3ikb + k^2b^2}{-3 + 3ikb + k^2b^2}
\end{aligned} \tag{12.108}
$$

or taking the logs,

$$
\begin{aligned}
\delta_0(k) &= -kb \\
\delta_1(k) &= -kb + \mathrm{Arctg}(kb) \\
\delta_2(k) &= -kb + \mathrm{Arctg}\left(\frac{kb}{1 - k^2b^2/3}\right)
\end{aligned} \tag{12.109}
$$

Note that in the low momentum limit, $kb \to 0$, one may obtain an approximate result valid for all $\ell$, using the asymptotic expansions of the spherical Bessel functions,

$$
\begin{aligned}
j_\ell(kb) &= \mathrm{Re}(h_\ell(kb)) \sim \frac{(kb)^\ell}{(2\ell + 1)!!} \\
n_\ell(kb) &= \mathrm{Im}(h_\ell(kb)) \sim -\frac{(2\ell - 1)!!}{(kb)^{\ell+1}}
\end{aligned} \tag{12.110}
$$

Since $j_\ell(kb) \ll n_\ell(kb)$ in this limit, we find that

$$\delta_\ell(k) \sim \frac{j_\ell(kb)}{n_\ell(kb)} \sim -\frac{(kb)^{2\ell+1}}{(2\ell + 1)!!(2\ell - 1)!!} \tag{12.111}$$

Thus, for $kb \ll 1$, it makes sense to neglect $\ell \geq 1$ in the low momentum limit, and we find

$$\sigma_{\mathrm{tot}} \sim \frac{4\pi}{k^2} \sin^2 \delta_0 \sim 4\pi b^2 \tag{12.112}$$

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At high energy, the particles behave classically and see only the aspect disk with area $\pi b^2$, but at low energy, the $s$-wave scattering sees the entire surface area of the sphere, which is $4\pi b^2$.

In terms of the Bessel functions, it is possible to write down an exact expression for the cross section, valid for all ranges of the momenta $k$,

$$\sigma_{\text{tot}} = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1) \frac{(j_\ell(kb))^2}{|h_\ell(kb)|^2} \tag{12.113}$$

Collecting the first two terms, $\ell \le 1$, we find,

$$\sigma_{\text{tot}} = \frac{4\pi}{k^2} \left( k^2 b^2 + \frac{3}{1+k^2 b^2}(-kb\cos kb + \sin kb)^2 \right) \tag{12.114}$$

At very high momentum $kb \gg 1$, we may use the asymptotic expressions for the Bessel functions to evaluate the cross section, so that

$$\frac{(j_\ell(kb))^2}{|h_\ell(kb)|^2} \sim \sin^2\left( kb - \frac{\pi\ell}{2} \right) \tag{12.115}$$

Summing over $\ell$ leads to a divergent total cross section ! This is now a UV effect, operating at high momentum scattering, and it is due to the fact that we are assuming that the sphere is perfectly reflecting even to the highest momenta. Physically, this assumption is not valid in fact. Sakurai proposes then to limit the sum over $\ell$ to $\ell\ell_{\text{max}} < kb$, and refers to this as a *reasonable assumption*. Please judge for yourself.

## 12.13   The hard spherical shell

Another very interesting special case is for a $\delta$-function shell of finite strength, given by

$$U(r) = -U_0 \delta(r-b) \tag{12.116}$$

where $U_0$ may be either positive or negative. To solve for the phase shifts, we use the potential $U(r)$ above in the integral equation (12.78). The integral over $r'$ is readily performed since the $\delta(r'-b)$ potential localizes the integral at $r'=b$, and we find,

$$R_\ell(r) = j_\ell(kr) - U_0 b^2 G_\ell(r,b) R_\ell(b) \tag{12.117}$$

To determine $R_\ell(b)$, we simply evaluate this equation at $r=b$, so that

$$R_\ell(b) = \frac{j_\ell(kb)}{1 + iU_0 kb^2 j_\ell(kb) h_\ell(kb)} \tag{12.118}$$

This result gives an exact expression for the partial wave functions $R_\ell(r)$ outside the spherical shell, where $r > b$ (the inside region may be solved for as well but is immaterial for the scattering problem), and we find,

$$R_\ell(r) = j_\ell(kr) + \frac{iU_0 kb^2 j_\ell(kb)^2 h_\ell(kr)}{1 - iU_0 kb^2 j_\ell(kb) h_\ell(kb)} \tag{12.119}$$

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Comparison of the asymptotics of this formula with the definition of the phase shifts in (12.93), we find, after some rearrangements, that

$$e^{2i\delta_\ell(k)} = \frac{1 + iU_0 kb^2 j_\ell(kb) h_\ell^*(kb)}{1 - iU_0 kb^2 j_\ell(kb) h_\ell(kb)}$$

(12.120)

Gottfried has a nice discussion of the physics of this problem.

## 12.14 Resonance scattering

There is a very interesting case of scattering potentials where quasi-stable bound states exist and affect the scattering process. This occurs when the effective potential

$$V_{\text{eff}}(r) = V(r) + \frac{\ell(\ell+1)}{r^2}$$

(12.121)

has a local minimum which is not a global minimum.
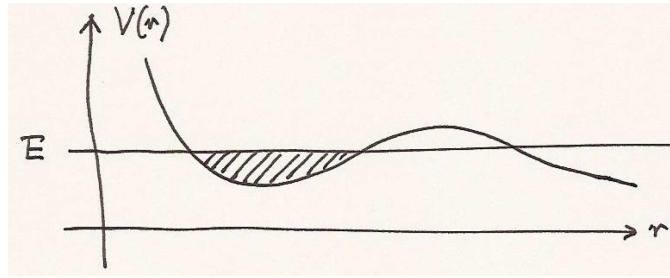


Figure 13: Potential with unstable minimum in shaded area

During a scattering process, the incident particle excites the potential and creates a quasi-stable bound state. This creates a resonance effect, since it will take some time for this bound state to decay, and the process is then referred to as *resonance scattering*. The scattering cross section in this channel reaches then a maximum. Note that this will always occur, for given $\ell$, when $\delta_\ell(k)$ crosses the value $\pi/2$. Given the partial cross section

$$\sigma_{\text{tot}}^{(\ell)} = \frac{4\pi}{k^2}(2\ell+1)\sin^2\delta_\ell(k)$$

(12.122)

we see that this partial cross section takes its maximal value at $\delta_\ell(k) = \pi/2$. Around this value, we may linearize as a function of momentum $k$ (or traditionally, more often as a function of energy $E$), we have

$$\text{cotg}\,\delta_\ell(k) = 2\frac{E - E_R}{\Gamma} + \mathcal{O}((E - E_R)^2) \qquad\qquad E = \frac{\hbar^2 k^2}{2m}$$

(12.123)

Since $\delta_\ell(k)$ is dimensionless, we need indeed two dimensionful parameters $E_R$, the position of the resonance, and $\Gamma$, the width of the resonance, to characterize the expansion to first order. Computing now the partial cross section, we use

$$\sin^2 \delta_\ell(k) = \frac{1}{1 + \text{cotg}^2\delta_\ell(k)} = \frac{\Gamma^2/4}{(E - E_R)^2 + \Gamma^2/4} \tag{12.124}$$

and thus the partial cross section

$$\sigma_{\text{tot}}^{(\ell)} = \frac{4\pi}{k^2} \frac{(2\ell + 1)\Gamma^2/4}{(E - E_R)^2 + \Gamma^2/4} \tag{12.125}$$

It turns out that this kind of curves fit experimental observations of resonance scattering processes very well.
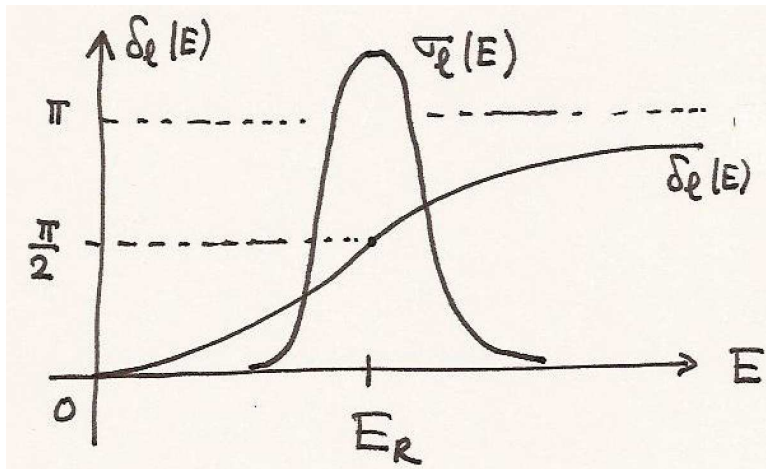


Figure 14: Behavior of the phase shift $\delta_\ell$ and of the partial cross section $\sigma_\ell$ near a resonance

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# 13 Time-dependent Processes

So far, we have studied problems in which the Hamiltonian is time-independent. This is suitable for any isolated system, in which the total energy is conserved. In many physical problems, however, it is inconvenient to treat the entire closed system, and views part of the system, instead, as an external source, which may be time dependent. The Hamiltonian for such systems then often takes the form of a sum of a time-independent unperturbed Hamiltonian $H_0$, and a time time-dependent perturbation $V(t)$,

$$H = H_0 + V(t) \tag{13.1}$$

and it will be assumed again that the spectrum and eigenstates of $H_0$ is exactly known. Very few such time dependent problems can be solved exactly, and often one will have to resort to carrying out perturbation theory in the strength of the potential $V(t)$.

## 13.1 Magnetic spin resonance and driven two-state systems

The problem of magnetic spin resonance is exactly solvable and is also of substantial practical significance. Actually, the problem is more general than magnetic spin would suggest, and the same methods may be applied for any two-state system driven by an external periodic oscillation. We deal with this problem first and then develop perturbation theory. The Hamiltonian is of the form

$$
\begin{aligned}
H_0 &= \omega_0 S_z \\
V(t) &= \omega_1 \cos(\omega t) S_x + \omega_1 \sin(\omega t) S_y
\end{aligned}
\tag{13.2}
$$

Here, $\omega$ is the driving frequency. As a magnetic problem, this Hamiltonian arises from a particle with spin $\mathbf{S}$ and magnetic moment $\mathbf{M} = \gamma \mathbf{S}$ in the presence of a constant magnetic field $\mathbf{B}_0$ along the $z$-axis, and an oscillating magnetic field $\mathbf{B}_1(t) = B_1 \cos(\omega t)\mathbf{n}_x + B_1 \sin(\omega t)\mathbf{n}_y$ in the $xy$-plane. The frequencies are then given by

$$
\begin{aligned}
\omega_0 &= \gamma B_0 \\
\omega_1 &= \gamma B_1
\end{aligned}
\tag{13.3}
$$

But the problem may be considered generally, without referring to the magnetic system.

Denote an orthonormal basis of the two state system by the vectors $|+|>$ and $|-\rangle$. In this basis, the Hamiltonian is given by

$$H = \frac{\hbar}{2} \begin{pmatrix} \omega_0 & \omega_1 e^{-i\omega t} \\ \omega_1 e^{+i\omega t} & -\omega_0 \end{pmatrix} \tag{13.4}$$

A general state $|\psi(t)\rangle$ may be decomposed onto $|+\rangle$ and $|-\rangle$,

$$|\psi(t)\rangle = a_+(t)|+\rangle + a_-(t)|-\rangle \tag{13.5}$$

The time-dependent Schrödinger equation for $|\psi(t)\rangle$ then reduces to the following set of equations for $a_\pm$,

$$
\begin{aligned}
i\dot{a}_+(t) &= \frac{\omega_0}{2}a_+(t) + \frac{\omega_1}{2}e^{-i\omega t}a_-(t) \\
i\dot{a}_-(t) &= \frac{\omega_1}{2}e^{+i\omega t}a_+(t) - \frac{\omega_0}{2}a_-(t)
\end{aligned}
\tag{13.6}
$$

In a comoving frame of states, defined by

$$
\begin{aligned}
b_+(t) &= a_+(t)e^{+i\omega t/2} \\
b_-(t) &= a_-(t)e^{-i\omega t/2}
\end{aligned}
\tag{13.7}
$$

the equations simplify in that they no longer involve any explicit time dependence,

$$
\begin{aligned}
i\dot{b}_+(t) &= \frac{\omega_0 - \omega}{2}b_+(t) + \frac{\omega_1}{2}b_-(t) \\
i\dot{b}_-(t) &= \frac{\omega_1}{2}b_+(t) - \frac{\omega_0 - \omega}{2}b_-(t)
\end{aligned}
\tag{13.8}
$$

The time evolution of the $b_\pm$ variables is thus effectively given by a reduced Hamiltonian,

$$
\tilde{H} = \frac{\hbar}{2}\begin{pmatrix} \omega_0 - \omega & \omega_1 \\ \omega_1 & -\omega_0 + \omega \end{pmatrix}
\tag{13.9}
$$

The eigenvalues of $\tilde{H}$ are $\pm\hbar\Omega$ with

$$
\Omega = \sqrt{(\omega_0 - \omega)^2 + \omega_1^2}
\tag{13.10}
$$

Thus, we get the following general solution,

$$
\begin{pmatrix} b_+(t) \\ b_-(t) \end{pmatrix} = \gamma_+ \begin{pmatrix} \omega_1 \\ \Omega + \omega - \omega_0 \end{pmatrix} e^{-i\Omega t/2} + \gamma_- \begin{pmatrix} \omega_1 \\ -\Omega + \omega - \omega_0 \end{pmatrix} e^{+i\Omega t/2}
\tag{13.11}
$$

where $\gamma_\pm$ are constants. This gives a complete solution of the problem.

We now introduce also physical initial conditions and a physical problem : suppose the system at time $t = 0$ is in the state $|+\rangle$, what is the probability of finding the system in the state $|-\rangle$ after time $t$ ? To solve this problem, we first enforce the initial condition on the general solution. This means that at time $t = 0$, we have $a_+(0) = b_+(0) = 1$ and $a_-(0) = b_-(0) = 0$, so that we must have

$$
\gamma_\pm = \frac{1}{2\omega_1}\left(1 \pm \frac{\omega_0 - \omega}{\Omega}\right)
\tag{13.12}
$$

The desired probability is then given by

$$
P_{+-}(t) = \frac{\omega_1^2}{(\omega - \omega_0)^2 + \omega_1^2}\sin^2\left(\sqrt{(\omega - \omega_0)^2 + \omega_1^2}\,\frac{t}{2}\right)
\tag{13.13}
$$

This is the Rabi formula for magnetic resonance. The resonance effect occurs when $\omega \sim \omega_0$, in which case the probability for the spin flip is maximal. In fact, when $\omega = \omega_0$, then this formula tells us that after a time $t = \pi/\omega_1$, the spin is flipped with probability 1.

## 13.2   The interaction picture

We now turn to time dependent problems in the general case where $H = H_0 + V(t)$. We shall assume that the eigenvalues and eigenstates of $H_0$ are known as follows,

$$H_0|n\rangle = E_n|n\rangle \tag{13.14}$$

For simplicity, we shall assume here that the spectrum of $H_0$ is discrete, but it is not hard to generalize to the continuous case, something we shall do later on. We prepare an initial state $|\phi_a\rangle$ at $t = 0$, which we may decompose in the basis of eigenstates $|n\rangle$ by

$$|\phi_a\rangle = \sum_n c_n(0)|n\rangle \tag{13.15}$$

In the absence of interaction potential, $V(t) = 0$, this state would evolve as follows,

$$|\phi_a; t\rangle = \sum_n c_n(0)e^{-itE_n/\hbar}|n\rangle \tag{13.16}$$

On the other hand, once the interaction potential is turned on, the time evolution will be more complicated, giving time dependence also to the coefficients $c_n$. The corresponding state will be denoted $|\psi_a; t\rangle$. It satisfies the full time dependent Schrödinger equation,

$$i\hbar\frac{d}{dt}|\psi_a; t\rangle = (H_0 + V(t))|\psi_a; t\rangle \tag{13.17}$$

and has the following decomposition,

$$|\psi_a; t\rangle = \sum_n c_n(t)e^{-itE_n/\hbar}|n\rangle \tag{13.18}$$

Notice that we can also write this time evolution as

$$|\psi_a; t\rangle = e^{-itE_n/\hbar}|\psi_a; t\rangle_I \tag{13.19}$$

where

$$|\psi_a; t\rangle_I = \sum_n c_n(t)|n\rangle \tag{13.20}$$

The subscript $I$ has been added to indicate that this state is now considered in the *interaction picture*, a method due to Dirac. The advantage is that the coefficients $c_n$ now have time dependence only through the effects of the time-dependent interaction potential, the effects of the free Hamiltonian having been factored out.

More generally, if $|\psi_a; t\rangle_S$ is a general state in the Schrödinger picture, satisfying the Schrödinger equation,

$$i\hbar\frac{d}{dt}|\psi_a; t\rangle_S = \left(H_0 + V(t)\right)|\psi_a; t\rangle_S \tag{13.21}$$

then we define the corresponding state $|\psi_a; t\rangle_I$ in the interaction picture by factoring out the time dependence induced by $H_0$ alone,

$$|\psi_a; t\rangle_I \equiv e^{itH_0/\hbar}|\psi_a; t\rangle_S \tag{13.22}$$

Correspondingly, any observable $A_S$ in the Schrödinger picture (which is by construction time independent), maps to an observable $A_I$ in the interaction picture, by

$$A_I(t) = e^{itH_0/\hbar} A_S e^{-itH_0/\hbar} \tag{13.23}$$

Thus, observables, in general, also become time dependent. The interaction picture is therefore intermediate between the Heisenberg and Schrödinger pictures.

The time evolution of the states $|\psi_a; t\rangle_I$ in the interaction picture may be deduced from their definition and from the Schrödinger equation, and we find,

$$i\hbar \frac{d}{dt}|\psi_a; t\rangle_I = V_I(t)|\psi_a; t\rangle_I \tag{13.24}$$

where the potential in the interaction picture is given by the relation between observables given above,

$$V_I(t) = e^{itH_0/\hbar} V(t) e^{-itH_0/\hbar} \tag{13.25}$$

The time-evolution of the coefficients $c_n$ is now simply given by the matrix elements of $V_I(t)$. Indeed, we have

$$|\psi_a; t\rangle_I = \sum_n c_n(t)|n\rangle \tag{13.26}$$

and

$$i\hbar \sum_n \dot{c}_n(t)|n\rangle = \sum_m c_m(t)V_I(t)|m\rangle \tag{13.27}$$

Taking the matrix elements with $\langle n|$,

$$
\begin{aligned}
i\hbar \dot{c}_n(t) &= \sum_m c_m(t)\langle n|V_I(t)|m\rangle \\
&= \sum_m c_m(t) e^{-it(E_m - E_n)/\hbar}\langle n|V(t)|m\rangle
\end{aligned}
\tag{13.28}
$$

In general, it is not possible to solve the resulting system of differential equations exactly (except in very special cases, such as magnetic resonnace treated earlier). Thus, we resort to carrying out a calculation which is perturbative in powers of $V_I$.

## 13.3  Time-dependent perturbation theory

A systematic way of organizing time-dependent perturbation theory is through the use the evolution operator in the interaction picture. After all, we have

$$|\psi_a; t\rangle_I = U_I(t, t_0)|\psi_a; t_0\rangle_I \tag{13.29}$$

where

$$
\begin{aligned}
i\hbar \frac{d}{dt} U_I(t, t_0) &= V_I(t) U_I(t, t_0) \\
U_I(t_0, t_0) &= I
\end{aligned} \tag{13.30}
$$

Notice that, since $V_I$ is time dependent, we need to keep the initial and final times in $U_I$, and not just their difference $t - t_0$, as we had done in the time independent case.

The differential equation, together with the initial value condition at $t_0$ may be reformulated in terms of a single integral equation,

$$U_I(t, t_0) = I - \frac{i}{\hbar} \int_{t_0}^{t} dt' \, V_I(t') \, U_I(t', t_0) \tag{13.31}$$

Clearly, the initial value problem is satisfied by this equation, and differentiation in $t$ immediately reproduces the differential equation. Its solution may be obtained order by order in perturbation theory by successive substitution and iteration. A first iteration gives

$$U_I(t, t_0) = I - \frac{i}{\hbar} \int_{t_0}^{t} dt' \, V_I(t') - \frac{1}{\hbar^2} \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' V_I(t') V_I(t'') U_I(t'', t_0) \tag{13.32}$$

Iterating again will yield the solution to second order in $V_I$,

$$U_I(t, t_0) = I - \frac{i}{\hbar} \int_{t_0}^{t} dt' \, V_I(t') - \frac{1}{\hbar^2} \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' V_I(t') V_I(t'') + \cdots \tag{13.33}$$

This is referred to as the *Dyson series*. Alternatively, we may derive an analogous formula directly on the coefficients $c_n$, and we get

$$c_n(t) = c_n(0) - \frac{i}{\hbar} \int_{t_0}^{t} dt' \sum_m \langle n|V_I(t')|m\rangle c_m(t') \tag{13.34}$$

and then this formula may be iterated in turn.

The difficulty of this integral solution is that the potential $V_I(t)$ is an operator, and in general, we will have

$$[V_I(t'), V_I(t'')] \neq 0 \tag{13.35}$$

Generally, it is difficult to go beyond the first order in any expliciit way. For short time intervals $t - t_0$, the expansion should yield reliable results given by the contributions of the leading orders. For long time evolution, however, predictions are much harder to come by. Below, we show that it is possible to obtain new results already just from the first order approximation to this formula. Below, we shall treat a special case to illuminate the procedure.

## 13.4  Switching on an interaction

We consider perhaps the simples of time-dependent potentials,

$$V(t) = \mathcal{V}\theta(t) \tag{13.36}$$

where $\theta(t)$ is the step function, and $\mathcal{V}$ is a time-independent operator. This potential represents an interaction that is turned on abruptly at time $t = 0$ and then stays on. This circumstance is a reasonable approximation to what happens in physical situations. For example, an atom prepared in a certain excited energy eigenstate may decay under the influence of an external perturbation, such as an incoming wave or a vacuum fluctuation. Or a probe may hit a target in a scattering experiment.

We use (13.34) to first order to compute the time evolution. For simplicity, we shall assume that the system has been prepared at time $t = 0$ in one of the eigenstates $n = i$, so that $c_n(0) = \delta_{n,i}$, and we obtain,

$$
\begin{aligned}
c_n(t) &= \delta_{n,i} - \frac{i}{\hbar}\mathcal{V}_{ni}\int_0^t dt'\, e^{i\omega_{ni}t} \\
&= \frac{\mathcal{V}_{ni}}{E_n - E_i}\left(1 - e^{i\omega_{ni}t}\right)
\end{aligned}
\tag{13.37}
$$

where we have used,

$$
\begin{aligned}
\mathcal{V}_{ni} &= \langle n|\mathcal{V}|i\rangle \\
\omega_{ni} &= (E_n - E_i)/\hbar
\end{aligned}
\tag{13.38}
$$

The probability for measuring the system in state $n \neq i$ after time $t$ is then given by

$$P_{ni}(t) = |c_n(t)|^2 = \frac{4|\mathcal{V}_{ni}|^2}{(E_n - E_i)^2}\sin^2\frac{(E_n - E_i)t}{2\hbar} \tag{13.39}$$

Clearly, this probability distribution is peaked towards the smallest values of $|E_n - E_i|$. To study this behavior more closely, it is convenient to introduce the density of states $\rho(E)$, so that we can treat discrete and continuous spectra on the same footing. The density of states is defined so that $\rho(E)dE$ equals the number of states between energies $E$ and $E + dE$. The probability for the decay of the initial state at energy $E_i$ into a state $E_n$ between $E$ and $E + dE$ is then given by

$$dP(E, t) = \rho(E)dE|c_n(t)|^2 = \rho(E)dE\,\frac{4|\mathcal{V}_{E,E_i}|^2}{(E - E_i)^2}\sin^2\frac{(E - E_i)t}{2\hbar} \tag{13.40}$$

This gives us the probability rate, per unit energy,

$$\frac{dP(E, t)}{dE} = \rho(E)\frac{4|\mathcal{V}_{E,E_i}|^2}{(E - E_i)^2}\sin^2\frac{(E - E_i)t}{2\hbar} \tag{13.41}$$

Now, we are primarily interested in this probability for long time scales, where we mean long compared to the transition energies $E - E_i$.

It is best to consider this problem mathematically first. We set $x = (E - E_i)/(2\hbar)$, and thus seek to obtain the following large $t$ behavior ($tx \gg 1$ for $x$ fixed)

$$\lim_{t \to \infty} \frac{\sin^2(tx)}{tx^2} \tag{13.42}$$

Clearly, when $x \neq 0$, this quantity tends to zero as $t \to \infty$. So, it can have support only at $x = 0$. In fact, at $x = 0$, its value is just $t$, so we suspect that the limit is of the form $\delta(x)$. To prove this, integrate the quantity against a smooth function $f(x)$,

$$\begin{aligned}
\lim_{t \to \infty} \int_{-\infty}^{\infty} dx\, f(x) \frac{\sin^2(tx)}{tx^2} &= \lim_{t \to \infty} \int_{-\infty}^{\infty} dy\, f(y/t) \frac{\sin^2 y}{y^2} \\
&= f(0) \int_{-\infty}^{\infty} dy \frac{\sin^2 y}{y^2} = \pi f(0)
\end{aligned} \tag{13.43}$$

As a result, we conclude that

$$\lim_{t \to \infty} \frac{\sin^2(tx)}{tx^2} = \pi \delta(x) \tag{13.44}$$

The object of interest may now be handled as follows,

$$\frac{4}{(E - E_i)^2} \sin^2 \frac{(E - E_i)t}{2\hbar} \sim t \times \frac{4}{(E - E_i)^2 t} \sin^2 \frac{(E - E_i)t}{2\hbar} \tag{13.45}$$

as $t \to \infty$. The second factor now has a limit, as computed above, and we have

$$\frac{4}{t(E - E_i)^2} \sin^2 \frac{(E - E_i)t}{2\hbar} \sim t \times \frac{2\pi}{\hbar} \delta(E - E_i) \tag{13.46}$$

Putting all together, we obtain still for large $t$,

$$\frac{dP(E, t)}{dE} \sim t \times \frac{2\pi}{\hbar} \rho(E) |\mathcal{V}_{E, E_i}|^2 \delta(E - E_i) \tag{13.47}$$

It is customary to express this result in terms of the *transition rate* per unit time, by taking the time derivative on both sides,

$$\omega_{i \to E} = \frac{d^2 P(E, t)}{dE\, dt} = \frac{2\pi}{\hbar} \rho(E) |\mathcal{V}_{E, E_i}|^2 \delta(E - E_i) \tag{13.48}$$

This formula is referred to as *Fermi's Golden Rule*.

The Fermi Golden Rule formula must be interpreted with some care. For finite $t$, as we are of course always assuming, it is not strictly true that only a state with energy $E = E_i$ will contribute. This is a simple reflection of the energy time uncertainty relation,

$$\Delta t \Delta E \geq \hbar \tag{13.49}$$

Thus, for finite time, we should really integrate over $E$ in a range around $E_i$ given by $\Delta E \sim \hbar/t$, where $t$ is large. The density of states may be assumed to be a smooth function of $E$, but the matrix elements may or may not vary smoothly. Thus, one defines an average matrix element squared $\overline{|\mathcal{V}_{E, E_i}|^2}$ in terms of which we have,

$$\omega_{i \to E} = \frac{2\pi}{\hbar} \rho(E) \overline{|\mathcal{V}_{E, E_i}|^2} \tag{13.50}$$

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## 13.5   Sinusoidal perturbation

Another very important special case, analogous to the problem of spin magnetic resonance, is when the time dependence of the perturbing potential is sinusoidal,

$$V(t) = \mathcal{V}e^{i\omega t} + \mathcal{V}^\dagger e^{-i\omega t} \tag{13.51}$$

where $\mathcal{V}$ is a time independent operator. We again use the perturbative formula for the coefficients $c_n$, given in (13.34), and assume that at time $t = 0$, the system has been prepared in one of the eigenstates $|i\rangle$ of $H_0$. We obtain,

$$
\begin{aligned}
c_n(t) &= \delta_{n,i} - \frac{i}{\hbar}\int_0^t dt' \left(\mathcal{V}e^{i\omega t'} + \mathcal{V}^\dagger e^{-i\omega t'}\right)e^{i\omega_{ni}t'} \\
&= \delta_{n,i} + \frac{1 - e^{i(\omega_{ni}+\omega)t}}{\hbar(\omega_{ni}+\omega)}\mathcal{V}_{ni} + \frac{1 - e^{i(\omega_{ni}-\omega)t}}{\hbar(\omega_{ni}-\omega)}\mathcal{V}_{ni}^\dagger
\end{aligned} \tag{13.52}
$$

We see that this formula is very similar to the switched on interaction, except that $\omega_{ni} \to \omega_{ni} \pm \omega$. Thus, the transition rate is supported not at $\omega_{ni} = 0$ as in the case of the switched on interaction, but rather at $\omega_{ni} \pm \omega = 0$. Thus the rates are given by

$$\omega_{i\to E} = \frac{d^2 P(E,t)}{dE\, dt} = \frac{2\pi}{\hbar}\rho(E)\,|\mathcal{V}_{E,E_i}|^2\delta(E - E_i \pm \hbar\omega) \tag{13.53}$$

The two cases correspond to absorption or emission a quantum with energy $\hbar$.

# 14    Path Integral Formulation of Quantum Mechanics

A quantum system associated with classical mechanics admits a formulation in terms of functional integrations over all possible paths. This path-integral formulation was pioneered by Dirac in 1933, and popularized by Feynman in the 1940's. It is quite useful in modern quantum mechanics, but it has become an indispensable tool especially in quantum field theory.

The key intuitive idea behind the path integral construction of the probability amplitudes of quantum mechanics is as follows. Classically, the system is deterministic, and we know the precise path followed by a particle, given initial $q$ and final $q'$ conditions. Quantum mechanically, each geometric path is a possible "trajectory" for the quantum particle, and its contribution to the full quantum probability amplitude will be given by some weight factor which remains to be determined. The full quantum probability amplitude will then be given by a sum over all possible paths, and a weight factor for each path.

$$\text{probability amplitude} = \sum_{\text{paths}} \text{weight factor for path} \tag{14.1}$$

A sketch of the (unique) path followed by a classical particle and possible quantum paths is depicted in the Figure below.
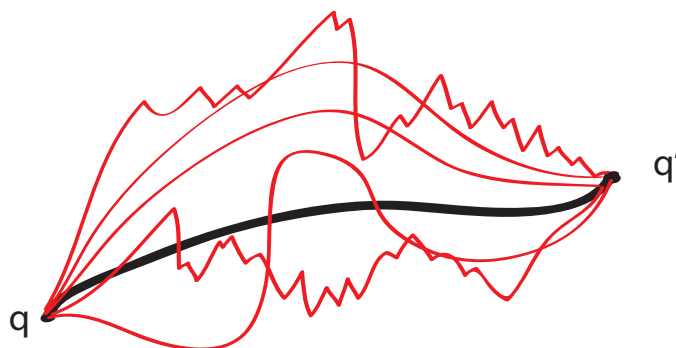


Figure 15: The black line represents the classical trajectory; the red lines represent various path which contribute to the path integral for the quantum probability amplitude.

In the present chapter, we shall give a detailed derivation of the sum over paths and the associated weight factor. The standard reference is the book by Feynman and Hibbs, but I will follow rather the more general derivation in phase space given originally by Dirac.

## 14.1    The time-evolution operator

Time evolution in the Schrödinger and Heisenberg pictures are given by a differential equation respectively for states and observables,

$$i\hbar \frac{d}{dt}|\varphi(t)\rangle = H(t)|\varphi(t)\rangle \qquad\qquad \text{Schroedinger picture}$$

$$i\hbar \frac{d}{dt}A(t) = [A(t), H(t)] \qquad\qquad \text{Heisenberg picture} \tag{14.2}$$

Actually, the time-evolution equations in both pictures may be solved with the use of the *time evolution operator* $U(t)$. This operator is defined to be *unitary*, and to satisfy,[13]

$$i\hbar \frac{d}{dt}U(t) = H(t)U(t) \qquad\qquad U(t)^{\dagger}U(t) = I \qquad\qquad (14.3)$$

It is often convenient to give an initial condition on $U$ such that at time $t_a$, the operator is unity. We shall denote this operator by $U(t; t_a)$. The solution to both equations in (14.2) may then be presented as follows,

$$
\begin{aligned}
|\varphi(t)\rangle &= U(t; t_a)|\varphi(t_a)\rangle \qquad\qquad U(t_a; t_a) = I \\
A(t) &= U(t; t_a)^{\dagger} A(t_a) U(t; t_a)
\end{aligned}
\qquad (14.4)
$$

This result may be verified by explicit calculation; to do so in the Heisenberg picture, the following intermediate step will be helpful,

$$i\hbar \frac{d}{dt}U(t)^{\dagger} = -U(t)^{\dagger}H(t) \qquad\qquad (14.5)$$

For a time-independent Hamiltonian $H$, the evolution operator is given by the exponential,

$$U(t; t_a) = U(t - t_a) \qquad\qquad U(t) = e^{-itH/\hbar} \qquad\qquad (14.6)$$

The evolution operator $U(t)$ now commutes with $H$ at all times $t$, and manifestly satisfies the following composition formula,

$$U(t_1 + t_2) = U(t_1)U(t_2) \qquad\qquad (14.7)$$

## 14.2 The evolution operator for quantum mechanical systems

Let us consider a quantum system which is associated with a classical mechanical one. As discussed in the preceding section, such systems may be formulated in terms of the position $Q$ and momentum $P$ operators, in terms of which the Hamiltonian is expressed, $H(Q, P)$. In general, we may have several such pairs, $Q_i$, $P_i$ with $i = 1, \cdots, N$. For simplicity, we shall start with the case $N = 1$; the generalization to higher $N$ will be straightforward. Recall the bases defined by these operators,

$$
\begin{aligned}
Q|q\rangle &= q|q\rangle \qquad\qquad [Q, P] = i\hbar \\
P|p\rangle &= p|p\rangle
\end{aligned}
\qquad (14.8)
$$

Orthonormality and completeness hold as follows,

$$\langle q'|q\rangle = \delta(q - q') \qquad\qquad I = \int dq\, |q\rangle\langle q|$$

$$\langle p'|p\rangle = 2\pi\hbar\, \delta(p - p') \qquad\qquad I = \int \frac{dp}{2\pi\hbar}\, |p\rangle\langle p| \qquad (14.9)$$

---

[13]Note the definite order in the product of $H(t)$ and $U(t)$; generally these operators do not commute.

Translation operators in both bases satisfy

$$
\begin{aligned}
e^{+iaP/\hbar} Q e^{-iaP/\hbar} &= Q + a \qquad\qquad\qquad e^{-iaP/\hbar}|q\rangle = |q + a\rangle \\
e^{-ibQ/\hbar} P e^{+ibQ/\hbar} &= P + b \qquad\qquad\qquad e^{+ibQ/\hbar}|p\rangle = |p + b\rangle
\end{aligned}
\tag{14.10}
$$

and their mutual overlap is

$$
\begin{aligned}
\langle q|p\rangle &= e^{+iqp/\hbar} \\
\langle p|q\rangle &= e^{-iqp/\hbar}
\end{aligned}
\tag{14.11}
$$

This summarizes all that will be needed to derive the functional integral representation.

We now use the position basis to express the time-evolution of the wave function $\varphi(q,t) = \langle q|\varphi(t)\rangle$ associated with a general state $|\varphi(t)\rangle$. It is given by

$$
\varphi(q_b, t_b) = \langle q_b|U(t_b - t_a)|\varphi(t_a)\rangle = \int dq_a \langle q_b|U(t_b - t_a)|q_a\rangle \varphi(q_a, t_a)
\tag{14.12}
$$

Hence, the evolution of the wave function is given by the matrix elements of the evolution operator in a position space basis. It is these matrix elements for which we shall derive a functional integral formulation. We can split this evolution into the consecutive evolutions of two shorter time intervals, $t_c - t_a = (t_c - t_b) + (t_b - t_a)$, with $t_c > t_b > t_a$. Inserting a complete set of position eigenstates in the product on the right hand side of the formula $U(t_c - t_a) = U(t_c - t_b)U(t_b - t_a)$, we obtain,

$$
\langle q_c|U(t_c - t_a)|q_a\rangle = \int dq_b \langle q_c|U(t_c - t_b)|q_b\rangle \langle q_b|U(t_b - t_a)|q_a\rangle
\tag{14.13}
$$

Clearly this process can be repeated.

## 14.3    The evolution operator for a free massive particle

Before launching a full attack on this problem, let us calculate the matrix elements of the evolution operator for a a free massless particle with Hamiltonian,

$$
H = \frac{1}{2m}P^2
\tag{14.14}
$$

Since $H$ is diagonal in the momentum basis, we calculate as follows,

$$
\begin{aligned}
\langle q_b|U(t_b - t_a)|q_a\rangle &= \int \frac{dp_b}{2\pi\hbar} \int \frac{dp_a}{2\pi\hbar} \langle q_b|p_b\rangle \langle p_b|U(t_b - t_a)|p_a\rangle \langle p_a|q_a\rangle \\
&= \int \frac{dp_b}{2\pi\hbar} \int \frac{dp_a}{2\pi\hbar} e^{i(p_b q_b - p_a q_a)/\hbar} \, \langle p_b|U(t_b - t_a)|p_a\rangle
\end{aligned}
\tag{14.15}
$$

Using the fact that $U(t_b - t_a)$ is diagonal in the momentum basis, we find,

$$
\langle p_b|U(t_b - t_a)|p_a\rangle = 2\pi\hbar\delta(p_b - p_a)\, e^{-i(t_b - t_a)p_a^2/(2m\hbar)}
\tag{14.16}
$$

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Putting all together, and using $\delta(p_b - p_a)$ to carry out the integration over $p_b$, we have

$$
\begin{aligned}
\langle q_b | U(t_b - t_a) | q_a \rangle &= \int \frac{dp_a}{2\pi\hbar} e^{-i(t_b - t_a)p_a^2/(2m\hbar)} \, e^{ip_a(q_b - q_a)/\hbar} \\
&= \left( \frac{m}{2\pi i(t_b - t_a)\hbar} \right)^{\frac{1}{2}} \exp\left\{ \frac{im(q_b - q_a)^2}{2\hbar(t_b - t_a)} \right\}
\end{aligned}
\tag{14.17}
$$

The full significance of the exponential factor will become clear later. Here, we notice simply that the quantity

$$
\dot{q} = \frac{q_b - q_a}{t_b - t_a}
\tag{14.18}
$$

is the velocity needed for a free particle in uniform motion departing from position $q_a$ at time $t_a$ to reach position the $q_b$ at time $t_b$. Its energy $E$ is just its kinetic energy, and the associated action $S$ are given by

$$
E(q_b, t_b; q_a, t_a) = \frac{m(q_b - q_a)^2}{2(t_b - t_a)^2} \qquad\qquad S(q_b, t_b; q_a, t_a) = \frac{m(q_b - q_a)^2}{2(t_b - t_a)}
\tag{14.19}
$$

For the free particle, the matrix elements of the evolution operator are given by

$$
\langle q_b | U(t_b - t_a) | q_a \rangle \sim \exp\{iS(q_b, t_b; q_a, t_a)/\hbar\}
\tag{14.20}
$$

Notice that for fixed $q_a, q_b$ and $t_b - t_a \to 0$, $S$ is becomes very large, unless $q_a \sim q_b$. As $t_b - t_a \to 0$, the evolution operator becomes local in $q$ and tends towards $\delta(q_b - q_a)$.

## 14.4   Derivation of the path integral

We now seek a formula for $\langle q_b | U(t_b - t_a) | q_a \rangle$ which will be valid for a general time-independent Hamiltonian $H(Q, P)$. It is convenient to begin by dividing the time interval $t_b - t_a > 0$ into $N$ consecutive segments of equal length $\varepsilon = (t_b - t_a)/N$. Using the multiplicative property of the exponential, we have

$$
U(t_b - t_a) = U(\varepsilon)^N
\tag{14.21}
$$

Inserting $N - 1$ times the identity operator, expressed as a completeness relation on position eigenstates, we obtain,

$$
\langle q_b | U(t_b - t_a) | q_a \rangle = \left( \prod_{n=1}^{N-1} \int_{\mathbf{R}} dq_n \right) \prod_{n=1}^{N} \langle q_n | U(\varepsilon) | q_{n-1} \rangle
\tag{14.22}
$$

where we have set $q_0 \equiv q_a$ and $q_N \equiv q_b$. The remaining $q_n$ for $n = 1, \cdots, N-1$ are integrated over in this formula, as may be seen schematically on the Figure below.

When $N \to \infty$ and $\varepsilon \to 0$, we may expand the evolution operator in a power series in $\varepsilon$,

$$
U(\varepsilon) = I - i\frac{\varepsilon}{\hbar} H + \mathcal{O}(\varepsilon^2)
\tag{14.23}
$$

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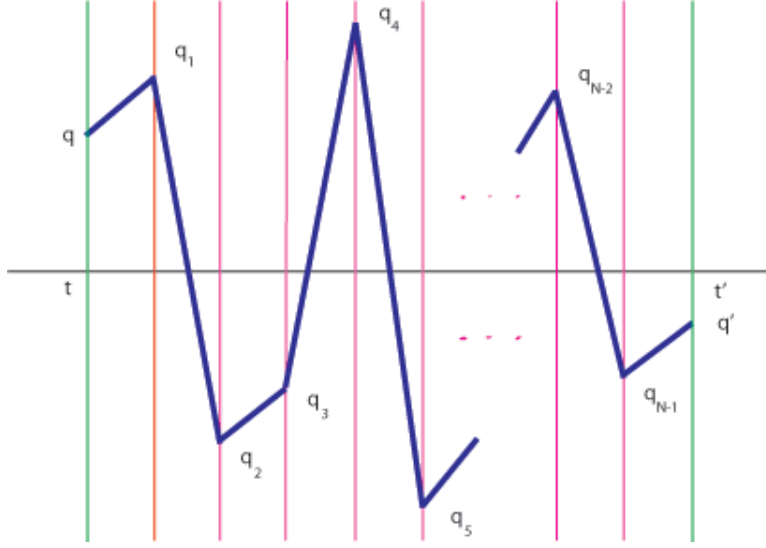
Figure 16: The evolution operator given as a summation over paths, $q_a = q$ and $q_b = q'$

The problem will be, however, that the Hamiltonian $H$ is not generally diagonal in the position basis (as was clear from the free particle Hamiltonian already). Of course we could use the momentum basis, in which the free particle Hamiltonian is diagonal, but a general Hamiltonian will not be diagonal in this basis either. The trick is to use a mixed basis. Consider for example a general *potential type Hamiltonian*, of the form,

$$H(Q, P) = \frac{1}{2m}P^2 + V(Q) \tag{14.24}$$

It is manifest that we have $\langle q|H(Q,P)|p\rangle = \langle q|p\rangle H(q,p)$, where $H(q,p)$ is just the classical Hamiltonian. Now, given a general Hamiltonian, $H(Q,P)$, it can always be rearranged so that all $P$ operators are on the right of all $Q$ operators. It is in this form that we can use it to define the classical Hamiltonian $H(q,p)$ by,

$$\langle q|H(Q,P)|p\rangle = \langle q|p\rangle H(q,p) \tag{14.25}$$

We are now in a position to complete our calculations. We shall define the classical Hamiltonian by

$$\langle q|U(\varepsilon)|p\rangle = \langle q|p\rangle \left(1 - i\frac{\varepsilon}{\hbar}H(q,p) + \mathcal{O}(\varepsilon^2)\right) = \langle q|p\rangle \exp\left\{-i\frac{\varepsilon}{\hbar}H(q,p)\right\} \tag{14.26}$$

and use this expression to compute the matrix element,

$$\langle q_n|U(\varepsilon)|q_{n-1}\rangle = \int \frac{dp_n}{2\pi\hbar}\langle q_n|U(\varepsilon)|p_n\rangle\langle p_n|q_{n-1}\rangle$$

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$$= \int \frac{dp_n}{2\pi\hbar} \langle q_n | p_n \rangle \langle p_n | q_{n-1} \rangle \exp\left\{ -i\frac{\varepsilon}{\hbar} H(q_n, p_n) \right\}$$

$$= \int \frac{dp_n}{2\pi\hbar} \exp\left\{ i(q_n - q_{n-1}) p_n / \hbar - i\frac{\varepsilon}{\hbar} H(q_n, p_n) \right\} \tag{14.27}$$

The final step consists of a change of notation,

$$
\begin{aligned}
t_n &= t + n\varepsilon \\
q_n &= q(t_n) \\
p_n &= p(t_n)
\end{aligned}
\tag{14.28}
$$

The argument of the exponential may now be recast as follows,

$$
\begin{aligned}
\frac{i}{\hbar}(q_n - q_{n-1}) p_n - i\frac{\varepsilon}{\hbar} H(q_n, p_n) &= \frac{i}{\hbar}\varepsilon\left( \frac{q(t_n) - q(t_n - \varepsilon)}{\varepsilon} p(t_n) - H(q_n, p_n) \right) \\
&= \frac{i}{\hbar} \int_{t_{n-1}}^{t_n} dt \left( \dot{q}(t) p(t) - H(q(t), p(t)) \right)
\end{aligned}
\tag{14.29}
$$

Putting all together,

$$\langle q_b | U(t_b - t_a) | q_a \rangle = \int \mathcal{D}q \int \mathcal{D}p \exp\left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt \left( \dot{q}(t) p(t) - H(q(t), p(t)) \right) \right\} \tag{14.30}$$

where the measures are defined by

$$
\begin{aligned}
\int \mathcal{D}q &= \lim_{N\to\infty} \prod_{n=1}^{N-1} \int_{\mathbf{R}} dq(t_n) \\
\int \mathcal{D}p &= \lim_{N\to\infty} \prod_{n=1}^{N} \int_{\mathbf{R}} \frac{dp(t_n)}{2\pi\hbar}
\end{aligned}
\tag{14.31}
$$

and the paths satisfy the following "boundary conditions"

$$
\begin{aligned}
q(t_a) &= q_a \\
q(t_b) &= q_b
\end{aligned}
\tag{14.32}
$$

Notice that there are no boundary conditions on $p(t)$. The combination $\dot{q}p - H(q, p)$ is nothing but the Lagrangian written in canonical coordinates $q$ and $p$, and the integral over $\tau$ that enters the path integral formula above is just the action in terms of $q$ and $p$.

An alternative formula is obtained by expressing $\langle q_b |$ as the Fourier transform of a momentum state,

$$\langle p_b | U(t_b - t_a) | q_a \rangle = \int \mathcal{D}q \int \mathcal{D}p \exp\left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt \left( \dot{q}(t) p(t) - H(q(t), p(t)) \right) \right\} \tag{14.33}$$

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where the combine measure is defined by

$$\int \mathcal{D}q \int \mathcal{D}p = \lim_{N \to \infty} \prod_{n=1}^{N-1} \int_{\mathbf{R}} \int_{\mathbf{R}} \frac{dq(t_n) dp(t_n)}{2\pi\hbar} \tag{14.34}$$

and the paths satisfy the following "boundary conditions"

$$\begin{aligned} q(t_a) &= q_a \\ p(t_b) &= p_b \end{aligned} \tag{14.35}$$

while the boundary conditions on $p(t_a)$ and $q(t_b)$ are now free. This form is particularly geometrical because the measure is intrinsic and invariant under canonical transformations. The volume element

$$\frac{dq(t_n) dp(t_n)}{2\pi\hbar} \tag{14.36}$$

gives a measure for the elementary volume of phase space in a quantum system. By the uncertainty relation, there is in some sense one state per elementary phase space volume element $\Delta q \Delta p$. The above measure naturally puts a measure on the number of quantum states for the system.

## 14.5 Integrating out the canonical momentum $p$

Whenever the Hamiltonian is simple enough so that its dependence on momentum and position enter separately, momentum may be "integrated out". Let us take the most customary form,

$$H = \frac{p^2}{2m} + V(q) \tag{14.37}$$

The combination under the integration is

$$\begin{aligned} \dot{q}p - H(q,p) &= \dot{q}p - \frac{p^2}{2m} - V(q) \\ &= -\frac{1}{2m}(p - m\dot{q})^2 + \frac{1}{2}m\dot{q}^2 - V(q) \end{aligned} \tag{14.38}$$

We now see that the integration over $\mathcal{D}p$ does not depend on $q$ any more, after an innocuous translation by $m\dot{q}$. The Gaussian integral involves an infinite number of integrations, so this gives a constant, which we shall absorb into the definition of the integration measure $\mathcal{D}q$,

$$\int \mathcal{D}q = \lim_{N \to \infty} \prod_{n=1}^{N-1} \left( \int_{\mathbf{R}} dq(t_n) \sqrt{\frac{m}{2\pi i \hbar \varepsilon}} \right) \tag{14.39}$$

Our final result is thus,

$$\langle q_b | U(t_b - t_a) | q_a \rangle = \int \mathcal{D}q \exp\left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt L(q, \dot{q}) \right\} \tag{14.40}$$

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where $L$ is the standard Lagrangian, formulated in terms of $q$ and $\dot{q}$, and given by

$$L(q, \dot{q}) \;=\; \frac{1}{2}m\dot{q}^2 - V(q) \tag{14.41}$$

The extra dynamics-dependent constant factor that appears in the measure after $p$ has been integrated out is a real nuisance and it is often "omitted", in the sense that one gives up on computing it. Instead, one writes that

$$\langle q_b|U(t_b - t_a)|q_a\rangle = \mathcal{N} \int \mathcal{D}q \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, L(q, \dot{q})\right\} \tag{14.42}$$

where $\mathcal{N}$ is a quantity which is independent of $q_a, q_b$. Often, $\mathcal{N}$ can be determined by considering limits of $q_a$ or $q_b$ in which the integral simplifies, but $\mathcal{N}$ remains unchanged.

## 14.6 Dominant paths

The space of all paths that contribute to the path integral is huge. Often, however, the physics of the problem produces a natural distinction between the paths that contribute most and paths that do not. We can see this by studying the free-particle weight factor in the path integral,

$$e^{iS_m/\hbar} \qquad\qquad S_m = \frac{m(q_b - q_a)^2}{2(t_b - t_a)} \tag{14.43}$$

Consider a particle traveling a distance of $q_b - q_a \sim 1mm$ in a time of $t_b - t_a \sim 1sec$. The phase factors for a particle of mass $m = 1g$, for an electron of mass $m_e \sim 10^{-27}g$, and a proton of mass $m_p \sim 2 \times 10^{-24}g$ are,

$$
\begin{aligned}
S_m/\hbar \;&\sim\; 0.5 \times 10^{25} & &\gg \pi \\
S_{m_e}/\hbar \;&\sim\; 0.005 & &\ll \pi \\
S_{m_p}/\hbar \;&\sim\; 1 & &\sim \pi
\end{aligned}
\tag{14.44}
$$

Clearly, for the particle of mass $1g$, the interference of all the paths but the classical one will cancel one another out. For the electron, paths other than the classical path interfere strongly with the contribution of the classical path, and the case of the proton is intermediate.

## 14.7 Stationary phase approximation

When the classical path has an action which is much larger than $\pi$, it makes sense to treat the functional integral by approximations. It is useful to consider an example of a rapidly oscillating integral first.

$$\int_{-\infty}^{+\infty} dk\; e^{i(\pi ak^2 - 2\pi bk)} = \frac{e^{-i\pi b^2/a}}{\sqrt{-ia}} \tag{14.45}$$

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Of course, we knw how to do this integral exactly; it is just a Gaussian. But if we were just interested in the $a \gg 1$ behavior of the integral, we can use stationary phase approximation. The rule is to approximate the integral by the value it takes when the phase is stationary,

$$\frac{d}{dk}(\pi a k^2 - 2\pi bk) = 0 \tag{14.46}$$

which is also $ak - b = 0$. Hence, in this approximation, we get

$$\int_{-\infty}^{+\infty} dk \, e^{i(\pi a k^2 - 2\pi bk)} \sim e^{-i\pi b^2/a} \tag{14.47}$$

Comparing with the exact result, we see that the exponential is correct, though the prefactor is missing. The prefactor is subdominant to the exponential though when $a \ll 1$, so this approximation is not too bad. The method is especially useful for integrals that we do not know how to evaluate exactly, eg,

$$\int_{-\infty}^{+\infty} dk \, e^{i(\pi a k^4 - 2\pi bk)} \sim e^{-3/2 i\pi b(b/2a)^{1/3}} \tag{14.48}$$

Here, we have assume that only the real stationary phase solution of $2ak^3 - b = 0$ contributes. In general, the issue of whether complex solutions contribute or not is a quite subtle one (see eg Mathews and Walker).

We shall now be interested in applying the stationary phase method to the path integral

$$\langle q_b | U(t_b - t_a) | q_a \rangle = \int \mathcal{D}q \exp\left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt \, L(q, \dot{q}) \right\} \tag{14.49}$$

We begin by assuming that there exists a classical trajectory $q_0(t)$ such that

$$\begin{aligned} q_0(t_a) &= q_a \\ q_0(t_b) &= q_b \end{aligned} \tag{14.50}$$

and such that $q_0(t)$ solves the Euler-Lagrange equations, and is thus a stationary path of the action. For simplicity, we shall assume that the solution $q_0(t)$ is unique. The stationary phase approximation to the path integral is then,

$$\langle q_b | U(t_b - t_a) | q_a \rangle \sim \exp\left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt \, L(q_0(t), \dot{q}_0(t)) \right\} \tag{14.51}$$

In the next subsection, we shall improve upon this result.

## 14.8    Gaussian fluctuations

It is possible to systematically improve upon the stationary phase approximation. Here, we shall discuss only the leading such correction, obtained by taking into account the Gaussian fluctuations

of paths around the classical one. As before, we assume that we have a classical solution $q_0(t)$ connecting initial and final positions. If $\hbar$ were zero, that is all there would be. So, it makes sense to think of the quantum fluctuations around $q_0(t)$ as small when $S/\hbar \gg \pi$. The correct expansion order is given by

$$q(t) = q_0(t) + \sqrt{\hbar}y(t) \qquad\qquad y(t_a) = y(t_b) = 0 \qquad\qquad (14.52)$$

The contribution from the Gaussian fluctuations is then obtained by expanding $S[q_0 + \sqrt{\hbar}y]$ in powers of $\hbar$. By the very fact that $q_0(t)$ is a classical solution, we know that the term of order $\sqrt{\hbar}$ in this expansion must vanish. Hence, we have

$$
\begin{aligned}
S[q_0 + \sqrt{\hbar}y] &= S[q_0] + \hbar S_2[y; q_0] + \mathcal{O}(\hbar^{3/2}) \\
S_2[y; q_0] &= \int_{t_a}^{t_b} dt \left( \frac{1}{2} L_{\dot{q}\dot{q}} \dot{y}^2 + L_{\dot{q}q} \dot{y}y + \frac{1}{2} L_{qq} y^2 \right)
\end{aligned} \qquad (14.53)
$$

where the coefficients are given by

$$L_{\dot{q}\dot{q}} = \left.\frac{\partial^2 L}{\partial \dot{q}^2}\right|_{q=q_0} \qquad\qquad L_{\dot{q}q} = \left.\frac{\partial^2 L}{\partial \dot{q}\partial q}\right|_{q=q_0} \qquad\qquad L_{qq} = \left.\frac{\partial^2 L}{\partial q^2}\right|_{q=q_0} \qquad (14.54)$$

Notice that, for a general Lagrangian $L$, all three coefficients $L_{\dot{q}\dot{q}}, L_{\dot{q}q}, L_{qq}$ will be non-vanishing and may be $\tau$-dependent. In the case of the standard Lagrangian,

$$L = \frac{1}{2}m\dot{q}^2 - V(q) \qquad\qquad (14.55)$$

the problem is much simplified though and we have

$$L_{\dot{q}\dot{q}} = m \qquad\qquad L_{\dot{q}q} = 0 \qquad\qquad L_{qq} = -V''(q_0(t)) \qquad (14.56)$$

The Gaussian action is then simply,

$$
\begin{aligned}
S_2[y; q_0] &= \int_{t_a}^{t_b} dt \left( \frac{1}{2}m\dot{y}^2 - \frac{1}{2}V''(q_0)y^2 \right) \\
&= \frac{1}{2} \int_{t_a}^{t_b} dt \, y(t) \left( -m\frac{d^2}{dt^2} - V''(q_0(t)) \right) y(t)
\end{aligned} \qquad (14.57)
$$

The energy levels and wave-functions of the harmonic oscillator could be recovered in this way (see homework problem).

## 14.9 Gaussian integrals

We shall compute the Gaussian integrals for real and complex variables, and show that

$$
\begin{aligned}
\int d^N X \, \exp\left\{ -\pi\tau X^t M X \right\} &= \frac{1}{(\det(\tau M))^{\frac{1}{2}}} \\
\int d^N Z d^N \bar{Z} \, \exp\left\{ -2\pi\tau Z^\dagger H Z \right\} &= \frac{1}{\det(\tau H)}
\end{aligned} \qquad (14.58)
$$

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Here, $X$ and $Z$ are respectively a real and a complex column matrix of height $N$. These variables and their associated measures may be parametrized as follows,

$$
X = \begin{pmatrix} x_1 \\ x_2 \\ . \\ x_N \end{pmatrix} \qquad
Z = \begin{pmatrix} z_1 \\ z_2 \\ . \\ z_N \end{pmatrix} \qquad
\begin{aligned}
d^N X &= dx_1 dx_2 \cdots dx_N \\[8pt]
d^N Z d^N \bar{Z} &= d^2 z_1 d^2 z_2 \cdots d^2 z_N
\end{aligned}
\tag{14.59}
$$

The measure on $z$ is defined by $d^2 z = d\mathrm{Re}(z)\, d\mathrm{Im}(z)$. The measures are invariant under orthogonal rotations of $X$ and unitary transformations of $Z$. The $N \times N$ matrices $M$ and $H$ are respectively real symmetric and Hermitian. Both $M$ and $H$ are assumed to be positive, i.e. all their eigenvalues, respectively $m_i$ and $h_i$ are positive. Finally, the complex parameter $\tau$ is required to have $\mathrm{Re}(\tau) > 0$ for absolute convergence of the integral.

We shall now prove the above Gaussian integral formulas. Using the fact that any real symmetric matrix $M$ can be diagonalized by an orthogonal change of basis, and that any Hermitian matrix $H$ may be diagonalized by a unitary change of basis, we have

$$
\int d^N X \, \exp\left\{ -\pi\tau X^t M X \right\} = \prod_{i=1}^{N} \left( \int dx_i \, e^{-\pi\tau m_i x_i^2} \right)
$$

$$
\int d^N Z d^N \bar{Z} \, \exp\left\{ -2\pi\tau Z^\dagger H Z \right\} = \prod_{i=1}^{N} \left( \int d^2 z_i \, e^{-2\pi\tau h_i |z_i|^2} \right)
\tag{14.60}
$$

It remains to carry out a single real or complex Gaussian integral. We do this first for $\tau$ real and then analytically continue in $\tau$. The complex integral is readily carried out in polar coordinates, $z_i = r_i e^{i\phi_i}$ for $0 \le r_i < \infty$ and $0 \le \phi_i < 2\pi$. We find,

$$
\int d^2 z_i \, e^{-2\pi\tau h_i |z_i|^2} = 2 \int_0^{2\pi} d\phi_i \int_0^\infty dr_i \, r_i \, e^{-2\pi\tau h_i r_i^2} = \frac{1}{\tau h_i}
\tag{14.61}
$$

Recasting this complex integral in real Cartesian coordinates, $z_i = (x_i + iy_i)/\sqrt{2}$, we see that the complex integral is the square of the real integral evaluated for $m_i = h_i$, and thus,

$$
\int dx_i \, e^{-\pi\tau m_i x_i^2} = \frac{1}{\sqrt{\tau m_i}}
\tag{14.62}
$$

Using the definition of the determinants for $\tau M$ and $\tau H$ in terms of the products of their eigenvalues, we immediately recover the desired integrals. Note that, as $\mathrm{Re}(\tau) \to 0$, we recover an integral which is not absolutely convergent, but which is conditionally convergent. Its conditional convergence prescription may be taken to be limit $\mathrm{Re}(\tau) \to 0$.

## 14.10 Evaluating the contribution of Gaussian fluctuations

The contribution of Gaussian fluctuations around a given dominant path $q_0(t)$ is given by the Gaussian functional integral,

$$
\int \mathcal{D}y \, \exp\left\{ \frac{i}{2} \int_{t_a}^{t_b} dt \, y(t) M(t) y(t) \right\}
\tag{14.63}
$$

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for the operator $M(t)$, defined by

$$M(t) = -m\frac{d^2}{dt^2} - V''(q_0(t)) \tag{14.64}$$

and subject to the boundary conditions $y(t_a) = y(t_b) = 0$. We will now show that, if the complete spectrum of the self-adjoint operator $M(t)$ (subject to the above boundary conditions) is known, then this functional integral of Gaussian fluctuations can be computed. Let the eigenfunctions $\phi_n(t)$ satisfy

$$M(t)\phi_n(t) = \lambda_n\phi_n(t) \tag{14.65}$$

subject to $\phi_n(t_a) = \phi_n(t_b) = 0$. Since $M(t)$ is self-adjoint, the eigenvalues $\lambda_n$ are real and the eigenfunctions $\phi_n(t)$ span an orthonormal basis of the function space for $y(t)$. Since $M(t)$ is actually real, we may choose a basis of real functions $\phi_n(t)$, obeying

$$\int_{t_a}^{t_b} dt\, \phi_n(t)\phi_{n'}(t) = \delta_{n,n'}$$
$$\sum_n \phi_n(t)\phi_n(t') = \delta(t - t') \qquad t_a \le t, t' \le t_b \tag{14.66}$$

The completeness of $\phi_n(t)$ allows us to expand

$$y(t) = \sum_n c_n\phi_n(t) \tag{14.67}$$

for real coefficients $c_n$. Since the metric on function space and on the $c_n$ are related by

$$\int_{t_a}^{t_b} dt\, \delta y(t)^2 = \sum_n (\delta c_n)^2 \tag{14.68}$$

the change of variables $y(t) \rightarrow \{c_n\}$ has unit Jacobian, and we have

$$\mathcal{D}y = \prod_n (dc_n) \tag{14.69}$$

It is now also straightforward to evaluate

$$\int_{t_a}^{t_b} dt\, y(t)M(t)y(t) = \sum_n \lambda_n(c_n)^2 \tag{14.70}$$

so that the entire functional integral over Gaussian fluctuations becomes,

$$\int \mathcal{D}y\, \exp\left\{\frac{i}{2}\int_{t_a}^{t_b} dt\, y(t)M(t)y(t)\right\} = \prod_n\left(\int dc_n \exp\left\{\frac{i}{2}\lambda_n(c_n)^2\right\}\right) = \prod_n \lambda_n^{-\frac{1}{2}} \tag{14.71}$$

Relating the product of the eigenvalues to the determinant, one often writes,

$$\int \mathcal{D}y\, \exp\left\{\frac{i}{2}\int_{t_a}^{t_b} dt\, y(t)M(t)y(t)\right\} = \mathrm{Det}\left(-m\frac{d^2}{dt^2} - V''(q_0(t))\right)^{-\frac{1}{2}} \tag{14.72}$$

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# 15 Applications and Examples of Path Integrals

In this section, we shall illustrate the use of path integrals and give examples of their calculation for simple examples. They include the harmonic oscillator, the Aharonov-Bohm effect, the Dirac magnetic monopole, imaginary time path integrals and the path integral formulation of statistical mechanics. We shall end by introducing the Ising model and solving it for the one dimensional case.

## 15.1 Path integral calculation for the harmonic oscillator

The classical Lagrangian is by now familiar,

$$L = \frac{1}{2}m\dot{q}^2 - \frac{1}{2}m\omega^2 q^2 \tag{15.1}$$

The dominant path is the classical trajectory between $(q_a, t_a)$ and $(q_b, t_b)$, which obeys the classical equation $\ddot{q}_0 + \omega^2 q_0 = 0$, and is given by

$$
\begin{aligned}
q_0(\tau) &= q_a \cos\omega(t - t_a) + B\sin\omega(t - t_a) \\
q_b &= q_a \cos\omega T + B\sin\omega T
\end{aligned}
\tag{15.2}
$$

where $T = t_b - t_a$, and the solution for $B$ is

$$B = \frac{q_b - q_a\cos\omega T}{\sin\omega T} \tag{15.3}$$

The associated classical action may be evaluated by exploiting the extremality of the action,

$$S = \frac{m}{2}\int_{t_a}^{t_b} dt\left(\frac{d}{dt}(q_0\dot{q}_0) - q_0\ddot{q}_0 - \omega^2 q_0^2\right) = \frac{m}{2}(q_0\dot{q}_0)(t)\bigg|_{t=t_a}^{t=t_b} \tag{15.4}$$

which yields explicitly,

$$e^{iS/\hbar} = \exp\left\{\frac{im\omega}{2\hbar\sin\omega T}\left[(q_a^2 + q_b^2)\cos\omega T - 2q_a q_b\right]\right\} \tag{15.5}$$

To compute the functional determinant, we solve for the eigenfunctions of

$$-m\frac{d^2}{dt^2}\phi_n(t) - m\omega^2\phi_n(t) = \lambda_n\phi_n(t) \tag{15.6}$$

subject to $\phi_n(t_a) = \phi_n(t_b) = 0$. The normalized solutions are

$$\phi_n(t) = \sqrt{\frac{2}{T}}\sin\left(\frac{n\pi(t - t_a)}{T}\right) \qquad\qquad n = 1, 2, 3, \cdots \tag{15.7}$$

and the eigenvalues are

$$\lambda_n = m\left(\frac{\pi^2 n^2}{T^2} - \omega^2\right) = \frac{m\pi^2 n^2}{T^2}\left(1 - \frac{\omega^2 T^2}{\pi^2 n^2}\right) \tag{15.8}$$

The product of the eigenvalues may first be defined up to a level $n \leq N$,

$$\prod_{n=1}^{N} \lambda_n = \prod_{n=1}^{N} \left[ \frac{m\pi^2 n^2}{T^2} \left( 1 - \frac{\omega^2 T^2}{\pi^2 n^2} \right) \right] \tag{15.9}$$

Clearly, the first factor in the product is independent of $\omega$, so we may write

$$\prod_{n=1}^{N} \lambda_n = \mathcal{N}_N \prod_{n=1}^{N} \left( 1 - \frac{\omega^2 T^2}{\pi^2 n^2} \right) \qquad \mathcal{N}_N = \prod_{n=1}^{N} \left( \frac{m\pi^2 n^2}{T^2} \right) \tag{15.10}$$

The $N \to \infty$ limit of the infinite product involving $\omega$ is convergent, and is related to the infinite product representation of the $\sin x$ function, which is given by

$$\sin x = x \prod_{n=1}^{\infty} \left( 1 - \frac{\pi^2 x^2}{n^2} \right) \tag{15.11}$$

Thus we have

$$\prod_{n=1}^{N} \left( 1 - \frac{\omega^2 T^2}{\pi^2 n^2} \right) = \frac{\sin \omega T}{\omega T} \tag{15.12}$$

The $N \to \infty$ limit of the product $\mathcal{N}_N$, however, does not converge. This divergence results from the fact that a precise calculation of the absolute overall normalization of the path integral would have required more care than we have applied here. But the most important property of $\mathcal{N}_N$ is that it is independent of $\omega$ for all values of $N$. Instead of attempting to calculate this proper normalization from first principles, we shall leave the overall normalization undetermined, and represent it by a multiplicative factor $\mathcal{N}$ which is independent of $\omega$. We shall then fix $\mathcal{N}$ by matching with the known case of the free particle corresponding to $\omega = 0$. Putting all together, we have,

$$\prod_{n=1}^{\infty} \lambda_n = \mathcal{N} \frac{\sin \omega T}{\omega T} \tag{15.13}$$

where $\mathcal{N}$ is independent of $\omega$. Assembling the entire path integral representation of the matrix elements of the evolution operator, and matching the overall normalization with that of the free particle for $\omega = 0$, given in (14.17), we find $\mathcal{N} = 2\pi i\hbar/m$, and thus,

$$\langle q_b | U(t_b - t_a) | q_a \rangle = \left( \frac{m\omega}{2\pi i\hbar \sin \omega T} \right)^{\frac{1}{2}} \exp \left\{ \frac{im\omega}{2\hbar \sin \omega T} \left[ (q_a^2 + q_b^2) \cos \omega T - 2q_a q_b \right] \right\} \tag{15.14}$$

It is good practice to double check this result in the following way. We compute the trace of the evolution operators by integrating over $q = q_a = q_b$,

$$\begin{aligned}
\mathrm{Tr}\left( U(T) \right) &= \int dq \langle q | U(T) | q \rangle \\
&= \int dq \left( \frac{m\omega}{2\pi i\hbar \sin \omega T} \right)^{\frac{1}{2}} \exp \left\{ \frac{im\omega q^2}{\hbar \sin \omega T} (\cos \omega T - 1) \right\} \\
&= \frac{-i}{2 \sin \omega T/2} = \frac{e^{-i\omega T/2}}{1 - e^{-i\omega T}}
\end{aligned} \tag{15.15}$$

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Expanding in powers of the exponential, we find,

$$\mathrm{Tr}\Big(U(T)\Big) = \sum_{n=0}^{\infty} e^{-iTE_n/\hbar} \qquad\qquad E_n = \hbar\omega\left(n+\frac{1}{2}\right) \qquad\qquad (15.16)$$

and recover the energy levels of the harmonic oscillator, each one with multiplicity 1.

## 15.2   The Aharonov-Bohm Effect

In classical electrodynamics, the motion of charged particles is completely determined by the electric $\mathbf{E}$ and magnetic $\mathbf{B}$ field strengths. This is because in classical physics, the equations of motion completely determine the dynamics, and for charged particles, the force is completely specified by the Lorentz formula,

$$\mathbf{F} = e\mathbf{E} + e\mathbf{v} \times \mathbf{B} \qquad\qquad (15.17)$$

Here, $\mathbf{F}$ is the force exerted on a particle of charge $e$ and velocity $\mathbf{v} = d\mathbf{x}/dt$. The gauge potentials $(\Phi, \mathbf{A})$ are usually introduced only as auxiliary variables, when deriving the field equations from a Lagrangian or from a Hamiltonian. Indeed, these quantities are given by

$$
\begin{aligned}
L &= \frac{1}{2}m\mathbf{v}^2 + e\mathbf{A}(t,\mathbf{x})\cdot\mathbf{v} - e\Phi(t,\mathbf{x}) \\
H &= \frac{1}{2m}\left(\mathbf{p} - e\mathbf{A}(t,\mathbf{x})\right)^2 + e\Phi(t,\mathbf{x}) \qquad\qquad (15.18)
\end{aligned}
$$

We have local gauge invariance, under $\Phi \to \Phi - \partial\Lambda/\partial t$ and $\mathbf{A} \to \mathbf{A} + \vec{\nabla}\Lambda$. For example, the Lagrangian transforms as follows, $L \to L + e\,d\Lambda/dt$.
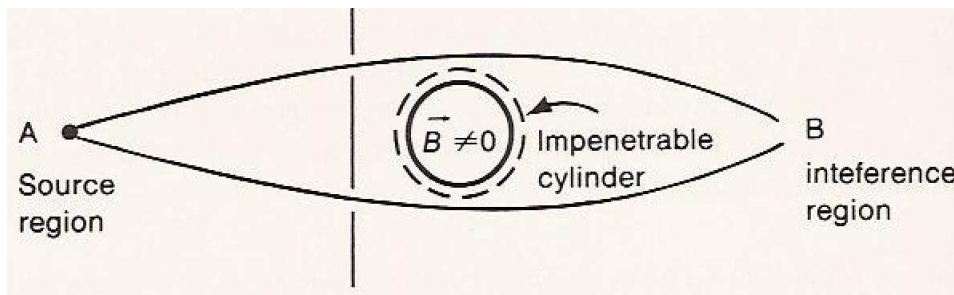


Figure 17: The Aharonov-Bohm set-up (figure from Sakurai)

In quantum mechanics, the dynamics of charged particles involves the vector potential in a fundamental way, either in the Hamiltonian operator formulation or in the Lagrangian path integral formulation. The Aharonov-Bohm effect is one of the most striking examples of the fundamental role played in quantum mechanics by the vector potential.

The set-up is as in Fig 9. Consider an infinite cylinder along the $z$-axis, of which only a cross-section in the $x-y$ plane in shown in Fig 9. The cylinder is impenetrable, so the particle we study

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can never penetrate inside. We assume vanishing electric field throughout, so that $\Phi = 0$. On the outside of the cylinder, the magnetic field vanishes identically. On the inside of the cylinder, there is a time-independent magnetic field **B**, which points in the $z$-direction, and produces a magnetic flux $\Phi_B$. Such a magnetic field may be produced by an infinite solenoid. Because of Stokes' theorem, the gauge potential outside the cylinder cannot vanish, because it must reproduce the total flux inside the cylinder,

$$\oint_C \mathbf{A} \cdot d\mathbf{x} = \Phi_B \tag{15.19}$$

where $C$ is any curve encircling the impenetrable cylinder once.

Next, we compare the probability amplitude for the charged particle to travel from point $A$ to point $B$ of Fig 9, either above or below the cylinder. We denote the paths above and below respectively by $C_+$ and $C_-$. The amplitudes are given by

$$\langle B|U(t_b - t_a)|A\rangle_{C_\pm} = \int \mathcal{D}\mathbf{x} \, \exp\left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt \, L_{C_\pm} \right\} \tag{15.20}$$

The actions may be compared by assuming that the path $C_-$ is exactly the mirror image of path $C_+$, so that the contribution of the kinetic terms in both are identical. The only difference is then due to the magnetic term, so that

$$
\begin{aligned}
\int_{t_a}^{t_b} dt \, L_{C_+} - \int_{t_a}^{t_b} dt \, L_{C_-} &= e \int_{t_a}^{t_b} dt \, \mathbf{A}(\mathbf{x}) \cdot \left. \frac{d\mathbf{x}}{dt} \right|_{C_+ - C_-} \\
&= e \int_{t_a}^{t_b} \mathbf{A}(\mathbf{x}) \cdot \left. d\mathbf{x} \right|_{C_+ - C_-} \\
&= e \int_C \mathbf{A}(\mathbf{x}) \cdot d\mathbf{x} = e\Phi_B
\end{aligned}
\tag{15.21}
$$

where we have used the fact that $C_+ - C_- = C$. As a result,

$$\langle B|U(t_b - t_a)|A\rangle_{C_+} = \langle B|U(t_b - t_a)|A\rangle_{C_-} \, \exp\left\{ \frac{ie\Phi_B}{\hbar} \right\} \tag{15.22}$$

For an arbitrary magnetic flux, $\Phi_B$, and electric charge $e$, there will be a non-trivial phase difference between the probability amplitudes along paths $C_+$ and $C_-$, and as a result, there will be interference when these paths merge at point $B$. On the other hand, the solenoid will be quantum mechanically unobservable provided the magnetic flux is *quantized*, and takes on integer multiple values of the basic magnetic flux quantum (for the electron charge $e$) of

$$\Phi_B^{(0)} = \frac{2\pi\hbar}{e} \ \sim \ 4.135 \times 10^{-7} \, Gauss \times cm^2 = 4.135 \times 10^{-15} \, Tm^2 \tag{15.23}$$

Note that the interference is purely quantum mechanical, it has no classical counterpart. Also, we have never needed the explicit form of the vector potential, only its role in generating a non-zero flux. It is possible to solve this problem using the Schrödinger equation, but then a specific **A** must be chosen.

## 15.3    Imaginary time path Integrals

If we formally replace $t \to -i\tau$ and consider $\tau$ real, then we obtain the *imaginary time* or *Euclidean* formulation of quantum mechanics. Often, one also refers to this procedure as *analytic continuation to imaginary time* because the substitution $t \to -i\tau$ can be regarded as an analytic continuation. The evolution operator becomes

$$U_E(\tau) = e^{-\tau H/\hbar} \tag{15.24}$$

and is formally related to the customary evolution operator by $U_E(\tau) = U(i\tau)$. Notice, however, that $U(t)$ and $U_E(\tau)$ are very different objects: most importantly, $U_E(\tau)$ is NOT a unitary operator for real $\tau$.

It is possible to obtain a path integral representation for the matrix elements of $U_E(\tau)$, just as we obtained one for $U(t)$. Instead of working out this path integral representation from scratch, we may simply obtain it by analytic continuation, $t \to -i\tau$,

$$\langle q_b | U_E(\tau_b - \tau_a) | q_a \rangle = \int \mathcal{D}q \exp\left\{ -\frac{1}{\hbar} \int_{\tau_a}^{\tau_b} d\tau\, L_E(q, \dot{q}) \right\} \tag{15.25}$$

subject to the boundary conditions,

$$
\begin{aligned}
q(\tau_a) &= q_a \\
q(\tau_b) &= q_b
\end{aligned} \tag{15.26}
$$

Here, the prefactor $-1/\hbar$, and the *Euclidean Lagrangian* $L_E$ are obtained as follows. In view of $t \to -i\tau$, we have,

$$\int dt \to -i \int d\tau \tag{15.27}$$

and the Euclidean Lagrangian becomes,

$$L\left( q(t), \frac{dq(t)}{dt} \right) = -L_E\left( q(\tau), \frac{dq(\tau)}{d\tau} \right) \tag{15.28}$$

Strictly speaking, we should also put a subscript $E$ on the basic variables $q$, so that $q(t) = q_E(\tau)$, but we shall omit this to save some notation. For the simplest Lagrangians, we have,

$$
\begin{aligned}
L &= \frac{1}{2}m \left( \frac{dq}{dt} \right)^2 - V(q) \\
L_E &= \frac{1}{2}m \left( \frac{dq}{d\tau} \right)^2 + V(q)
\end{aligned} \tag{15.29}
$$

Note that, at least for these simplest cases, the argument of the exponential in the path integral is now real and generally leads to a damped fall-off for large $q(\tau)$. This renders the Euclidean path integral well-defined even to the standards of mathematical rigor !

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For the free case ($V = 0$), we have $L_E = \frac{1}{2}m\dot{q}^2$, so that

$$\langle q_b | U_E(\tau_b - \tau_a) | q_a \rangle = \sqrt{\frac{m}{2\pi\hbar(\tau_b - \tau_a)}} \, \exp\left\{ -\frac{m(q_b - q_a)^2}{2\hbar(\tau_b - \tau_a)} \right\} \tag{15.30}$$

which is truly a Gaussian. Notice that for the free particle, this matrix element satisfies the heat equation,

$$\left( \frac{\partial}{\partial\tau} + \frac{\hbar}{2m}\frac{\partial^2}{\partial q^2} \right) \langle q | U_E(\tau - \tau_a) | q_a \rangle = 0 \tag{15.31}$$

with the initial condition that

$$\langle q | U_E(\tau_a - \tau_a) | q_a \rangle = \delta(q - q_a) \tag{15.32}$$

Its physical interpretation is as follows. We place a $\delta$-function heat distribution at the point $q_a$ at time $t_a$, and then observe the heat diffuse over $q$ as a function of time $\tau$; this is given by the function $\langle q | U_E(\tau - \tau_a) | q_a \rangle$.

## 15.4   Quantum Statistical Mechanics

The operator $e^{-\tau H/\hbar}$ is closely related to the Boltzmann operator $e^{-\beta H}$ of statistical mechanics. We introduce the standard notation,

$$\beta \equiv \frac{1}{k_B T} \tag{15.33}$$

where $T$ is temperature and $k_B$ is the Boltzmann constant. In any energy eigenstate $|E_n\rangle$ of $H$, the Boltzmann operator takes on the definite value

$$e^{-\beta H} |E_n\rangle = e^{-\beta E_n} |E_n\rangle \tag{15.34}$$

and thus provides the standard Boltzmann weight for a state with energy $E_n$.

The starting point of equilibrium statistical mechanics in the canonical ensemble is the *partition function*, which is defined by

$$Z \equiv \mathrm{Tr}\left( e^{-\beta H} \right) = \sum_n e^{-\beta E_n} \tag{15.35}$$

In the second equality, we have expanded the trace in a basis of eigenstates of $H$ which are labeled by $n$, and whose energy is $E_n$. Their multiplicities are properly included by summing, for each $E_n$ over all the states with energy $E_n$. All other thermodynamic functions may be expressed in terms of the partition function. The *free energy* $F$ is defined by

$$Z = e^{-\beta F} \qquad \text{or} \qquad F = -\frac{1}{\beta}\ln Z = -k_B T \ln Z \tag{15.36}$$

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The *internal energy* $E$ and the *entropy* $S$ are related to the free energy by

$$F = E - TS \tag{15.37}$$

Both may be expressed in terms of the partition function as well,

$$
\begin{aligned}
E &= -\frac{\partial \ln Z}{\partial \beta} \\
S &= -\frac{\partial F}{\partial T}
\end{aligned}
\tag{15.38}
$$

It is instructive to work out the internal energy in a basis of energy eigenstates,

$$E = \frac{1}{Z} \sum_n E_n e^{-\beta E_n} \tag{15.39}$$

A useful interpretation of these expressions is obtained by introducing the notion of *the statistical probability* $P_n$ for finding the system in a state $n$ with energy $E_n$. The statistical probability is defined as the normalized Boltzmann weight,

$$P_n \equiv \frac{e^{-\beta E_n}}{Z} \qquad\qquad \sum_n P_n = 1 \tag{15.40}$$

The internal energy then takes on a natural form,

$$E = \sum_n E_n P_n \tag{15.41}$$

The entropy may also be conveniently expressed in terms of the $P_n$,

$$S = -k_B \sum_n P_n \ln P_n \tag{15.42}$$

Some authors (such as Feynman) actually take the last formula as the definition for the entropy. This definition is also closely related to information theory definition of entropy (see Shannon).

## 15.5 Path integral formulation of quantum statistical mechanics

There is a simple and suggestive formula for the partition function (and in view of the preceding subsection, thus for all thermodynamic quantities) in terms of the Euclidean path integral. The correspondence between the Boltzmann operator $e^{-\beta H}$ and the Euclidean evolution operator $e^{-\tau_\beta H/\hbar}$ is fully brought out by the equality

$$\hbar\beta = \tau_\beta \tag{15.43}$$

The trace, needed for the partition function, may be expressed as an integral over $q$,

$$Z = \mathrm{Tr}\, e^{-\beta H} = \int dq \, \langle q | e^{-\beta H} | q \rangle \tag{15.44}$$

The general matrix elements of the Boltzmann operator may now be expressed using the Euclidean path integral,

$$\langle q'|e^{-\beta H}|q\rangle = \int \mathcal{D}q \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\, L_E(q,\dot{q})\right\} \tag{15.45}$$

subject to the boundary conditions,

$$
\begin{aligned}
q(0) &= q \\
q(\hbar\beta) &= q'
\end{aligned}
\tag{15.46}
$$

Here, $L_E$ is the Euclidean Lagrangian corresponding to the Hamiltonian $H$. To complete the construction of the partition function, we need to set $q' = q$ and then integrate over all $q$. But this instruction simply means that we should integrate in the path integral over all functions $q(\tau)$ which are periodic in $\tau$ with period $\hbar\beta$. Thus, we arrive at the following final formula for the partition function,

$$Z = \int \mathcal{D}q \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\, L_E(q,\dot{q})\right\} \qquad q(\hbar\beta) = q(0) \tag{15.47}$$

and it is understood that the actual value of $q(\hbar\beta) = q(0)$ is also integrated over, as part of the functional integral $\int \mathcal{D}q$.

## 15.6  Classical Statistical Mechanics as the high temperature limit

In the large $T$ (equivalently, small $\beta$) limit, many quantum states are occupied, and the system is expected to behave classically. It is possible to recover this limit from the general path integral formula given above. We carry out the limit here as an illustration of path integral methods.

In the limit $\beta \to 0$, the interval of periodicity of $q(\tau)$ becomes small. It is useful to decompose $q(\tau)$ in an orthonormal basis of periodic functions on the interval $[0, \hbar\beta]$,

$$q(\tau) = \sum_{n=-\infty}^{+\infty} c_n\, e^{2\pi i n\tau/(\hbar\beta)} \qquad\qquad c_n^* = c_{-n} \tag{15.48}$$

The *reality condition* $c_n^* = c_{-n}$ is needed to guarantee that the functions $q(\tau)$ be real. The *thermal* or *Matsubara frequencies*

$$\omega_n = \frac{2\pi n}{\hbar\beta} \tag{15.49}$$

govern the magnitude of the kinetic terms in $L_E$. When $\beta \to 0$, the frequencies $\omega_n$ become large as long as $n \neq 0$. The frequency $\omega_0$ vanishes for all $\beta$ and requires zero cost in kinetic energy for this mode. Thus, the kinetic energy will suppress all the modes with $n \neq 0$, and only the mode $n = 0$ will survive at high temperature. We shall denote this mode by $c_0 = q$. As a result,

$$Z(\beta \to 0) = \int_{-\infty}^{+\infty} dq\, e^{-\beta V(q)} \int \mathcal{D}'q \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\, \frac{1}{2}m\dot{q}^2\right\} \tag{15.50}$$

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The contribution of the second factor is being kept as a subdominant effect, which may be evaluated since it corresponds to the partition function of the free particle. Here, $\mathcal{D}'q$ stands for the instruction that the constant mode corresponding to $c_0$ has to be removed from this integration. In terms of the Fourrier component modes, this measure is given by

$$\mathcal{D}'q = \prod_{n \neq 0} dc_n \tag{15.51}$$

We then have

$$\int \mathcal{D}'q \exp\left\{ -\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \, \frac{1}{2} m\dot{q}^2 \right\} = \sqrt{\frac{m}{2\pi\hbar^2\beta}} \tag{15.52}$$

Comparing with the partition function of classical statistical mechanics,

$$Z_{\text{classical}} = \iint dp\,dq \, e^{-\beta H(q,p)} = \int_{-\infty}^{+\infty} dq \, e^{-\beta V(q)} \int_{-\infty}^{+\infty} dp \, e^{-\beta p^2/(2m)} \tag{15.53}$$

we find that

$$Z(\beta \to 0) = \frac{1}{\sqrt{2\pi^2\hbar^2}} Z_{\text{classical}} \tag{15.54}$$

The constant factor merely reflects an unphysical overall normalization. It implies that the classical free energy differs from the quantum one by a constant shift, which is physically unobservable.

# 16  Mixtures and Statistical Entropy

In this section, the notion of statistically mixed ensembles, of pure and mixed states, of coherent and incoherent superpositions are introduced and the corresponding formalism of the *density operator* or equivalently, of the *density matrix* is developed.

## 16.1  Polarized versus unpolarized beams

In chapter 2, we introduced the interference properties of quantum mechanics using the physical examples of the polarization states of light or of a spin $1/2$ particle. In any of these set-ups, the first piece of apparatus used was always a polarizer, which was responsible for filtering a definite polarization out of an unpolarized beam. We have then obtained a complete mathematical description of the polarized beam in terms of vectors in a Hilbert space of states. In particular, a *polarized beam* of light should be viewed as an ensemble of photons which are all in the same quantum state. Similarly, a polarized beam of Silver atoms in the Stern-Gerlach experiment should be viewed as an ensemble of spins which are all in the same quantum state. In each case, the quantum state of all particles in the beam are identical to one another. The phases of the various individual photons are all the same, and the ensemble of states in the beam is said to be *coherent*.

What we have not yet given is a mathematical description for a beam which is unpolarized (or partially polarized). The defining property of an unpolarized beam of light is as follows. We consider a beam propagating in the $z$-direction, and insert a (perfect) polarizer transverse to the beam at an angle $\theta$ with respect to the $x$-axis. Next, we measure the probability $P_\theta$ for observing photons as a function of the angle $\theta$. (Recall that for a beam polarized in the $x$-direction, we have $P_\theta = \cos^2\theta$.) The beam is *upolarized* provided the probability $P_\theta$ is *independent of the angle* $\theta$.

Analogously, the defining property of an *unpolarized beam of spin 1/2 particles* is as follows. Take a beam propagating in the $x$-direction, and insert a Stern-Gerlach apparatus oriented in a direction $\mathbf{n}$ where $\mathbf{n}^2 = 1$. Next, we measure the probability $P_\mathbf{n}$ for observing the spins in the quantum state $\mathbf{n} \cdot \mathbf{S} = +\hbar/2$ as a function of $\mathbf{n}$. (Recall that for a beam of spins with $S_z = +\hbar/2$, this probability is $n_z^2$.) The beam is *unpolarized* provided the probability for observing $\mathbf{n} \cdot \mathbf{S} = +\hbar/2$ is $P_\mathbf{n} = 1/2$ *for any angle* $\mathbf{n}$.

An unpolarized beam cannot be described mathematically as a state in Hilbert space. We can easily see why for the spin $1/2$ case, for example. If the unpolarized beam did correspond to a state $\Psi\rangle$ in Hilbert space, then measuring the probability for observing the spins in a quantum state with $\mathbf{n} \cdot \mathbf{S} = +\hbar/2$ would amount to

$$P_\mathbf{n} = |\langle \mathbf{n}|\Psi\rangle|^2 \tag{16.1}$$

where $|\mathbf{n}\rangle$ is the $+\hbar/2$ eigenstate of $\mathbf{n}\cdot\mathbf{S}$. If $|\Psi\rangle$ is a state in this same 2-dimensional Hilbert space, then we may decompose it onto the basis $|\pm\rangle$ as well, $|\Psi\rangle = a|+\rangle + b|-\rangle$, with $|a|^2 + |b|^2 = 1$. Using the result of Problem 1 in Problem set 2 of 221A, every unit vector $\mathbf{n}$ corresponds to a unitary rotation $U(\mathbf{n})$ in Hilbert space, $\mathbf{n} \cdot \mathbf{S} = U(\mathbf{n})S_z U^\dagger(\mathbf{n})$, so that the eigenstate $|\mathbf{n}\rangle$ of $\mathbf{n} \cdot \mathbf{S}$ with eigenvalue $+\hbar/2$ is concretely given by $|\mathbf{n}\rangle = U(\mathbf{n})|+\rangle$. Parametrizing $\mathbf{n}$ by Euler angles, $\theta, \psi$, we

get, up to an immaterial overall phase,

$$|\mathbf{n}\rangle = \cos\theta\, e^{i\psi}|+\rangle + \sin\theta\, e^{-i\psi}|-\rangle \tag{16.2}$$

so that

$$P_{\mathbf{n}} = \left| a\cos\theta\, e^{-i\psi} + b\sin\theta\, e^{i\psi} \right|^2 \tag{16.3}$$

Demanding that the probability be independent of $\mathbf{n}$ is tantamount to demanding that it be independent of $\theta$ and $\psi$. Evaluating it for $\alpha = 0, \pi/2$ gives $|a| = |b|$, so that we may set $a = |a|e^{i\alpha}$ and $b = |a|e^{i\beta}$, so that

$$P_{\mathbf{n}} = |a|^2 \left| \cos\theta + \sin\theta\, e^{2i\psi + i\beta - i\alpha} \right|^2 = |a|^2 \tag{16.4}$$

which requires $|a|^2 \cos(2\psi + \beta - \alpha) = 0$, for all $\psi$. This is possible only if $|a| = 0$, but then we would have $|a|^2 + |b|^2 = 0$, which contradicts the normalization of the state. We conclude that an unpolarized beam cannot be described mathematically by a state in Hilbert space.

## 16.2   The Density Operator

A new mathematical tool is needed to describe the particles in both polarized, unpolarized and partially polarized beams. This formalism was introduced by John von Neumann in 1927, and the key object is referred to traditionally referred to as the *density operator*, but it is actually more accurate to designate it as the *state operator*, since this object will characterize a state of a quantum system.

A *pure ensemble*, by definition, is a collection of physical systems such that every member of the ensemble is characterized by the same element $|\psi\rangle$ in Hilbert space.

A *mixed ensemble*, by definition, is a collection of physical systems such that a fraction of the members is characterized by a pure state $|\psi_1\rangle$, another fraction of the members is characterized by a pure state $|\psi_2\rangle$, and so on. We shall assume that each pure state ket $|\psi_i\rangle$ is normalized. Thus, a mixed ensemble is characterized by a number $N$ of pure states, $|\psi_i\rangle$ for $i = 1, \cdots, N$. Each pure state $|\psi_i\rangle$ enters into the mixed state with a *population fraction $w_i \geq 0$*, which quantitatively indicates the proportion of state $|\psi_i\rangle$ in the mixture. The population fractions are normalized by

$$\sum_{i=1}^{N} w_i = 1 \tag{16.5}$$

A mixture is an *incoherent superposition of pure states* which means that all relative phase information of the pure states must be lost in the mixture. This is achieved by superimposing, not the states $|\psi_i\rangle$ in Hilbert space, but rather the projection operators $|\psi_i\rangle\langle\psi_i|$ associated with each pure state. The *density operator* $\rho$ for an ensemble of $N$ pure states $|\psi_i\rangle$ incoherently superimposed with population fractions $w_i$ is defined by

$$\rho = \sum_{i=1}^{N} |\psi_i\rangle w_i \langle\psi_i| \tag{16.6}$$

Since the superpositions involved here are incoherent, the weights $w_i$ may be thought of as classical probability weights assigned to each population. Note that *we do not require that the various different pure states $|\psi_i\rangle$ be orthogonal to one another*, since it should certainly be possible to superimpose pure states which are not orthogonal to one another.

The following properties of the density operator immediately result,

1. Self-adjointness : $\rho^\dagger = \rho$;

2. Unit trace : $\mathrm{Tr}(\rho) = 1$;

3. Non-negative : $\langle \psi | \rho | \psi \rangle \geq 0$ for all $|\psi\rangle \in \mathcal{H}$.

Conversely, any operator in $\mathcal{H}$ with the above three properties is of the form of (16.6) with normalization (16.5), but some subtleties must be noted. Self-adjointness guarantees that $\rho$ can be diagonalized in an orthonormal basis $|\phi_i\rangle$, with real eigenvalues $p_i$,

$$\rho = \sum_i |\phi_i\rangle p_i \langle \phi_i| \tag{16.7}$$

Non-negativity then implies that $p_i \geq 0$ for all $i$, and unit trace forces

$$\sum_i p_i = 1 \tag{16.8}$$

Note that $|\phi_i\rangle$ need not coincide with $|\psi_i\rangle$, not even up to a phase, and $p_i$ need not coincide with $w_i$. Thus, a given density operator will have several equivalent representations in terms of pure states. We shall now illustrate this phenomenon by some examples.

Pure states are also described by the density operator formalism. A pure state $|\psi_j\rangle$ corresponds to the case where the mixture actually consists of only a single pure state, $w_j = 1$, and $w_i = 0$ for all $i \neq j$. In that case, $\rho^2 = \rho$, so that the density operator is a projection operator, namely onto the pure state $|\psi_j\rangle$. Conversely, a density operator $\rho$ (i.e. an operator which satisfies the above three properties) which is also a projection operator $\rho^2 = \rho$ correspond to a pure state. It is easiest to show this in the orthonormal representation of $\rho$ derived in (16.7). The condition $\rho^2 = \rho$ then implies

$$\sum_i |\phi_i\rangle p_i(p_i - 1)\langle \phi_i| = 0 \tag{16.9}$$

As a result, we must have $p_i(p_i - 1) = 0$ for all $i$, so that either $p_i = 0$ or $p_i = 1$. The normalization condition (16.77) then implies that $p_i$ can be equal to 1 only for exactly a single pure state. Note that the density operator is an economical way to describe pure states, since the normalization of the states, and the omission of the overall phase have automatically been incorporated.

### 16.2.1 Ensemble averages of expectation values in mixtures

In a pure normalized state $|\psi\rangle$, we defined the *expectation value of an observable A* by the matrix element $\langle\psi|A|\psi\rangle = \mathrm{Tr}\big(A|\psi\rangle\langle\psi|\big)$, a quantity that gives the quantum mechanical weighed probability average of the eigenvalues of $A$.

In a mixed state, these quantum mechanical expectation values must be further weighed by the population fraction of each pure state in the mixture. One defines the *ensemble average* of the observable $A$ by

$$
\begin{aligned}
\mathrm{Tr}(\rho A) &= \sum_i \mathrm{Tr}\big(A|\psi_i\rangle w_i\langle\psi_i|\big) \\
&= \sum_i w_i\langle\psi_i|A|\psi_i\rangle
\end{aligned}
\tag{16.10}
$$

It follows from the properties of the density operator that the ensemble average of any self-adjoint operator is real.

### 16.2.2 Time evolution of the density operator

Any quantum state $|\psi(t)\rangle$ in the Schrödinger picture evolves in time under the Schrödinger equation,

$$
i\hbar\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle
\tag{16.11}
$$

Assuming that the population fractions $w_i$ and $p_i$ do not change in time during this evolution, the density operator $\rho(t)$ then obeys the following time evolution equation,

$$
i\hbar\frac{d}{dt}\rho(t) = [H, \rho(t)]
\tag{16.12}
$$

To prove this formula, one first derives the time evolution equation for $|\psi(t)\rangle\langle\psi(t)|$ and then takes the weighed average with the time-indepenent population fractions. This time evolution may be solved for in terms of the unitary evolution operator $U(t) = e^{-itH/\hbar}$, by

$$
\rho(t) = U(t)\rho(0)U(t)^\dagger
\tag{16.13}
$$

Notice that the normalization condition $\mathrm{Tr}(\rho) = 1$ is automatically preserved under time evolution.

## 16.3 Example of the two-state system

Consider the two-state system of a spin $1/2$, expressed in the eigenbasis of $S^z$, given by the states $|\mathbf{z}+\rangle$ and $|\mathbf{z}-\rangle$. Below are three examples of the density matrix evaluated for pure states.

- Polarized along the $S^z$ direction with eigenvalue $+\hbar/2$, the state is $|\mathbf{z}+\rangle$, and the corresponding density operator is $\rho = |\mathbf{z}+\rangle\langle\mathbf{z}+|$. The ensemble averages are $\mathrm{tr}(\rho S^x) = \mathrm{tr}(\rho S^y) = 0$, and $\mathrm{tr}(\rho S^z) = +\hbar/2$.

- Polarized along the $S^z$ direction with eigenvalue $-\hbar/2$, the state is $|\mathbf{z}-\rangle$, and the corresponding density operator is $\rho = |\mathbf{z}-\rangle\langle \mathbf{z} - |$.

- Polarized along the $S^x$ direction with eigenvalue $\pm\hbar/2$, the state is $|\mathbf{x}\pm\rangle = (|\mathbf{z}+\rangle\pm|\mathbf{z}-\rangle)/\sqrt{2}$, and the corresponding density operator is $\rho = (|\mathbf{z}+\rangle \pm |\mathbf{z}-\rangle)(\langle \mathbf{z} + | \pm \langle \mathbf{z} - |)/2$.

From these pure states, we construct mixed states, and their associated density operators. First, we compute the density operators for unpolarized mixtures. Mixing 50% of $|\mathbf{z}+\rangle$ and 50% of $|\mathbf{z}-\rangle$ states produces the density matrix

$$
\begin{aligned}
\rho &= \frac{1}{2}|\mathbf{z}+\rangle\langle \mathbf{z} + | + \frac{1}{2}|\mathbf{z}-\rangle\langle \mathbf{z} - | \\
&= \frac{1}{2}I
\end{aligned}
\tag{16.14}
$$

Mixing 50% of $|\mathbf{x}+\rangle$ and 50% of $|\mathbf{x}-\rangle$ states produces the density matrix

$$
\begin{aligned}
\rho &= \frac{1}{2}|\mathbf{x}+\rangle\langle \mathbf{x} + | + \frac{1}{2}|\mathbf{x}-\rangle\langle \mathbf{x} - | \\
&= \frac{1}{4}\Big(|\mathbf{z}+\rangle + |\mathbf{z}-\rangle\Big)\Big(\langle \mathbf{z} + | + \langle \mathbf{z} - |\Big) + \frac{1}{4}\Big(|\mathbf{z}+\rangle - |\mathbf{z}-\rangle\Big)\Big(\langle \mathbf{z} + | - \langle \mathbf{z} - |\Big) \\
&= \frac{1}{2}I
\end{aligned}
\tag{16.15}
$$

We see that equal mixture of $|\mathbf{z}\pm\rangle$ states produce the same quantum mechanical state as the equal mixture of $|\mathbf{x}\pm\rangle$ states. This is good new, because after all, we aimed at constructing a characterization of an unpolarized beam. The ensemble averages of $\mathbf{S}$ all vanish $\mathrm{tr}(\rho \mathbf{S}) = 0$ in the unpolarized state.

Finally, let us derive the density matrix for the mixture of 50% of $|\mathbf{z}+\rangle$ and 50% of $|\mathbf{x}+\rangle$ pure states,

$$
\rho = \frac{1}{2}|\mathbf{z}+\rangle\langle \mathbf{z} + | + \frac{1}{2}|\mathbf{x}+\rangle\langle \mathbf{x} + | = \begin{pmatrix} \frac{3}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} \end{pmatrix}
\tag{16.16}
$$

Even though the pure states $|\mathbf{z}+\rangle$ and $|\mathbf{x}+\rangle$ are not orthogonal to one another, the resulting density matrix is perfectly fine. The eigenvalues of $\rho$ are $(2\pm\sqrt{2})/4$ and represent the population fractions in an orthonormal basis. The ensemble averages are $\mathrm{tr}(\rho S^x) = \hbar/4$, $\mathrm{tr}(\rho S^y) = 0$, and $\mathrm{tr}(\rho S^z) = \hbar/4$, indicating that the mixture is partially polarized.

The most general density matrix for the two-state system may be constructed by solving for its axioms one by one. Hermiticity of a $2 \times 2$ matrix $\rho$ allows us to put it in the following

$$
\rho = \frac{1}{2}\Big(a_0 I + a_1\sigma^1 + a_2\sigma^2 + a_3\sigma^3\Big) = \frac{1}{2}\Big(a_0 I + \mathbf{a}\cdot\sigma\Big)
\tag{16.17}
$$

where $\sigma^{1,2,3}$ are the three Pauli matrices, and $a_0, a_1, a_2, a_3$ are real. The unit trace condition forces $a_0 = 1$. Finally, positivity of the the matrix is equivalent to positivity of its eigenvalues. Since

$\text{tr}(\rho) = 1$, at least one of the eigenvalues must be positive. The sign of the other eigenvalue is then determined by the sign of $\det(\rho)$, since this is just the product of the two eigenvalues. The determinant is readily computed, and we find,

$$\det(\rho) = \frac{1}{4}(1 - \mathbf{a}^2) \tag{16.18}$$

Thus, positivity of the eigenvalues will be guaranteed by

$$\rho = \frac{1}{2}\Big(I + \mathbf{a} \cdot \sigma\Big) \qquad\qquad |\mathbf{a}| \leq 1 \tag{16.19}$$

This space is referred to as the *Bloch ball*, parametrized by $|\mathbf{a}| \leq 1$. Pure states, for which $\rho$ is a rank 1 projection operator, precisely correspond to the boundary $|\mathbf{a}| = 1$ sphere, called the *Bloch sphere*. On the other hand, any density operator with $|\mathbf{a}| < 1$ corresponds to a mixed state. The state is unpolarized $|\mathbf{a}| = 0$, and partially polarized for $0 < |\mathbf{a}| < 1$. This gives a geometrical presentation of the space of density matrices for the two-state system.

## 16.4  Non-uniqueness of state preparation

The set of all density operators for a given system forms a *convex set*. Thus, if $\rho_1$ and $\rho_2$ are two arbitrary density operators, then the operator

$$\rho(\lambda) = \lambda\rho_1 + (1 - \lambda)\rho_2 \tag{16.20}$$

is again a density operator for any $\lambda$ such that $0 \leq \lambda \leq 1$. This is shown by verifying that $\rho(\lambda)$ indeed satisfies the three defining properties of a density operator.

The physical interpretation of this property leads to one of the key distinctions between classical and quantum information theory. Consider an experimental set up where the system may be prepared either in the state associated with $\rho_1$ or in the state corresponding to $\rho_2$. We assign a probability $\lambda$ that the system be prepared in state $\rho_1$ and a probability $1 - \lambda$ that it be prepared in state $\rho_2$. The ensemble average of the expectation value of any observable $A$ is then obtained by taking the quantum mechanical expectation value, weighted by the probabilities for preparation either in state $\rho_1$ or in state $\rho_2$,

$$\langle A \rangle = \lambda\text{tr}(\rho_1 A) + (1 - \lambda)\text{tr}(\rho_2 A) = \text{tr}\Big(\rho(\lambda)A\Big) \tag{16.21}$$

Thus, the expectation value of any observable are indistinguishable from what we would obtain if they had been computed directly in the state $\rho(\lambda)$. In fact, our two-state example of the preceding subsection illustrated already this property. The totally unpolarized density operator could have been gotten either by equal populations of $S_z = \pm\hbar/2$, or equal populations of $S_x = \pm\hbar/2$, and in the final state, you could never tell the difference. Clearly, for any mixed state, there would be an infinite number of different ways of preparing the state, unless the state was actually pure and then there is only a single way. For the sake of completeness, we note that if the eigenvalues of $\rho$ are distinct, then there is a *unique way of preparing the system in terms mutually orthogonal density operators*, but allowing for non-orthogonal density operators, the preparation is again not unique.

This situation is to be contrasted with the preparation of a classical ensemble, which is unique, given the probabilities.

## 16.5　Quantum Statistical Mechanics

One particularly important special case of mixed states and ensembles is provided by equilibrium quantum statistical mechanics. Consider a system described by a time independent Hamiltonian $H$, whose eigenstates and eigenvalues will be denoted by $|E_n; \alpha\rangle$ and $E_n$ respectively. Here $\alpha$ stands for additional quantum numbers which characterize different states at the same energy $E_n$. The states $|E_n; \alpha\rangle$ will be assumed to be orthonormal. Already in Chapter 8 have we introduced the standard statistical mechanical quantities such as the partition function $Z$, and the Boltzmann weight $p_n$ of a state with energy $E_n$, given by

$$
\begin{aligned}
Z &= \text{Tr}\left(e^{-\beta H}\right) \qquad\qquad \beta = \frac{1}{k_B T} \\
p_n &= \frac{e^{-\beta E_n}}{Z}
\end{aligned}
\tag{16.22}
$$

From the Boltzmann weights, we can now compute the density operator,

$$
\rho = \sum_{n,\alpha} |E_n; \alpha\rangle p_n \langle E_n; \alpha|
\tag{16.23}
$$

Using the fact that in the orthonormal basis $|E_n; \alpha\rangle$ we have,

$$
\sum_{n,\alpha} |E_n; \alpha\rangle e^{-\beta E_n} \langle E_n; \alpha| = e^{-\beta H}
\tag{16.24}
$$

the density operator takes on a particularly simple form,

$$
\rho = \frac{e^{-\beta H}}{\text{Tr}\left(e^{-\beta H}\right)}
\tag{16.25}
$$

This expression makes the defining properties of the density operator manifest; it is self-adjoint, since $H$ is; it has unit trace; and it is non-negative since $H$ is self-adjoint and has only real eigenvalues. Other thermodynamic quantities similarly have simple expressions. The internal energy is the ensemble average of the Hamiltonian,

$$
E = \frac{1}{Z} \sum_{n,\alpha} E_n \, e^{-\beta E_n} = \text{Tr}(\rho E)
\tag{16.26}
$$

Similarly, the entropy is given by

$$
S = -k_B \sum_{n,\alpha} p_n \ln p_n = -k_B \text{Tr}\left(\rho \ln \rho\right)
\tag{16.27}
$$

In fact, one may take the entropy as the starting point for thermodynamics, and then use it to derive the Boltzmann distribution. Working in the canonical ensemble, one keeps the energy fixed and maximizes the entropy given this constraint. The standard way of doing this in practice is to

introduce Lagrange multipliers for the constant energy condition, as well as for the condition of unit trace of $\rho$. Thus, we extremize, as a function of $\rho$, the quantity

$$-\text{Tr}\left(\rho \ln \rho\right) - \beta \text{Tr}(\rho H) - \gamma \text{Tr}(\rho) \tag{16.28}$$

under the condition that

$$\text{Tr}(\rho) = 1 \tag{16.29}$$

The corresponding equation reads,

$$\text{Tr}\delta\rho\left(-\ln \rho - I - \beta H + \gamma I\right) = 0 \tag{16.30}$$

The operator in parentheses is self-adjoint, and the variations $\delta\rho$ of $\rho$ are also self-adjoint. Thus, if the above variational equation is to hold for arbitrary self-adjoint variations $\delta\rho$, we must have

$$\ln \rho = -\beta H + \text{constant} \times I \tag{16.31}$$

Enforcing now the unit trace condition guarantees that we recover (16.25), and that $\beta$ is indeed related to temperature as given above.

### 16.5.1 Generalized equilibrium ensembles

The derivation of the Boltzmann weights and associated density matrix corresponds to the canonical ensemble, in which only the energy of the system is kept constant. In the grand canonical ensemble, both the energy and the number of particles in the system is kept constant. More generally, we consider an ensemble in which the ensemble average of a number of commuting observables $A_i$, $i = 1, \cdots, K$ is kept constant. To compute the associated density operator $\rho$ of this ensemble, we extremize with respect to variations in $\rho$ the entropy, under the constraint that the ensemble averages $\text{Tr}(\rho A_i)$ are kept constant. Using again Lagrange multipliers $\beta_i$, $i = 1, \cdots, K$, we extremize

$$-\text{Tr}\left(\rho \ln \rho\right) - \sum_{i=1}^{K} \beta_i \text{Tr}(\rho A_i) \tag{16.32}$$

Upon enforcing the normalization $\text{Tr}(\rho) = 1$, this gives,

$$\begin{aligned}
\rho &= \frac{1}{Z} \exp\left\{-\sum_{i=1}^{K} \beta_i A_i\right\} \\
Z &= \text{Tr}\left(\exp\left\{-\sum_{i=1}^{K} \beta_i A_i\right\}\right)
\end{aligned} \tag{16.33}$$

In the grand canonical ensemble, for example, these quantities are

$$\begin{aligned}
\rho &= \frac{1}{Z} e^{-\beta H - \mu N} \\
Z &= \text{Tr}\left(e^{-\beta H - \mu N}\right)
\end{aligned} \tag{16.34}$$

where $N$ is the number operator and $\mu$ is the chemical potential. Other observables whose ensemble averages are often kept fixed in this way are electric charge, baryon number, electron number etc.

## 16.6 Classical information and Shannon entropy

Entropy may be given a meaning beyond traditional statistical mechanics. In developing a theory of classical (non-quantum mechanical) information, Claude Shannon was led to a generalized notion of entropy that characterizes the amount of *missing information* for a given ensemble. In the case of information theory, the ensembles consist of messages, sent in words and sentences. To make contact with the previous sections, a message may be viewed as a mixture of a certain number of letters and words.

Consider an ensemble with $n$ possible outcomes, for example, by the number of different letters or words in a text. A probability $p_i$ is assigned to each outcome $i = 1, \cdots, n$, and total probability is normalized to 1. This assignment of probabilities characterizes a *macro-state*. The *statistical or Shannon entropy* associated with this macro-state is defined by

$$S(p_1, \cdots, p_n) = -k \sum_{i=1}^{n} p_i \ln p_i \qquad\qquad \sum_{i=1}^{n} p_i = 1 \qquad (16.35)$$

Here, $k$ is a positive constant. For statistical mechanics, $k$ is the Boltzmann constant, but in information theory, one usually sets $k = 1$.

Shannon derived this formula from a number of simple basic assumptions. Here, we shall contents ourselves by arguing that the formula follows from a *large numbers approach* to the possible outcomes in a message. Suppose we have a message of length $N$ formed out of $n$ different letters $a_i$, $i = 1, \cdots, n$. We consider this problem in the limit where $N \gg n$. A message then takes the form

$$\ell_1 \, \ell_2 \, \ell_3 \, \cdots \, \ell_N \qquad (16.36)$$

Since the probability $p_i$ for the letter $i$ to occur in this message is given, we expect the letter $i$ to occur $p_i N$ times. The number $\Omega$ of distinct messages with this assignment of letters gives a quantitative measure of the amount of *missing information*. Namely, if you are given the information that the message contains the letter $i$ precisely $p_i N$ times, the more possible messages there are, the more information is lacking. This number $\Omega$ of possible messages is also referred to as the number of *micro-states* corresponding to a given probability assgnment.

With this mixture of letters, and the assumption that the occurrence of the letters in the message is uncorrelated, $\Omega$ is given by the multinomial coefficient. To make contact with the statistical entropy formula, we take its logarithm,

$$\ln \Omega = \ln \left( \frac{N!}{(p_1 N)!(p_2 N)! \cdots (p_n N)!} \right) \qquad (16.37)$$

Since $N \gg 1$, we can use the Sterling formula to approximate the factorial, $\ln k! = k(\ln k - 1)$, and we get

$$\begin{aligned} \ln \Omega &= N(\ln N - 1) - \sum_{i=1}^{n} (p_i N)\Big( \ln(p_i N) - 1 \Big) \\ &= -N \sum_{i=1}^{n} p_i \ln p_i \end{aligned} \qquad (16.38)$$

Thus, the logarithm of the number of micro-states $\Omega$ is an extensive quantity, proportional to the length $N$ of the message. The statistical entropy is the corresponding intensive quantity, up to a multiplicative factor.

Some basic properties of the statistical entropy are as follows.

1. Positivity, $S(p_1, \cdots, p_n) \geq 0$;

2. The minimum is $S = 0$, attained when all probability assignments are 0, except for a single entry $p_j = 1$;

3. The maximum is attained when all probabilities are equal, $p_i = 1/n$, giving $S_{\max} = \ln n$.

## 16.7  Quantum statistical entropy

A quantum mechanical macro-state is characterized by the density operator $\rho$. The state may be obtained as an incoherent mixture of *orthogonal* pure states $|\phi_i\rangle$, with population fractions $p_i$, so that

$$\rho = \sum_i |\phi_i\rangle p_i \langle \phi_i| \qquad\qquad \sum_i p_i = 1 \qquad\qquad (16.39)$$

The population fractions $p_i$ may be measured *simultaneously* by the commuting (actually orthogonal) observables $\mathcal{P}_i = |\phi_i\rangle\langle\phi_i|$. Thus, the $p_i$ may be viewed essentially as classical probabilities, and the statistical entropy may be generalized immediately,[14]

$$S(\rho) = -k\mathrm{Tr}\Big(\rho\ln\rho\Big) \qquad\qquad (16.40)$$

Here again, $k$ is a positive constant, left arbitrary in information theory, but equal to Boltzmann's constant $k_B$ for statistical mechanics. This is the statistical entropy for a macro-state specified by the density operator $\rho$, and is sometimes referred to as the von Neumann entropy.

Some fundamental properties of the statistical entropy are given as follows,

1. **Positivity**, $S(\rho) \geq 0$;

2. **Minimum** is $S(\rho) = 0$ attained if and only if $\rho$ is a projection operator and thus corresponds to a pure state;

3. **Maximum** is attained as follows. If the possible probabilities are non-zero for a subspace $\mathcal{H}_n \subset \mathcal{H}$ of finite dimension $n$, then the maximum entropy is $S_{\max} = k\ln n$;

4. **Invariance** under conjugation of the density operator by a unitary transformation. In particular, the entropy is invariant under time evolution, under the assumption that the population fractions remain unchanged in time;

---

[14]Note that when the density matrix is written as a weighted sum involving non-orthogonal states as in (16.6), the weights $w_i$ cannot be measured simultaneously, as the corresponding states are not orthogonal. Thus, the entropy is *not equal* to the replacement $p_i \to w_i$.

5. **Additivity** upon combination of two subsystems which are *statistically uncorrelated*. Let the systems be described by Hilbert spaces $\mathcal{H}_a$ and $\mathcal{H}_b$, with density operators $\rho_a$ and $\rho_b$ respectively, then the full Hilbert space is $\mathcal{H}_{ab} = \mathcal{H}_a \otimes \mathcal{H}_b$ and the density matrix for the combined system is $\rho_{ab} = \rho_a \otimes \rho_b$. The entropy is then additive,

$$S(\rho_{ab}) = S(\rho_a) + S(\rho_b) \tag{16.41}$$

6. **Subadditivity** upon dividing a system with Hilbert space $\mathcal{H}_{ab}$ and density operator $\rho_{ab}$ into two subsystems with Hilbert spaces $\mathcal{H}_a$ and $\mathcal{H}_b$, and density matrices $\rho_a$ and $\rho_b$ which are *statistically correlated*. The full density operator $\rho_{ab}$ is *not the tensor product of $\rho_a$ and $\rho_b$*, in view of the non-trivial statistical correlations between the two subsystems. Instead, one only has an inequality,

$$S(\rho_{ab}) \leq S(\rho_a) + S(\rho_b) \tag{16.42}$$

with equality being attained iff there are no statistical correlations and $\rho_{ab} = \rho_a \otimes \rho_b$.

7. **Strong subadditivity** upon dividing a system with density operator $\rho_{abc}$ into three subsystems with density operators $\rho_a$, $\rho_b$, and $\rho_c$, and their pairwise combinations with density operators $\rho_{ab}$, $\rho_{bc}$, and $\rho_{ac}$, the entropy satisfies

$$S(\rho_{abc}) + S(\rho_b) \leq S(\rho_{ab}) + S(\rho_{bc}) \tag{16.43}$$

or any rearrangement thereof.

8. **Concavity** For $\lambda_1, \lambda_2, \cdots, \lambda_r \geq 0$, and $\lambda_1 + \cdots + \lambda_r = 1$, we have

$$S(\lambda_1 \rho_1 + \cdots + \lambda_r \rho_r) \geq \lambda_1 S(\rho_1) + \cdots + \lambda_r S(\rho_r) \tag{16.44}$$

Properties 1, 2, 3, and 4 are straightforward. To prove property 5, we have to make careful use of the definitions. Each density matrix is normalized,

$$\mathrm{Tr}_{\mathcal{H}_a} \rho_a = \mathrm{Tr}_{\mathcal{H}_b} \rho_b = 1 \tag{16.45}$$

and the corresponding entropies are defined by

$$
\begin{aligned}
S(\rho_a) &= -k \mathrm{Tr}_{\mathcal{H}_a} \left( \rho_a \ln \rho_a \right) \\
S(\rho_b) &= -k \mathrm{Tr}_{\mathcal{H}_b} \left( \rho_b \ln \rho_b \right)
\end{aligned}
\tag{16.46}
$$

The total entropy for the tensor product density operator $\rho_{ab} = \rho_a \otimes \rho_b$ is then given by

$$
\begin{aligned}
S(\rho_{ab}) &= -k \mathrm{Tr}_{\mathcal{H}_a} \mathrm{Tr}_{\mathcal{H}_b} \left( (\rho_a \otimes \rho_b) \ln(\rho_a \otimes \rho_b) \right) \\
&= -k \mathrm{Tr}_{\mathcal{H}_a} \mathrm{Tr}_{\mathcal{H}_b} \left( (\rho_a \otimes \rho_b)(\ln \rho_a \otimes I_b) \oplus (\rho_a \otimes \rho_b)(I_a \otimes \ln \rho_b) \right) \\
&= -k \mathrm{Tr}_{\mathcal{H}_a} \left( \rho_a \ln \rho_a \right) - k \mathrm{Tr}_{\mathcal{H}_b} \left( \rho_b \ln \rho_b \right)
\end{aligned}
\tag{16.47}
$$

which proves the formula of 5. To prove 6, we first prove the following intermediate results.

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### 16.7.1 Density matrix for a subsystem

Let $\mathcal{H}_{ab} = \mathcal{H}_a \otimes \mathcal{H}_b$ be the Hilbert space organized as the tensor product of two subspaces $\mathcal{H}_a$ and $\mathcal{H}_b$. Let $\rho_{ab}$ be the density matrix corresponding to a state of the system. Suppose now that we observe the system with observables that act only on the subsystem $a$. In all generality, such observables are of the form,

$$A = A_a \otimes I_b \tag{16.48}$$

The expectation value of $A$ of this type of operators in the full system reduces in a systematic manner to the expectation value with respect to the density matrix of the subsystem. To see this, we compute the expectation values,

$$
\begin{aligned}
\langle A \rangle &= \mathrm{Tr}_{\mathcal{H}_{ab}}\Big(\rho_{ab} A\Big) = \mathrm{Tr}_{\mathcal{H}_a} \mathrm{Tr}_{\mathcal{H}_b}\Big(\rho_{ab}\,(A_a \otimes I_b)\Big) \\
&= \mathrm{Tr}_{\mathcal{H}_a}\Big(A_a \rho_a\Big)
\end{aligned}
\tag{16.49}
$$

where

$$\rho_a = \mathrm{Tr}_{\mathcal{H}_b}\Big(\rho_{ab}\Big) \tag{16.50}$$

Note that the normalization $\mathrm{Tr}_{\mathcal{H}_a}(\rho_a) = 1$ as a result of the normalization of $\rho_{ab}$. In particular, the population fraction of a pure state $|\psi_a\rangle\langle\psi_a|$ is given by

$$p_a = \mathrm{Tr}_{\mathcal{H}_a}\Big(\rho_a|\psi_a\rangle\langle\psi_a|\Big) = \langle\psi_a|\rho_a|\psi_a\rangle \tag{16.51}$$

### 16.7.2 Example of relations between density matrices of subsystems

It will be helpful to clarify the relations between $\rho_{ab}$, $\rho_a$, $\rho_b$ and the tensor product $\rho_a \otimes \rho_b$ with the help of an example involving two spin $1/2$ systems. We denote the Pauli matrices for these systems respectively by $\sigma_a^i$ and $\sigma_b^i$ where $i = 1, 2, 3$. Consider general density matrices for each subsystem,

$$
\begin{aligned}
\rho_a &= \frac{1}{2}\left(I_a + \vec{a} \cdot \vec{\sigma}_a\right) & |\vec{a}| \leq 1 \\
\rho_b &= \frac{1}{2}\left(I_b + \vec{b} \cdot \vec{\sigma}_b\right) & |\vec{b}| \leq 1
\end{aligned}
\tag{16.52}
$$

The tensor product is given by

$$\rho_a \otimes \rho_b = \frac{1}{4}\Big(I_a \otimes I_b + I_a \otimes (\vec{b} \cdot \vec{\sigma}_b) + (\vec{a} \cdot \vec{\sigma}_a) \otimes I_b + (\vec{a} \cdot \vec{\sigma}_a) \otimes (\vec{b} \cdot \vec{\sigma}_b)\Big) \tag{16.53}$$

Clearly, when we compute the partial traces, we recover the density matrices of the subsystems,

$$
\begin{aligned}
\mathrm{tr}_{\mathcal{H}_a}(\rho_a \otimes \rho_b) &= \rho_b \\
\mathrm{tr}_{\mathcal{H}_b}(\rho_a \otimes \rho_b) &= \rho_a
\end{aligned}
\tag{16.54}
$$

The general density matrix $\rho_{ab}$ of the combined system may be parametrized as follows,

$$\rho_{ab} = \rho_a \otimes \rho_b + \sum_{i,j=1}^{3} C_{ij} \sigma_a^i \otimes \sigma_b^j \tag{16.55}$$

where $C_{ij}$ is an arbitrary $3 \times 3$ real matrix. For any choice of $C_{ij}$, we have

$$\begin{aligned} \text{tr}_{\mathcal{H}_a}(\rho_{ab}) &= \rho_b \\ \text{tr}_{\mathcal{H}_b}(\rho_{ab}) &= \rho_a \end{aligned} \tag{16.56}$$

so that the reduced density matrices $\rho_a$ and $\rho_b$ are independent of $C_{ij}$. Only for $C_{ij} = 0$ is the density matrix $\rho_{ab}$ the tensor product of $\rho_a$ and $\rho_b$.

### 16.7.3   Lemma 1

*For any two density operator $\rho$ and $\rho'$ in the same Hilbert space $\mathcal{H}$, we have the inequality,*

$$S(\rho) \leq -k \text{Tr} \left( \rho \ln \rho' \right) \tag{16.57}$$

*with equality being attained iff $\rho' = \rho$.*

To prove this, we write both density matrices in diagonal form, in orthonormal bases,

$$\begin{aligned} \rho &= \sum_i |\phi_i\rangle p_i \langle \phi_i| \\ \rho' &= \sum_i |\phi_i'\rangle p_i' \langle \phi_i'| \end{aligned} \tag{16.58}$$

The bases $|\phi_i\rangle$ and $|\phi_i'\rangle$ are in general different. We now consider

$$\begin{aligned} S(\rho) + k \text{Tr} \left( \rho \ln \rho' \right) &= -k \sum_i p_i \ln p_i + k \sum_{i,j} p_i \ln p_j' |\langle \phi_i | \phi_j' \rangle|^2 \\ &= k \sum_{i,j} p_i (\ln p_j' - \ln p_i) |\langle \phi_i | \phi_j' \rangle|^2 \end{aligned} \tag{16.59}$$

where we have used the completeness relation $\sum_j |\phi_j'\rangle\langle \phi_j'| = I$ in recasting the simple sum on the first line in the form of a double sum on the last line. Next, we introduce the function

$$f(x) \equiv x - 1 - \ln x \tag{16.60}$$

We set $x = p_j'/p_i$ and recast the above double sum in the following way,

$$S(\rho) + k \text{Tr} \left( \rho \ln \rho' \right) = k \sum_{i,j} p_i \left( 1 - \frac{p_j'}{p_i} - f\left( \frac{p_j'}{p_i} \right) \right) |\langle \phi_i | \phi_j' \rangle|^2 \tag{16.61}$$

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The first two terms on the right hand side simplify as follows,

$$\sum_{i,j}(p_i - p'_j)|\langle\phi_i|\phi'_j\rangle|^2 = \sum_i p_i - \sum_{j'} p_{j'} = 0 \tag{16.62}$$

in view of the completeness relations of the both orthonormal bases. This gives us an expression directly in terms of the function $f$,

$$S(\rho) + k\mathrm{Tr}\left(\rho\ln\rho'\right) = -k\sum_{i,j}p_i f\left(\frac{p'_j}{p_i}\right)|\langle\phi_i|\phi'_j\rangle|^2 \tag{16.63}$$

To derive the lemma, we use the following simple properties of the function $f(x)$,

- $f(1) = 0$;

- $f(x) > 0$ for all $x \geq 0$ and $x \neq 1$.

The first property is obvious, the second may be established from the first by noticing that $f'(x) < 0$ for $0 \leq x < 1$, and $f'(x) > 0$ for $1 < x$. Thus, we have $f(x) \geq 0$ for all $x \geq 0$, and as a result, we have the inequality of the lemma, since in all terms we have $p_i|\langle\phi_i|\phi'_j\rangle|^2 \geq 0$.

To complete the proof of the lemma, we assume that the equality holds. Problems with possible degeneracies of the population fractions force us to be more precise in our analysis. Thus, we shall decompose the density matrices as follows,

$$\rho = \sum_{i=0}^{N} p_i P_i \qquad\qquad \sum_{i=0}^{N} P_i = I$$
$$\rho' = \sum_{i=0}^{N'} p'_i P'_i \qquad\qquad \sum_{i=0}^{N'} P'_i = I \tag{16.64}$$

where we shall now assume that all population fractions $p_i$ and distinct from one another, same for $p'_i$, so that we can order them as follows,

$$p_0 = 0 < p_1 < p_2 < \cdots < p_N$$
$$p'_0 = 0 < p'_1 < p'_2 < \cdots < p'_{N'} \tag{16.65}$$

We shall also assume that each contribution for $i \neq 0$ is non-trivial, in the sense that

$$\begin{aligned} \dim(P_i) &= \mathrm{tr}(P_i) \geq 1 & i \geq 1 \\ \dim(P'_i) &= \mathrm{tr}(P'_i) \geq 1 & i \geq 1 \end{aligned} \tag{16.66}$$

In this notation, the combination of the lemma may be recast in the following form,

$$S(\rho) + k\mathrm{Tr}\left(\rho\ln\rho'\right) = -k\sum_{i,j}\left(p'_j - p_i - p_i\ln\left(\frac{p'_j}{p_i}\right)\right)\mathrm{tr}\left(P_iP'_j\right) \tag{16.67}$$

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The combinations of projectors obeys

$$\text{tr}\left(P_i P_j'\right) \geq 0 \tag{16.68}$$

As a result, every term in the double sum is either positive or zero. The equality in the lemma is achieved if and only if every term separately vanishes for all $i, j$,

$$\left(p_j' - p_i - p_i \ln\left(\frac{p_j'}{p_i}\right)\right) \text{tr}\left(P_i P_j'\right) = 0 \tag{16.69}$$

If $\text{tr}(P_i P_j') \neq 0$, then we must have $p_j' = p_i$, even when $p_i = 0$. Now fix the index $i$, and let $j$ run through $j = 0, 1, 2, \cdots, N'$. If $\text{tr}(P_i P_j') = 0$ for all values $j$, then $\dim(P_i) = 0$, since $P_j'$ span the entire Hilbert space. Thus, we must have $i = 0$, and $\dim(P_0) = 0$, in which case the result is trivial. Thus, for all $i \neq 0$, there must be a unique $j$ such that $\text{tr}(P_i P_j') \neq 0$, and for which $p_i = p_j'$. Reversing the argument, fixing $j$, and letting $i$ run through the values $i = 0, 1, 2, \cdots, N$, we see that every $j \neq 0$, there must be a unique $i$ such that $\text{tr}(P_i P_j') \neq 0$ and $p_j' = p_i$. Given the ordering (16.65) that we assumed, this implies a one-to-one and onto map between the $p_i$ and the $p_i'$, so that $N' = N$. As a result we have

$$\rho = \sum_{i=1}^{N} p_i P_i \qquad\qquad \sum_{i=0}^{N} P_i = I$$
$$\rho' = \sum_{i=1}^{N} p_i P_i' \qquad\qquad \sum_{i=0}^{N} P_i' = I \tag{16.70}$$

where

$$\text{tr}(P_i P_j') \begin{cases} = 0 & j \neq i \\ \neq 0 & j = i \end{cases} \tag{16.71}$$

Finally, using these results, we compute

$$\text{tr}\left(P_i P_i'\right) = \text{tr}P_i - \sum_{j \neq i} \text{tr}(P_i P_j') \tag{16.72}$$

Each term under the sum on the rhs vanishes, so that $\text{tr}\left(P_i(I - P_i')\right) = 0$ As a result, we have $P_i' = P_i$, and thus $\rho' = \rho$, which completes the proof of the lemma.

### 16.7.4 Completing the proof of subadditivity

To complete the proof of 6, we proceed as follows. First, define the density operators of the subsystems $a$ and $b$ by

$$\begin{aligned} \rho_a &= \text{Tr}_{\mathcal{H}_b}(\rho) \\ \rho_b &= \text{Tr}_{\mathcal{H}_a}(\rho) \end{aligned} \tag{16.73}$$

Next, we take $\rho' = \rho_a \otimes \rho_b$, so that

$$
\begin{aligned}
S(\rho_{ab}) \;&\leq\; -k\mathrm{Tr}_{\mathcal{H}_a}\mathrm{Tr}_{\mathcal{H}_b}\Big(\rho(\ln\rho_a \otimes I_b) \oplus \rho(I_a \otimes \ln\rho_b)\Big) \\
&\leq\; -k\mathrm{Tr}_{\mathcal{H}_a}\Big(\rho_a \ln\rho_a\Big) - k\mathrm{Tr}_{\mathcal{H}_b}\Big(\rho_b \ln\rho_b\Big)
\end{aligned}
\tag{16.74}
$$

which proves 6. Properties 7 and 8 may be proven along the same lines of reasoning, and use of the Lemma.

## 16.8   Examples of the use of statistical entropy

We illustrate the property of *subadditivity*, in 6, by considering a pure state of the full system, and then viewing this pure state from the vantage point of a bi-partite subsystem. Thus we view the full Hamiltonian $\mathcal{H}_{ab} = \mathcal{H}_a \otimes \mathcal{H}_b$, and construct the density operator

$$
\begin{aligned}
\rho_{ab} \;&=\; |\psi\rangle \otimes \langle\psi| \\
|\psi\rangle \;&=\; \sum_{\alpha,\beta} C_{\alpha\beta}|\phi_\alpha; a\rangle \otimes |\phi_\beta; b\rangle
\end{aligned}
\tag{16.75}
$$

Here, $|\phi_\alpha; a\rangle$ is an orthonormal basis of $\mathcal{H}_a$ and $|\phi_\beta; b\rangle$ is an orthonormal basis of $\mathcal{H}_b$. Since $\rho_{ab}$ corresponds to a pure state, we clearly have $S(\rho_{ab}) = 0$. By subadditivity, however, we only have and inequality for $S(\rho_a)$ and $S(\rho_b)$,

$$
0 \leq S(\rho_a) + S(\rho_b)
\tag{16.76}
$$

and neither quantity, in general, should be expected to have to vanish. Physically, this result may be interpreted as follows. Even though the full system is in a pure quantum state, the fact that we "average" over subspace $\mathcal{H}_b$ to get $\rho_a$ (and "average" over subspace $\mathcal{H}_a$ to get $\rho_b$) means that the quantum information contained in $\mathcal{H}_b$ has been lost and this translates into a non-zero value of the statistical entropy.

It is instructive to work out the corresponding density operators, and check that they do not, in general, correspond to pure states. We have,

$$
\begin{aligned}
\rho_a \;&=\; \mathrm{Tr}_{\mathcal{H}_b}(\rho_{ab}) = \sum_\beta w_\beta^{(a)}|\psi_\beta; a\rangle \otimes \langle\psi_\beta; a| \\
\rho_b \;&=\; \mathrm{Tr}_{\mathcal{H}_a}(\rho_{ab}) = \sum_\alpha w_\alpha^{(b)}|\psi_\alpha; b\rangle \otimes \langle\psi_\alpha; b|
\end{aligned}
\tag{16.77}
$$

Here, the weights $w_\beta^{(a)}$ and $w_\alpha^{(b)}$ are positive and less or equal to 1, and $|\psi_\beta; a\rangle$, and $|\psi_\alpha; b\rangle$ are normalized pure states, defined by

$$
\begin{aligned}
\left(w_\beta^{(a)}\right)^{\frac{1}{2}}|\psi_\beta; a\rangle &= \sum_\alpha C_{\alpha\beta}|\phi_\alpha; a\rangle & w_\beta^{(a)} &= \sum_\alpha |C_{\alpha\beta}|^2 \\
\left(w_\alpha^{(b)}\right)^{\frac{1}{2}}|\psi_\alpha; b\rangle &= \sum_\beta C_{\alpha\beta}|\phi_\beta; b\rangle & w_\alpha^{(b)} &= \sum_\beta |C_{\alpha\beta}|^2
\end{aligned}
\tag{16.78}
$$

The formulas for the population fractions directly result from the normalization of the pure states $|\psi_\beta; a\rangle$, and $|\psi_\alpha; b\rangle$. Notice that states $|\psi_\beta; a\rangle$ for different values of $\beta$ need not be orthogonal to one another. The above result may be applied to two different physical situations.

### 16.8.1  Second law of thermodynamics

First, suppose we view the entire universe as divided into a certain system $a$, in which we are interested, and the environment $b$ which we do not study directly. The Hilbert space of the entire universe $\mathcal{H} = \mathcal{H} \otimes \mathcal{H}_b$. Suppose $a$ and $b$ interact with one another, for example by exchanging energy. Now, at an initial time $t_0$, we prepare the system $a$ in such a way that it has no statistical correlations with the environment. This is clearly an idealized set-up, which is certainly hard to realize experimentally. But if we assume absence of correlations at time $t_0$, then the density operator of the universe $\rho(t_0)$ is a tensor product,

$$\rho(t_0) = \rho_a \otimes \rho_b \tag{16.79}$$

From the property of additivity of the statistical entropy, we then have

$$S(\rho(t_0)) = S(\rho_a) + S(\rho_b) \tag{16.80}$$

Unitary time evolution of the entire universe implies that at a later time $t > t_0$, we will have

$$S(\rho(t)) = S(\rho(t_0)) \tag{16.81}$$

But the density matrices $\rho_a(t)$ and $\rho_b(t)$ at time $t$ will not be the same as the density matrices $\rho_a = \rho_a(t_0)$ and $\rho_b = \rho_b(t_0)$ respectively. In fact, they will not even be unitary evolutions of these because the Hamiltonian will mix the time evolutions of states in $\mathcal{H}_a$ and $\mathcal{H}_b$, since the system $a$ interacts with the environment. All we can do is use the definition of these density operators,

$$\begin{aligned} \rho_a(t) &= \mathrm{Tr}_{\mathcal{H}_b}(\rho(t)) \\ \rho_b(t) &= \mathrm{Tr}_{\mathcal{H}_a}(\rho(t)) \end{aligned} \tag{16.82}$$

But now, in general, the system at time $t$ will have statistical correlations with its environment $b$, so that the density matrix $\rho(t)$ will no longer be the tensor product of $\rho_a(t)$ and $\rho_b(t)$. As a result, by the subadditivity property of the statistical entropy, we have,

$$S(\rho(t)) \leq S(\rho_a(t)) + S(\rho_b(t)) \tag{16.83}$$

putting this together with (16.80) and (16.81), we obtain,

$$S(\rho_a(t_0)) + S(\rho_b(t_0)) \leq S(\rho_a(t)) + S(\rho_b(t)) \tag{16.84}$$

for times $t > t_0$. We have just derived the second law of thermodynamics, under the assumptions we have advocated: the sum of the entropy of the system and of its environment cannot decrease with time.

### 16.8.2  Entropy resulting from coarse graining

# 17  Entanglement, EPR, and Bell's inequalities

Quantum systems exhibit correlations (entanglement) that appear counter-intuitive from the classical viewpoint. The examination of these questions can be traced back to a 1932 book by von Neumann, but especially to a 1935 paper by Einstein-Podolsky-Rosen (EPR). Both addressed the question as to whether quantum mechanics can be a complete theory of physical phenomena or whether there exists a full theory with extra *hidden variables*. These investigations remained somewhat philosophical until John Bell (1964) derived concrete and experimentally testable predictions (Bell's inequalities) of hidden variables. In the early 1980's, various experiments on the correlations of photon systems by Aspect, Gragnier, and Roger have shown experimental agreement with quantum mechanics, and contradictory to hidden variable theory. Since then, however, entanglement has been explored as a fundamental property of quantum theory, and applied to physical processes, such as quantum computation. Here, we shall concentrate on the basics.

## 17.1  Entangled States for two spin 1/2

Consider the spin degrees of freedom of a two-electron system. In fact, the analysis applies to the tensor product $\mathcal{H}_{ab} = \mathcal{H}_a \otimes \mathcal{H}_b$ of any two-state systems $a$ and $b$, with respective Hilbert spaces $\mathcal{H}_a$ and $\mathcal{H}_b$, in the notation of the preceding section. For any unit vector $\mathbf{n}$, we shall denote the two eigenstates of $\mathbf{n} \cdot \mathbf{S}$ with eigenvalue $\pm \hbar/2$ by $|\mathbf{n}+\rangle$ and $|\mathbf{n}-\rangle$. We use the notation $\mathbf{n} = \mathbf{x}, \mathbf{y}, \mathbf{z}$ for the unit vectors in the direction of the coordinate axes. The tensor product states for the two electrons will be denoted by

$$|\mathbf{n}_a \alpha\rangle \otimes |\mathbf{n}_b \beta\rangle = |\mathbf{n}_a \alpha; \mathbf{n}_b \beta\rangle \qquad\qquad \alpha, \beta = \pm \qquad\qquad (17.1)$$

The state of 0 total spin, or singlet, corresponds to the following combination of the two electron states,

$$|\Phi\rangle = \frac{1}{\sqrt{2}}\Big(|\mathbf{z}+; \mathbf{z}-\rangle - |\mathbf{z}-; \mathbf{z}+\rangle\Big) \qquad\qquad (17.2)$$

The state $|\Phi\rangle$ has been expressed here with respect to the basis in which $S_z$ is diagonal. Since $|\Phi\rangle$ has total spin zero, however, it is invariant under arbitrary rotations of the full system, so that $(\mathbf{S}_a + \mathbf{S}_b)|\Phi\rangle = 0$. As a result, the state $|\Phi\rangle$ may be expressed in the same way in terms of the eigenstates of $\mathbf{n} \cdot \mathbf{S}$ for an arbitrary direction $\mathbf{n}$,

$$|\Phi\rangle = \frac{1}{\sqrt{2}}\Big(|\mathbf{n}+; \mathbf{n}-\rangle - |\mathbf{n}-; \mathbf{n}+\rangle\Big) \qquad\qquad (17.3)$$

Thus, the preparation of the state $|\Phi\rangle$ could have been made in terms of eigenstates along any direction $\mathbf{n}$. The three remaining states of the two-electron system are the triplet states

$$
\begin{aligned}
|T^+\rangle &= |\mathbf{z}+; \mathbf{z}+\rangle \\
|T^0\rangle &= \frac{1}{\sqrt{2}}\Big(|\mathbf{z}+; \mathbf{z}-\rangle + |\mathbf{z}-; \mathbf{z}+\rangle\Big) \\
|T^-\rangle &= |\mathbf{z}-; \mathbf{z}-\rangle
\end{aligned}
\qquad\qquad (17.4)
$$

expressed here with respect to the $z$-basis.

Basic observables in $\mathcal{H}_a$ and in $\mathcal{H}_b$ respectively are the spin $\mathbf{n}_a \cdot \mathbf{S}_a$ and $\mathbf{n}_b \cdot \mathbf{S}_b$. In addition, we have observables defined only in the full Hilbert space $\mathcal{H}_{ab}$, such as $(\mathbf{n}_a \cdot \mathbf{S}_a) \otimes (\mathbf{n}_b \cdot \mathbf{S}_b)$.

To understand the concept of entanglement of two states $a$ and $b$, we begin by evaluating various observables on the state $|\Phi\rangle$. First, $|\Phi\rangle$ is an eigenstate of the observable $S_a^z \otimes S_b^z$,

$$S_a^z \otimes S_b^z |\Phi\rangle = -\frac{\hbar^2}{4}|\Phi\rangle \tag{17.5}$$

Thus, in the state $|\Phi\rangle$, the eigenvalues of $S_a^z$ and of $S_b^z$ are always opposite to one another (with probability 1). Expressed alternatively, the spins of electrons $a$ and $b$ are perfectly correlated with one another; when $S_a^z$ is $+$, then $S_b^z$ is $-$ and vice-versa. The same correlation exists in the triplet states,

$$S_a^z \otimes S_b^z |T^0\rangle = -\frac{\hbar^2}{4}|T^0\rangle$$
$$S_a^z \otimes S_b^z |T^\pm\rangle = +\frac{\hbar^2}{4}|T^\pm\rangle \tag{17.6}$$

The analysis could be repeated with respect to any orientation $\mathbf{n}$.

The key distinction appears when we investigate observables measuring properties of only subsystem $a$, but not $b$ (or vice-versa). Take for example the operator $S_a^z = S_a^z \otimes I_b$. From the construction of the states $|T^\pm\rangle$, it is immediate that

$$S_a^z |T^\pm\rangle = \pm\frac{\hbar}{2}|T^\pm\rangle \tag{17.7}$$

When observed from the point of view of subsystem $a$ alone, the states $|T^\pm\rangle$ behaves as pure states, as if subsystem $b$ were absent. These states are examples of *non-entangled states* (we shall present a general definition of such states later on). On the other hand, applying the operator $S_a^z$ to the states $|\Phi\rangle$ and $|T^0\rangle$, we find,

$$S_a^z |\Phi\rangle = \frac{\hbar}{2}|T^0\rangle$$
$$S_a^z |T^0\rangle = \frac{\hbar}{2}|\Phi\rangle \tag{17.8}$$

Neither $|\Phi\rangle$, nor $|T^0\rangle$ are eigenstates of $S_a^z$. Hence, measurements of $S_a^z$ in the state $|\Phi\rangle$ will give both the results $+\hbar/2$ and $-\hbar/2$. By computing the expectation value of $S_a^z$ in the state $|\Phi\rangle$, we gain information on the quantum mechanical probabilities with which either eigenvalues $\pm\hbar/2$ will be measured. The expectation values are given by

$$\langle\Phi|S_a^z|\Phi\rangle = \langle T^0|S_a^z|T^0\rangle = 0 \tag{17.9}$$

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so that the probability for measuring the eigenvalues $\pm\hbar/2$ are actually equal to one another. This is not really surprising, since both eigenstates $\pm$ of the electron $a$ entered into the state $|\Phi\rangle$. In fact, the expectation value of $\mathbf{n}_a \cdot \mathbf{S}_a$ in the state $|\Phi\rangle$ vanishes for any $\mathbf{n}_a$,

$$\langle\Phi|\left(\mathbf{n}_a \cdot \mathbf{S}_a\right)|\Phi\rangle = 0 \tag{17.10}$$

This is an immediate result of the rotation invariance of the state $|\Phi\rangle$.

Therefore, the probabilities for measuring the eigenvalues $\pm\hbar/2$ for $\mathbf{n}_a \cdot \mathbf{S}_a$ are equal to one another, for any orientation $\mathbf{n}_a$. This behavior of the observable $S_a^z$, from the viewpoint of the subsystem $a$, is unlike that of any pure state of $a$, but in fact precisely coincides with the behavior of an unpolarized state of $a$. We see that by summing, or "averaging", over the states in the subsystem $b$, the full system reduces to subsystem $a$, and the state $|\Phi\rangle$, which is a pure state of the full system $\mathcal{H}_{ab}$, reduces to a mixed state of the subsystem $a$. Mathematically, this may be expressed as follow,

$$\begin{aligned}
\langle\Phi|S_a^z|\Phi\rangle &= \mathrm{tr}_{\mathcal{H}_{ab}}\left(|\Phi\rangle\langle\Phi|S_a^z\right) \\
&= \mathrm{tr}_{\mathcal{H}_a}\mathrm{tr}_{\mathcal{H}_b}\left(|\Phi\rangle\langle\Phi|S_a^z\right) \\
&= \mathrm{tr}_{\mathcal{H}_a}\left(\rho_a S_a^z\right)
\end{aligned} \tag{17.11}$$

where we have defined

$$\rho_a \equiv \mathrm{tr}_{\mathcal{H}_b}\left(|\Phi\rangle\langle\Phi|\right) \tag{17.12}$$

This quantity may be computed explicitly, using the form of $|\Phi\rangle$, and we get

$$\begin{aligned}
\rho_a &= \frac{1}{2}\mathrm{tr}_{\mathcal{H}_b}\left(|\mathbf{z}+;\mathbf{z}-\rangle - |\mathbf{z}-;\mathbf{z}+\rangle\right)\left(<\mathbf{z}+;\mathbf{z}-| - \langle\mathbf{z}-;\mathbf{z}+|\right) \\
&= \frac{1}{2}\left(|\mathbf{z}+\rangle\langle\mathbf{z}+| + |\mathbf{z}-\rangle\langle\mathbf{z}-|\right) = \frac{1}{2}I_a
\end{aligned} \tag{17.13}$$

The value $\rho_a = I_a/2$ indeed confirms that subsystem $a$ appears in an unpolarized state. From the point of view of subsystem $a$, the state $|\Phi\rangle$ is *entangled* with subsystem $b$

## 17.2   Entangled states from non-entangled states

Entangled states naturally appear in the time evolution of a system that was originally in a non-entangled state. This may be illustrated concretely in the above two spin $1/2$ system as well. Let the time evolution be determined by the simplest non-trivial Hamiltonian,

$$H = \frac{2\omega}{\hbar}\mathbf{S}_a \cdot \mathbf{S}_b = \frac{\omega}{\hbar}\left(\mathbf{S}^2 - \frac{3}{2}\hbar^2\right) \tag{17.14}$$

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where $\mathbf{S} = \mathbf{S}_a + \mathbf{S}_b$ is the total spin. The Hamiltonian is diagonal on the states $|\Phi\rangle$, and $|T^{0,\pm}\rangle$, and has eigenvalues $-3\hbar\omega/2$ and $\hbar\omega/2$ respectively. Consider now a state $|\Psi(t)\rangle$ for which $|\Psi(0)\rangle = |\mathbf{z}+;\mathbf{z}-\rangle$, then time evolution under Hamiltonian $H$ produces

$$|\Psi(t)\rangle = e^{i\omega t/2}\left(\cos(\omega t)|\mathbf{z}+;\mathbf{z}-\rangle - i\sin(\omega t)|\mathbf{z}-;\mathbf{z}+\rangle\right) \tag{17.15}$$

The state $|\Psi(0)\rangle$ was chosen to be *non-entangled*, but we see that time evolution entangles and then un-entangles the state. In particular, we may compute the density matrix

$$\begin{aligned}
\rho_a(t) &= \operatorname{tr}_{\mathcal{H}_b}|\Psi(t)\rangle\langle\Psi(t)| \\
&= \cos^2(\omega t)|\mathbf{z}+\rangle\langle\mathbf{z}+| + \sin^2(\omega t)|\mathbf{z}-\rangle\langle\mathbf{z}-|
\end{aligned} \tag{17.16}$$

This state is non-entangled when $t = k\pi/(2\omega)$ for any integer $k$, and maximally entangled (unpolarized) when $t = \pi/(4\omega) + k\pi/(2\omega)$ for any integer $k$.

## 17.3 The Schmidt purification theorem

Consider now, more generally, a full quantum system with Hilbert space $\mathcal{H}_{ab}$, built out of two subsystems $a$ and $b$ with respective Hilbert spaces $\mathcal{H}_a$ and $\mathcal{H}_b$, so that $\mathcal{H}_{ab} = \mathcal{H}_a \otimes \mathcal{H}_b$. In this general system, let $|\Psi\rangle$ be a *pure state* in $\mathcal{H}_{ab}$. The division of the system into the two subsystems $a$ and $b$ allows us to define the two density operators,

$$\begin{aligned}
\rho_a &\equiv \operatorname{tr}_{\mathcal{H}_b}\left(|\Psi\rangle\langle\Psi|\right) \\
\rho_b &\equiv \operatorname{tr}_{\mathcal{H}_a}\left(|\Psi\rangle\langle\Psi|\right)
\end{aligned} \tag{17.17}$$

By construction, $\rho_a$ is a density operator for subsystem $a$, while $\rho_b$ is a density matrix for subsystem $b$. The density operators $\rho_a$ and $\rho_b$ are not independent. In particular, we always have $\operatorname{rank}(\rho_a) = \operatorname{rank}(\rho_b)$. In fact, even more precise relations hold between $\rho_a$ and $\rho_b$, which we now exhibit.

The Schmidt purification theorem states that, for any $|\Psi\rangle \in \mathcal{H}_{ab}$, there exists an orthonormal set $|i,a\rangle$ in $\mathcal{H}_a$ and an orthonormal set $|i,b\rangle$ in $\mathcal{H}_b$, such that

$$|\Psi\rangle = \sum_i \sqrt{p_i}\,|i,a\rangle \otimes |i,b\rangle \tag{17.18}$$

Notice that the sum is over a common index $i$, even though the Hilbert spaces $\mathcal{H}_a$ and $\mathcal{H}_b$ need not have the same dimension. The numbers $p_i$ are real and satisfy $0 \le p_i \le 1$. Finally, note that the sets $\{|i,a\rangle\}_i$ and $\{|i,b\rangle\}_i$ depend on the state $|\Psi\rangle$.

To prove this theorem, we begin by decomposing the pure state in an orthonromal basis $|i,a\rangle$ of $\mathcal{H}_a$ and $|m,b'\rangle$ of $\mathcal{H}_b$,

$$|\Psi\rangle = \sum_{i,m} C_{im}|i,a\rangle \otimes |m,b'\rangle \tag{17.19}$$

We choose the basis $|i,a\rangle$ to be such that $\rho_a$ is diagonal in this basis, and given by the sum,

$$\sum_i p_i|i,a\rangle\langle i,a| \tag{17.20}$$

where $0 \le p_i \le 1$. In this special basis, we define the following states of $\mathcal{H}_b$,

$$|i, b''\rangle \equiv \sum_m C_{im} |m, b'\rangle \tag{17.21}$$

Note that these states need to be neither orthogonal to one another, nor normalized. Hence the pure state may be expressed as

$$|\Psi\rangle = \sum_i |i, a\rangle \otimes |i, b''\rangle \tag{17.22}$$

We now use this expression to evaluate the density operator $\rho_a$, and find,

$$\rho_a = \sum_{i,j} \langle j, b'' | i, b'' \rangle |i, a\rangle \langle j, a| \tag{17.23}$$

But, we had already assume that $\rho_a$ was actually diagonal in the basis $|i, a\rangle$, with eigenvalues $p_i$, so that we must have

$$\langle j, b'' | i, b'' \rangle = p_i \delta_{ij} \tag{17.24}$$

Thus, we conclude that the states $|i, b''\rangle$ are in fact orthogonal to one another. It now suffices to normalize the states by

$$|i, b\rangle = \frac{1}{\sqrt{p_i}} |i, b''\rangle \tag{17.25}$$

to recover the formula (17.18) of Schmidt's theorem. In this basis now, we may compute also $\rho_b$, and we find,

$$\rho_b = \sum_i p_i |i, b\rangle \langle i, b| \tag{17.26}$$

Thus, the probability assignments of $\rho_a$ and $\rho_b$, in this basis, are identically the same. In particular, the rank of $\rho_a$ coincides with the rank of $\rho_b$, and this is referred to as the *Schmidt number*. It is obviously a positive integer.

## 17.4  Generalized description of entangled states

Consider again, as in the preceding subsection, a full quantum system with Hilbert space $\mathcal{H}_{ab}$, built out of two subsystems $a$ and $b$ with respective Hilbert spaces $\mathcal{H}_a$ and $\mathcal{H}_b$, so that $\mathcal{H}_{ab} = \mathcal{H}_a \otimes \mathcal{H}_b$. By the Schmidt purification theorem, we then have

$$\begin{aligned}
\rho_a &= \sum_{i=1}^s p_i |i, a\rangle \langle i, a| \\
\rho_b &= \sum_{i=1}^s p_i |i, b\rangle \langle i, b| \\
|\Psi\rangle &= \sum_{i=1}^s \sqrt{p_i} |i, a\rangle \otimes |i, b\rangle
\end{aligned} \tag{17.27}$$

Henceforth, we shall assume that $p_i > 0$, and omit those contributions for which $p_I = 0$ from the sum. The number $s$ is then the common rank of $\rho_a$ and $\rho_b$, which is nothing but the Schmidt number of the state $|\Psi\rangle$,

$$s = \text{rank}(\rho_a) = \text{rank}(\rho_b) \tag{17.28}$$

- If $s = 1$, the state $|\Psi\rangle$ is *non-entangled*. In this case, the density operators $\rho_a$ and $\rho_b$ correspond to pure states of $\mathcal{H}_a$ and $\mathcal{H}_b$ respectively.

- If $s > 1$, the state $|\Psi\rangle$ is *entangled*. In this case, the density operators $\rho_a$ and $\rho_b$ *do not correspond to pure states of $\mathcal{H}_a$ and $\mathcal{H}_b$ respectively* but represent a mixture instead.

## 17.5  Entanglement entropy

The Schmidt number gives a discrete measure of the degree of entanglement of a bipartite division. But there is also value in having a continuously varying measure of the entanglement of a state. This is provided by the *entanglement entropy*. Recall that the state $|\Psi\rangle$ in the full Hilbert space is pure, so its statistical entropy vanishes. But when the state is considered from the point of view of the bipartite division into systems $a$ and $b$, it makes sense to talk about entropies $S(\rho_a)$ and $S(\rho_b)$ associated with the density operators $\rho_a$ or $\rho_b$. By the Schmidt purification theorem, we have $S(\rho_a) = S(\rho_b)$, so that we may consistently defined an entanglement entropy by

$$S_{\text{entang}} \equiv S(\rho_a) = S(\rho_b) = -\sum_{i=1}^{s} p_i \ln p_i \tag{17.29}$$

As the state $|\Psi\rangle$ approaches a non-entangled state $|\Psi; j\rangle$ (in which $p_i = 0$ for all $i \neq j$, and $p_j = 1$), the entanglement entropy of $|\Psi\rangle$ tends to 0 in a continuous manner.

## 17.6  The two-state system once more

Consider the following pure state in the system of two spin $1/2$ particles,

$$|\Psi\rangle = \cos\theta \, |\mathbf{z}+, a; bz-, b\rangle + \sin\theta \, |\mathbf{z}-, a; \mathbf{z}+, b\rangle \tag{17.30}$$

The density operators of the subsystems $a$ and $b$ are readily evaluated,

$$\begin{aligned} \rho_a &= \cos^2\theta \, |\mathbf{z}+, a\rangle\langle\mathbf{z}+, a| + \sin^2\theta \, |\mathbf{z}-, a\rangle\langle\mathbf{z}-, a| \\ \rho_b &= \cos^2\theta \, |\mathbf{z}-, b\rangle\langle\mathbf{z}-, b| + \sin^2\theta \, |\mathbf{z}+, b\rangle\langle\mathbf{z}+, b| \end{aligned} \tag{17.31}$$

Note the reversal of probability assignments for spin $+$ and spin $-$. The Schmidt number is

- $s = 1$ when $\sin(2\theta) = 0$: the state $|\Psi\rangle$ is not entangled;

- $s = 2$ when $\sin(2\theta) \neq 0$: the state $|\Psi\rangle$ is entangled.

The entanglement entropy is given by

$$S_{\text{entang}} = -\cos^2\theta \ln(\cos^2\theta) - \sin^2\theta \ln(\sin^2\theta) \tag{17.32}$$

When $\theta \to 0$, for example, we approach the non-entangled state $|\mathbf{z}+, a; bz-, b\rangle$, and the entanglement entropy $S_{\text{entang}} \sim -\theta^2 \ln\theta^2$ tends to zero in a smooth way.

## 17.7　Entanglement in the EPR paradox

Einstein Podolsky and Rosen (EPR) proposed a *gedanken* experiment in 1935 the outcome of which they viewed as a paradox, namely a contradiction between the principles of causality in relativity and the principles of quantum mechanics.

The set-up (as re-interpreted by David Bohm) is as follows. Consider a spin 0 particle which decays into two stable particles $a$ and $b$. To make this interesting, we consider a case where the particles $a$ and $b$ have both spin 1 (typically photons) or spin $1/2$ (electrons). Physical examples are

$$
\begin{aligned}
\pi^0 &\rightarrow & \gamma + \gamma \\
\pi^0 &\rightarrow & e^+ + e^-
\end{aligned}
\tag{17.33}
$$

The first is the dominant decay mode of the $\pi^0$, whose life-time is $10^{-16}s$. The branching ratio for the second decay is $10^{-7}$. Let us concentrate on the example of $\pi^0 \rightarrow e^+ + e^-$, so that the two subsystems both correspond to spin $1/2$.

Because the $\pi^0$ has zero spin, and angular momentum is conserved, the spins of the electron and positron must be opposite. This means that the electron/positron state produced by the decay of $\pi^0$ must be

$$
|\Phi\rangle = \frac{1}{\sqrt{2}}\Big(|\mathbf{z}+;\mathbf{z}-\rangle - |\mathbf{z}-;\mathbf{z}+\rangle\Big) = \frac{1}{\sqrt{2}}\Big(|\mathbf{n}+;\mathbf{n}-\rangle - |\mathbf{n}-;\mathbf{n}+\rangle\Big)
\tag{17.34}
$$

following the notations of the preceding sections. Here, we ignore all extra quantum numbers the particles carry, such as energy, momentum, and electric charge.

Assuming that the $e^+$ and $e^-$ can travel a long distance without any interaction with other particles or with electric and magnetic fields, this correlation between the spins of $e^+$ and $e^-$ will persist, and the quantum state of the spins will remain $|\Phi\rangle$. We now imagine two observers $A$ and $B$ far away in opposite directions from where the $\pi^0$ decays. These observers can measure the spins of the $e^+$ and $e^-$.

$$
\begin{array}{ccccc}
& e^+ & & e^- & \\
A <----- & \pi^0 & ------> B
\end{array}
\tag{17.35}
$$

Assume that $A$ measures the spin of the electron along the $S_a^z$ direction. The probability for $A$ to measure $+\hbar/2$ is 50%, and the probability for $A$ to measure $-\hbar/2$ is also 50%. But now, if $A$ measures spin $+\hbar/2$ in the $S_a^z$ direction, then $A$ knows for sure (with probability 1) that, if $B$ measures spin in the $S_b^z$ direction as well, $B$ must necessarily find $-\hbar/2$, since these spins are opposite in the state $|\Phi\rangle$. The same would be true if $A$ and $B$ measured spin along any other direction $\mathbf{n}$.

At first sight, one may conclude that because of these correlations, there must be some information that can travel from $B$ to $A$ instantaneously. This would appear to be so because as soon as $A$ has measured spin $S_a^z = +\hbar/2$, then the outcome of the measurement that $B$ can perform will be known to $A$ instantaneously. This issue, however, is not where the EPR paradox lies. After

all, this is a question of causality in special relativity, and could be considered purely classically. Suppose two travelers originating at $\pi^0$ are each given a ball. Both travelers know that the ball given to one of them is black, while the ball given to the other is white, but they do not know whether the ball each one received is black or white. They now travel apart for a long long time, until one of the travelers decides to open his present and finds out this his ball is black. He then instantaneously knows that the other guy's ball is white. Nonetheless, no information has really traveled faster than light, and again, this is not the key problem in the EPR paradox. After all, if both $A$ and $B$ only measure along commuting observables, such as $S_a^z$ and $S_b^z$, their measurements are analogous to classical ones.

The real distinction brought by quantum behavior is that one can make measurements along $S_a^z$ or along $S_a^x$, for example, and these operators do not commute. It is this realization that was new in Bell's work. If we allow for these observables to be measured, then the possible outcomes are as given in Table 1 below.

| spin component measured by A | result | spin component measured by B | result |
|:---:|:---:|:---:|:---:|
| $z$ | $+$ | $z$ | $-$ |
| $z$ | $-$ | $z$ | $+$ |
| $z$ | $+$ | $x$ | $+$ |
| $z$ | $+$ | $x$ | $-$ |
| $z$ | $-$ | $x$ | $+$ |
| $z$ | $-$ | $x$ | $-$ |
| $x$ | $+$ | $x$ | $-$ |
| $x$ | $-$ | $x$ | $+$ |
| $x$ | $+$ | $z$ | $+$ |
| $x$ | $+$ | $z$ | $-$ |
| $x$ | $-$ | $z$ | $+$ |
| $x$ | $-$ | $z$ | $-$ |

For example,

1. If both $A$ and $B$ measure $S^z$ or both measure $S^x$, the spins measured are opposite;

2. If $A$ makes no measurement, then the measurements of $B$ are 50% spin $+\hbar/2$ and 50% spin $-\hbar/2$;

3. If $A$ measures $S_a^z$ and $B$ measures $S_b^x$, there is completely random correlation between the two measurements. Even if $S_a^z$ is measured to be $+\hbar/2$, the measurement of $S_b^x$ will yield 50% spin $+$ and 50% spin $-$.

Thus, the outcome of the measurements of $B$ depend on what kind of measurement $A$ decides to perform. And $A$ can decide to orient his measurement direction $\mathbf{n}$ long after the two particles have separated. It is as though particle $b$ knows which spin component of particle $a$ is being measured.

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The *orthodox quantum interpretation* of this situation is as follows. We must accept that when $A$ performs a measurement on the spin of one of the particles, this is really a measurement on the entire system, even though it would appear that $A$ is making a measurement on only part of the system (namely only one of the two particles). If $A$ makes a measurement of $S_a^z$, then the act of performing the measurement will select an eigenstate of $s_a^z$ out of the full state $|\Phi\rangle$. Depending on the eigenvalue of $S_a^z$ observed, the state selected will be

$$S_a^z = +\frac{\hbar}{2} \qquad\qquad |\mathbf{z}+;\mathbf{z}-\rangle$$

$$S_a^z = -\frac{\hbar}{2} \qquad\qquad |\mathbf{z}-;\mathbf{z}+\rangle \qquad\qquad (17.36)$$

This then explains why measuring then $S_b^z$ gives perfectly anti-correlated outcomes, and why measuring $S_b^x$ gives 50% spin + and 50% spin −.

The real novelty in EPR is that the measurement at $A$ changes the whole state and in particular the state as $B$ will measure it.

## 17.8    Einstein's locality principle

Einstein Podolsky and Rosen could not accept as part of a complete theory the fact that a measurement at $A$ could change the state as measured by $B$ in violation of macroscopic causality. To quote them

> If, without in any way disturbing a system, we can predict with certainty (i.e. with probability equal to unity) the value of a physical reality, then there exists an element of physical reality corresponding to this physical quantity.

and also

> The real factual situation of the system $B$ is independent of what is done with the system $A$, which is spatially separated from $B$.

The first principle led to *theories with hidden variables*, in which the measured values of $S_b^x$ in an eigenstate of $S_a^z$ actually have a physical reality, but this reality remains hidden from us, and we can probe these deterministic hidden variables only in a statistical sense. Hidden variable theories seemed so generally possible that it seemed always possible to mimic the predictions of quantum mechanics (and their experimental verifications) by introducing some extra degrees of freedom of this type.

## 17.9    Bell's inequalities

The situation changed dramatically in 1964, when John Bell made verifiable and falsifiable predictions that could distinguish between quantum mechanics and theories of hidden variables.[15] The key is to trigger on these entanglements typical of quantum theory.

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[15] J.S. Bell, Physics **1** (1964) 195; *Speakable and unspeakable in quantum mechanics*, Cambridge, 1991.

We all agree that $S^z$ and $S^x$ cannot be measured simultaneously. However, for a large number of spin 1/2 particles, we can assign a fraction of them to have the following property

1. If $S^z$ is measured, we obtain $+\hbar/2$ with certainty;

2. If $S^x$ is measured, we obtain $-\hbar/2$ with certainty.

What this means is that *if we measure $S^z$ on one of these particles, we agree not to measure $S^x$ on that same particle*, and *if we measure $S^x$ on another one of these particles, we agree not to measure $S^x$ on that particle.* In this way, we are never led to actually measure $S^z$ and $S^x$ simultaneously, since of course, we agreed that we cannot. We denote a particle of this type by $(\mathbf{z}+, \mathbf{x}-)$. Even though this model is very different from quantum mechanics, it can actually reproduce the quantum measurements of $S^z$ and $S^x$, provided there are equal numbers of particles of type $(\mathbf{z}+, \mathbf{x}+)$ as there are particles of type $(\mathbf{z}+, \mathbf{x}-)$.

Next, let us see how this model can reproduce the predictions of the spin-singlet correlated measurements. For a particular pair, there should be a perfect match between particles 1 and 2. For example,

$$1: \quad \text{type} \quad (\mathbf{z}+, \mathbf{x}-) \quad \longleftrightarrow \quad 2: \quad \text{type} \quad (\mathbf{z}-, \mathbf{x}+) \tag{17.37}$$

The results of correlations in Table 1 can be reproduced if particle 1 and 2 are matched as follows,

| particle 1 | | particle 2 |
|---|---|---|
| $(\mathbf{z}+, \mathbf{x}-)$ | $\longleftrightarrow$ | $(\mathbf{z}-, \mathbf{x}+)$ |
| $(\mathbf{z}+, \mathbf{x}+)$ | $\longleftrightarrow$ | $(\mathbf{z}-, \mathbf{x}-)$ |
| $(\mathbf{z}-, \mathbf{x}+)$ | $\longleftrightarrow$ | $(\mathbf{z}+, \mathbf{x}-)$ |
| $(\mathbf{z}-, \mathbf{x}-)$ | $\longleftrightarrow$ | $(\mathbf{z}+, \mathbf{x}+)$ |

$$\tag{17.38}$$

with equal populations, 25% for each pair. The key assumption, as always with hidden variable theory, is that the results measured by $A$ are *predetermined* independently of $B$'s choice of what to measure.

So far, correlated measurements involving 2 directions can be accounted for by a theory of hidden variables. But new things happen when we consider correlated measurements of 3 spins. To do this, we consider again a problem of spin 1/2, but we now measure in three directions, indicated by three unit vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$, which, in general, need not be orthogonal to one another.

Extending the above analysis on two measurements, we now assume that the particles belong to a definite type $(\mathbf{a}+, \mathbf{b}-, \mathbf{c}+)$. This means that on any given particle, one decides to measure either $\mathbf{a} \cdot \mathbf{S}$, or $\mathbf{b} \cdot \mathbf{S}$ or $\mathbf{c} \cdot \mathbf{S}$, but never more than one of these for any given particle. The eigenvalues are then given by the $\pm$ assignments. Now, to ensure conservation of total angular momentum, there must again be a perfect match between the spins measured on particles 1 and 2. The particle pair must then be a member of one of eight types, given this matching. In hidden variable theory, these eight types are mutually exclusive, and the corresponding sets are mutually disjoint. They

are listed in the table below,

| population | particle 1 | particle 2 | |
|---|---|---|---|
| $N_1$ | $(\mathbf{a}+, \mathbf{b}+, \mathbf{c}+)$ | $(\mathbf{a}-, \mathbf{b}-, \mathbf{c}-)$ | |
| $N_2$ | $(\mathbf{a}+, \mathbf{b}+, \mathbf{c}-)$ | $(\mathbf{a}-, \mathbf{b}-, \mathbf{c}+)$ | |
| $N_3$ | $(\mathbf{a}+, \mathbf{b}-, \mathbf{c}+)$ | $(\mathbf{a}-, \mathbf{b}+, \mathbf{c}-)$ | |
| $N_4$ | $(\mathbf{a}-, \mathbf{b}+, \mathbf{c}+)$ | $(\mathbf{a}+, \mathbf{b}-, \mathbf{c}-)$ | |
| $N_5$ | $(\mathbf{a}+, \mathbf{b}-, \mathbf{c}-)$ | $(\mathbf{a}-, \mathbf{b}+, \mathbf{c}+)$ | |
| $N_6$ | $(\mathbf{a}-, \mathbf{b}+, \mathbf{c}-)$ | $(\mathbf{a}+, \mathbf{b}-, \mathbf{c}+)$ | |
| $N_7$ | $(\mathbf{a}-, \mathbf{b}-, \mathbf{c}+)$ | $(\mathbf{a}+, \mathbf{b}+, \mathbf{c}-)$ | |
| $N_8$ | $(\mathbf{a}-, \mathbf{b}-, \mathbf{c}-)$ | $(\mathbf{a}+, \mathbf{b}+, \mathbf{c}+)$ | (17.39) |

Needless to say, each population number is positive $N_i \geq 0$ for $i = 1, \cdots, 8$. Now, we consider pairs of measurements by observers $A$ and $B$ in the following fashion.

Suppose $A$ finds $\mathbf{a} \cdot \mathbf{S}_1$ to be $+$, and $B$ finds $\mathbf{b} \cdot \mathbf{S}_2$ to be $+$ as well. This can happen if the pair of particles belongs to type 3 or to type 5. Hence the number of particles found for this particular measurement will be $N_3 + N_5$. We can associate a probability with this particular measurement,

$$P(\mathbf{a}+, \mathbf{b}+) = (N_3 + N_5)/N_{\text{tot}} \qquad\qquad N_{\text{tot}} = \sum_{i=1}^{8} N_i \qquad\qquad (17.40)$$

In a similar manner, we have

$$\begin{aligned} P(\mathbf{a}+, \mathbf{c}+) &= (N_2 + N_5)/N_{\text{tot}} \\ P(\mathbf{c}+, \mathbf{b}+) &= (N_3 + N_7)/N_{\text{tot}} \end{aligned} \qquad\qquad (17.41)$$

Now, since $N_2, N_7 \geq 0$, we find that there must be an inequality obeyed by these probabilities,

$$P(\mathbf{a}+, \mathbf{b}+) \leq P(\mathbf{a}+, \mathbf{c}+) + P(\mathbf{c}+, \mathbf{b}+) \qquad\qquad (17.42)$$

or more generally,

$$P(\mathbf{a}\alpha, \mathbf{b}\beta) \leq P(\mathbf{a}\alpha, \mathbf{c}\gamma) + P(\mathbf{c}\gamma, \mathbf{b}\beta) \qquad\qquad (17.43)$$

where $\alpha, \beta, \gamma$ now take any values $\pm$. These are the Bell inequalities for this system. They follow from assigning an independent reality to the spin measured in each of the directions $\mathbf{a}, \mathbf{b}$, and $\mathbf{c}$, which in turn follows from Einstein's locality argument.

## 17.10   Quantum predictions for Bell's inequalities

We shall here calculate those same probabilities $P(\mathbf{a}\alpha, \mathbf{b}\beta)$ etc. using the standard rules of quantum theory. The state $|\Phi\rangle$, being a spin singlet, may be represented in either one of the following three

ways,

$$
\begin{aligned}
|\Phi\rangle &= \frac{1}{\sqrt{2}}|\mathbf{a}+;\mathbf{a}-\rangle - \frac{1}{\sqrt{2}}|\mathbf{a}-;\mathbf{a}+\rangle \\
|\Phi\rangle &= \frac{1}{\sqrt{2}}|\mathbf{b}+;\mathbf{b}-\rangle - \frac{1}{\sqrt{2}}|\mathbf{b}-;\mathbf{b}+\rangle \\
|\Phi\rangle &= \frac{1}{\sqrt{2}}|\mathbf{c}+;\mathbf{c}-\rangle - \frac{1}{\sqrt{2}}|\mathbf{c}-;\mathbf{c}+\rangle
\end{aligned}
\tag{17.44}
$$

The probability amplitude for measuring $|\Phi\rangle$ in a state $|\mathbf{a}+;\mathbf{b}+\rangle$ is given by

$$
\langle \mathbf{a}+;\mathbf{b}+|\Phi\rangle = \frac{1}{\sqrt{2}}\langle \mathbf{a}+;\mathbf{b}+|\mathbf{a}+;\mathbf{a}-\rangle - \frac{1}{\sqrt{2}}\langle \mathbf{a}+;\mathbf{b}+|\mathbf{a}-;\mathbf{a}+\rangle
\tag{17.45}
$$

The last term vanishes because it involves the inner product $\langle \mathbf{a}+|\mathbf{a}-\rangle = 0$ for the first particle. The first term also simplifies by using $\langle \mathbf{a}+|\mathbf{a}+\rangle = 1$ for the first particle, and we are left with,

$$
\langle \mathbf{a}+;\mathbf{b}+|\Phi\rangle = \frac{1}{\sqrt{2}}\langle \mathbf{b}+|\mathbf{a}-\rangle
\tag{17.46}
$$

where the inner product is for the particle 2. Hence, the probability we seek is given by

$$
P(\mathbf{a}+,\mathbf{b}+) = |\langle \mathbf{a}+;\mathbf{b}+|\Phi\rangle|^2 = \frac{1}{2}|\langle \mathbf{b}+|\mathbf{a}-\rangle|^2
\tag{17.47}
$$

To compute the last inner product, we express the states $|\mathbf{b}\beta\rangle$ in terms of the states $|\mathbf{a}\alpha\rangle$. This is the same formula as for expressing a general state $|\mathbf{n}\pm\rangle$ in terms of $|\mathbf{z}\pm\rangle$, but now the angle $\theta$ between $\mathbf{n}$ and $\mathbf{z}$ becomes the angle $\theta_{ab}$ between the vectors $\mathbf{a}$ and $\mathbf{b}$,

$$
\begin{aligned}
|\mathbf{b}+\rangle &= \cos\frac{\theta_{ab}}{2}|\mathbf{a}+\rangle + e^{i\phi}\sin\frac{\theta_{ab}}{2}|\mathbf{a}-\rangle \\
|\mathbf{b}-\rangle &= \cos\frac{\theta_{ab}}{2}|\mathbf{a}-\rangle - e^{-i\phi}\sin\frac{\theta_{ab}}{2}|\mathbf{a}+\rangle
\end{aligned}
\tag{17.48}
$$

Here, we have omitted an overall phase which is immaterial in evaluating the probabilities, and we find the probability amplitude to be,

$$
\langle \mathbf{a}+|\mathbf{b}-\rangle = -e^{-i\phi}\sin\frac{\theta_{ab}}{2}
\tag{17.49}
$$

and the probability,

$$
P(\mathbf{a}+,\mathbf{b}+) = \frac{1}{2}\sin^2\frac{\theta_{ab}}{2}
\tag{17.50}
$$

The phase $\phi$ is immaterial in calculating this probability. Note that, in the limit where $\mathbf{b} \to \mathbf{a}$, the probability $P(\mathbf{a}+,\mathbf{b}+) \to 0$. This is consistent with the fact that the spin must be perfectly anti-correlated when measured along the same axis by $A$ and $B$. Also, we have $P(\mathbf{a}+,\mathbf{b}+) \to 1/2$ as

$\mathbf{b} \to -\mathbf{a}$, which is consistent with the fact that the spins measured by $A$ and $B$ should be perfectly anti-correlated in the state $|\Phi\rangle$.

Are the Bell inequalities obeyed by quantum mechanics ? To find that out, consider the combination

$$P(\mathbf{a}+, \mathbf{c}+) + P(\mathbf{c}+, \mathbf{b}+) - P(\mathbf{a}+, \mathbf{b}+) \tag{17.51}$$

The Bell inequalities require that this combination be always $\geq 0$. The quantum mechanical computation gives,

$$P(\mathbf{a}+, \mathbf{c}+) + P(\mathbf{c}+, \mathbf{b}+) - P(\mathbf{a}+, \mathbf{b}+) = \frac{1}{2} \left( \sin^2 \frac{\theta_{ac}}{2} + \sin^2 \frac{\theta_{cb}}{2} - \sin^2 \frac{\theta_{ab}}{2} \right) \tag{17.52}$$

It is easiest to analyze the expression on the right hand side when the directions $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are coplanar. We then have

$$\theta_{ab} = \theta_{ac} + \theta_{cb} \tag{17.53}$$

If the $\theta_{ab}$ angle is taken to be *the smallest angle subtended between the vectors* $\mathbf{a}$ *and* $\mathbf{b}$ (i.e. $0 \leq \theta_{ab} \leq \pi$), then the above planar relation between angles requires that

$$0 \leq \theta_{ab} \leq \pi$$
$$0 \leq \theta_{ac} \leq \pi$$
$$0 \leq \theta_{cb} \leq \pi \tag{17.54}$$

In this sense, the direction $\mathbf{c}$ lies between $\mathbf{a}$ and $\mathbf{b}$. Using

$$\sin^2 \frac{\theta_{ab}}{2} = \sin^2 \frac{\theta_{ac} + \theta_{cb}}{2} = \left( \sin \frac{\theta_{ac}}{2} \cos \frac{\theta_{cb}}{2} + \sin \frac{\theta_{cb}}{2} \cos \frac{\theta_{ac}}{2} \right)^2 \tag{17.55}$$

and combining with the other terms, we get

$$P(\mathbf{a}+, \mathbf{c}+) + P(\mathbf{c}+, \mathbf{b}+) - P(\mathbf{a}+, \mathbf{b}+) = - \sin \frac{\theta_{ac}}{2} \sin \frac{\theta_{cb}}{2} \cos \frac{\theta_{ab}}{2} \tag{17.56}$$

Given the ranges of the angles, the combination on the right is always negative or zero. Sakurai quotes an even more special case where $\theta_{ab} = 2\theta$ and $\theta_{ac} = \theta_{cb} = \theta$. The above formula then reduces to

$$P(\mathbf{a}+, \mathbf{c}+) + P(\mathbf{c}+, \mathbf{b}+) - P(\mathbf{a}+, \mathbf{b}+) = - \sin^2 \frac{\theta}{2} \cos \theta \tag{17.57}$$

which is manifestly negative when $0 \leq \theta \leq \pi$.

Thus, quantum mechanics gives a radically different prediction for these combinations of probabilities. The measurements can actually be carried out on pairs of linearly polarized photons, produced in cascade decays of atoms such as $Ca$ or $Hg$, excited by laser pumping.[16] The experiments clearly confirm quantum mechanics and thus invalidate hidden variable theories.

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[16]A. Aspect, P. Gragnier, G. Roger, Phys. Rev. Lett. **47** (1981) 460; Phys. Rev. Lett. **49** (1982) 91.

## 17.11 Three particle entangled states

Even more drastic violations of hidden variable type theories may be obtained by considering the decay of an entangled state into three particles. We imagine a system of three spin $1/2$ particles, with associated 8-dimensional Hilbert space $\mathcal{H}_{abc} = \mathcal{H}_a \otimes \mathcal{H}_b \otimes \mathcal{H}_c$. Instead of working with spin components, we shall work directly with components of the Pauli matrices $\sigma_a^i$, $\sigma_b^i$ and $\sigma_c^i$ where $i = x, y, z$.

A basis for all observables on this Hilbert space is given by 64 matrices $\sigma_a^I \otimes \sigma_b^J \otimes \sigma_c^K$, where $J$ can take the values $x, y, z$ or $0$, and $\sigma^0 = I$ is the identity matrix. Of special interest are sets of observables that mutually commute with one another. The maximal number is 3, excluding the identity operator itself. For example, one could pick the set

$$
\begin{aligned}
&I_a \otimes I_b \otimes \sigma_c^z \\
&I_a \otimes \sigma_b^z \otimes I_c \\
&\sigma_a^z \otimes I_b \otimes I_c
\end{aligned}
\tag{17.58}
$$

Any operator commuting with all three must be functionally dependent on these three, as may be easily verified.

But it is possible to choose a more interesting set of mutually commuting observables that shows some degree of entanglement. One may also choose,

$$
\begin{aligned}
\Sigma_a &= \sigma_a^x \otimes \sigma_b^y \otimes \sigma_c^y \\
\Sigma_b &= \sigma_a^y \otimes \sigma_b^x \otimes \sigma_c^y \\
\Sigma_c &= \sigma_a^y \otimes \sigma_b^y \otimes \sigma_c^x
\end{aligned}
\tag{17.59}
$$

Using the commutation relations for the $\sigma^i$ and the fact that the matrix product commutes with the tensor product, such as for example, $(\sigma_a^i \otimes \sigma_b^j)(\sigma_a^{i'} \otimes \sigma_b^{j'}) = (\sigma_a^i \sigma_a^{i'}) \otimes (\sigma_b^j \sigma_b^{j'})$. we easily verify that these operators mutually commute,

$$
[\Sigma_a, \Sigma_b] = [\Sigma_b, \Sigma_c] = [\Sigma_c, \Sigma_a] = 0
\tag{17.60}
$$

Furthermore, we have

$$
(\Sigma_a)^2 = (\Sigma_b)^2 = (\Sigma_c)^2 = I
\tag{17.61}
$$

so that each of these operators has eigenvalues $\pm 1$. We now define a state $|\Phi\rangle$ which satisfies,

$$
\Sigma_a |\Phi\rangle = \Sigma_b |\Phi\rangle = \Sigma_c |\Phi\rangle = +|\Phi\rangle
\tag{17.62}
$$

The condition becomes easier to solve if translated to the equivalent conditions

$$
\Sigma_a \Sigma_b |\Phi\rangle = \Sigma_b \Sigma_c |\Phi\rangle = \Sigma_c \Sigma_a |\Phi\rangle = +|\Phi\rangle
\tag{17.63}
$$

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and

$$\begin{aligned}
\Sigma_a \Sigma_b &= \sigma_a^z \otimes \sigma_b^z \otimes I_c \\
\Sigma_b \Sigma_c &= I_a \otimes \sigma_b^z \otimes \sigma_c^z \\
\Sigma_c \Sigma_a &= \sigma_a^z \otimes I_b \otimes \sigma_c^z
\end{aligned} \tag{17.64}$$

The eigenvalue conditions of $\Sigma_a \Sigma_b$, $\Sigma_b \Sigma_c$, and $\Sigma_c \Sigma_a$, on $|\Phi\rangle$ then translate to the fact that in a basis where $\sigma_a^z, \sigma_b^z, \sigma_c^z$ are diagonal, the eigenvalues of these three operators must be the same. This allows for the states $|+++\rangle$ and $|---\rangle$. Separately, these states are not eigenstates of $\Sigma_a, \Sigma_b$, and $\Sigma_c$, however, and only then combination

$$|\Phi\rangle = \frac{1}{\sqrt{2}}\Big(|+++\rangle - |---\rangle\Big) \tag{17.65}$$

satisfies the original conditions (17.62). This is an entangled 3-particle state of total spin 3/2. It is referred to as a GHZ (Greenberger-Horne-Zeilinger) state. Such entangled states have remarkable properties. They also allow one to exhibit the conflict between the predictions of quantum theory and of hidden variable theory even more dramatically.

The product of the operators $\Sigma_a, \Sigma_b$, and $\Sigma_c$ is also an observable,

$$\begin{aligned}
\Sigma &= \sigma_a^x \otimes \sigma_b^x \otimes \sigma_c^x \\
&= -\Sigma_a \Sigma_b \Sigma_c
\end{aligned} \tag{17.66}$$

of which $|\Phi\rangle$ is obviously an eigenstate with eigenvalue $-1$.

Now if the measurements of $\sigma_{a,b,c}^{x,y}$ really had independent physical reality, as hidden variable theory proclaims, then we can again make a list of all possible outcomes of measurements by three observers $A, B, C$. Denoting these outcomes $A_x, B_y, C_y$ etc, we are led to the following relations in view of the fact that the state $|\Phi\rangle$ measured here satisfies (17.62),

$$\begin{aligned}
A_x B_y C_y &= +1 \\
A_y B_x C_y &= +1 \\
A_y B_y C_x &= +1
\end{aligned} \tag{17.67}$$

As a result, the measurement of the observable $\sigma_a^x \otimes \sigma_b^x \otimes \sigma_c^x$ will yield

$$A_x B_x C_x = (A_x B_y C_y)(A_y B_x C_y)(A_y B_y C_x) = +1 \tag{17.68}$$

since we have $A_y^2 = B_y^2 = C_y^2 = +1$. But this is in blatant contradiction with the eigenvalue of the operator $\Sigma$ which is $-1$.

# 18 Introductory Remarks on Quantized Fields

Quantum Field Theory (abbreviated QFT) deals with the quantization of fields. A familiar example of a field is provided by the electromagnetic field. Classical electromagnetism describes the dynamics of electric charges and currents, as well as electro-magnetic waves, such as radio waves and light, in terms of Maxwell's equations. At the atomic level, however, the quantum nature of atoms as well as the quantum nature of electromagnetic radiation must be taken into account. Quantum mechanically, electromagnetic waves turn out to be composed of quanta of light, whose individual behavior is closer to that of a particle than to a wave. Remarkably, the quantization of the electromagnetic field is in terms of the quanta of this field, which are particles, also called *photons*. In QFT, this field particle correspondence is used both ways, and it is one of the key assumptions of QFT that to every elementary particle, there corresponds a field. Thus, the electron will have its own field, and so will every quark.

Quantum Field Theory provides an elaborate general formalism for the field–particle correspondence. The advantage of QFT will be that it can naturally account for the creation and annihilation of particles, which ordinary quantum mechanics of the Schrödinger equation could not describe. The fact that the number of particles in a system can change over time is a very important phenomenon, which takes place continuously in everyone's daily surroundings, but whose significance may not have been previously noticed.

In *classical mechanics*, the number of particles in a closed system is conserved, i.e. the total number of particles is unchanged in time. To each pointlike particle, one associates a set of position and momentum coordinates, the time evolution of which is governed by the dynamics of the system. *Quantum mechanics* may be formulated in two stages.

1. The *principles of quantum mechanics*, such as the definitions of states, observables, are general and do not make assumptions on whether the number of particles in the system is conserved during time evolution.

2. The *specific dynamics of the quantum system*, described by the Hamiltonian, may or may not assume particle number conservation. In introductory quantum mechanics, dynamics is usually associated with non-relativistic mechanical systems (augmented with spin degrees of freedom) and therefore assumes a fixed number of particles. In many important quantum systems, however, *the number of particles is not conserved*.

A familiar and ubiquitous example is that of *electromagnetic radiation*. An excited atom may decay into its ground state by emitting a single quantum of light or photon. The photon was not "inside" the excited atom prior to the emission; it was "created" by the excited atom during its transition to the grounds state. This is well illustrated as follows. An atom in a state of sufficiently high excitation may decay to its ground state in a single step by emitting a single photon. However, it may also emit a first photon to a lower excited state which in turn re-emits one or more photons in order to decay to the ground state (see Figure **??**, (a) and (b)). Thus, given initial and final states, the number of photons emitted may vary, lending further support to the fact that no photons are "inside" the excited state to begin with.

Other systems where particle number is not conserved involve *phonons* and *spin waves* in condensed matter problems. Phonons are the quanta associated with vibrational modes of a crystal or fluid, while spin waves are associated with fluctuating spins. The number of particles is also not conserved in nuclear processes like fusion and fission.

## 18.1  Relativity and quantum mechanics

Special relativity invariably implies that the number of particles is not conserved. Indeed, one of the key results of special relativity is the fact that mass is a form of energy. A particle at rest with mass $m$ has a rest energy given by the famous formula

$$E = mc^2 \tag{18.1}$$

The formula also implies that, given enough energy, one can *create particles* out of just energy – kinetic energy for example. This mechanism is at work in fire and light bulbs, where energy is being provided from chemical combustion or electrical input to excite atoms which then emit light in the form of photons. The mechanism is also being used in particle accelerators to produce new particles through the collision of two incoming particles. In Figure **??** the example of a photon scattering off an electron is illustrated. In (c), a photon of low energy ($\ll m_e c^2$) is being scattered elastically which results simply in a deflection of the photon and a recoil of the electron. In (d), a photon of high energy ($\gg m_e c^2$) is being scattered inelastically, resulting not only in a deflection of the photon and a recoil of the electron, but also in the *production of new particles*.

The particle data table also provides numerous examples of particles that are unstable and decay. In each of these processes, the number of particles is *not conserved*. To list just a few,

$$
\begin{aligned}
n &\rightarrow p^+ + e^- + \bar{\nu}_e \\
\pi^0 &\rightarrow \gamma + \gamma \\
\pi^+ &\rightarrow \mu^+ + \nu_\mu \\
\mu^+ &\rightarrow e^+ + \nu_e + \bar{\nu}_\mu
\end{aligned}
$$
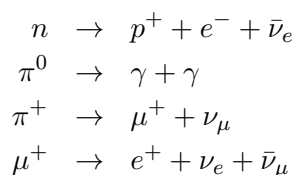
As already mentioned, nuclear processes such as fusion and fission are further examples of systems in which the number of particles is not conserved.

## 18.2  Why Quantum Field Theory ?

Quantum Field Theory is a formulation of a quantum system in which the number of particles does not have to be conserved but may vary freely. QFT does not require a change in the principles of either quantum mechanics or relativity. QFT requires a different formulation of the dynamics of the particles involved in the system.

Clearly, such a description must go well beyond the usual Schrödinger equation, whose very formulation requires that the number of particles in a system be fixed. Quantum field theory may be formulated for non-relativistic systems in which the number of particles is not conserved, (recall

spin waves, phonons, spinons etc). Here, however, we shall concentrate on *relativistic quantum field theory* because relativity forces the number of particles not to be conserved. In addition, relativity is one of the great fundamental principles of Nature, so that its incorporation into the theory is mandated at a fundamental level.

## 18.3   Further conceptual changes required by relativity

Relativity introduces some further fundamental changes in both the nature and the formalism of quantum mechanics. We shall just mention a few.

- **Space versus time**

    In non-relativistic quantum mechanics, the position $x$, the momentum $p$ and the energy $E$ of free or interacting particles are all observables. This means that each of these quantities *separately* can be *measured* to arbitrary precision in an arbitrarily short time. By contrast, the accurarcy of the simultaneous measurement of $x$ and $p$ is limited by the Heisenberg uncertainty relations,

$$\Delta x \ \Delta p \ \sim \hbar$$

There is also an energy-time uncertainty relation $\Delta E \ \Delta t \sim \hbar$, but its interpretation is quite different from the relation $\Delta x \ \Delta p \ \sim \hbar$, because in ordinary quantum mechanics, time is viewed as a parameter and not as an observable. Instead the energy-time uncertainty relation governs the time evolution of an interacting system. In relativistic dynamics, particle-antiparticle pairs can always be created, which subjects an interacting particle always to a cloud of pairs, and thus inherently to an uncertainty as to which particle one is describing. Therefore, the momentum itself is no longer an instantaneous observable, but will be subject to the a momentum-time uncertainty relation $\Delta p \ \Delta t \sim \hbar/c$. As $c \to \infty$, this effect would disappear, but it is relevant for relativistic processes. Thus, momentum can only be observed with precision away from the interaction region.

   Special relativity puts space and time on the same footing, so we have the choice of either treating space and time both as observables (a bad idea, even in quantum mechanics) or to treat them both as parameters, which is how QFT will be formulated.

- **"Negative energy" solutions and anti-particles**

    The kinetic law for a relativistic particle of mass $m$ is

$$E^2 = m^2 c^4 + p^2 c^2$$

Positive and negative square roots for $E$ naturally arise. Classically of course one may just keep positive energy particles. Quantum mechanically, interactions induce transitions to negative energy states, which therefore cannot be excluded arbitrarily. Following Feynman, the correct interpretation is that these solutions correspond to negative frequencies, which describe physical anti-particles with positive energy traveling "backward in time".

- **Local Fields and Local Interactions**

    Instantaneous forces acting at a distance, such as appear in Newton's gravitational force and Coulomb's electrostatic force, are incompatible with special relativity. No signal can travel faster

than the speed of light. Instead, in a relativistic theory, the interaction must be *mediated* by another particle. That particle is the graviton for the gravitational force and the photon for the electromagnetic force. The true interaction then occurs at an instant in time and at a point in space, thus expressing the forces in terms of *local interactions* only. Thus, the Coulomb force is really a limit of relativistic "retarded" and "advanced" interactions, mediated by the exchange of photons. The exchange is pictorially represented in Figure **??**.

One may realize this picture concretely in terms of local fields, which have local couplings to one another. The most basic prototype for such a field is the electro-magnetic field. Once a field has been associated to the photon, then it will become natural to associate a field to every particle that is viewed as *elementary* in the theory. Thus, electrons and positrons will have their (Dirac) field. There was a time that a field was associated also to the proton, but we now know that the proton is composite and thus, instead, there are now fields for quarks and gluons, which are the elementary particles that make up a proton. The gluons are the analogs for the strong force of the photon for the electro-magnetic force, namely the gluons mediate the strong force. Analogously, the $W^{\pm}$ and $Z^0$ mediate the weak interactions.

## 18.4   Some History and present significance of QFT

The quantization of the elctro-magnetic field was initiated by Born, Heisenberg and Jordan in 1926, right after quantum mechanics had been given its definitive formulation by Heisenberg and Schrödinger in 1925. The complete formulation of the dynamics was given by Dirac Heiseberg and Pauli in 1927. Infinities in perturbative corrections due to high energy (or UV – ultraviolet) effects were first studied by Oppenheimer and Bethe in the 1930's. It took until 1945-49 until Tomonaga, Schwinger and Feynman gave a completely relativistic formulation of Quantum Electrodynamics (or QED) and evaluated the radiative corrections to the magnetic moment of the electron. In 1950, Dyson showed that the UV divergences of QED can be systematically dealt with by the process of renormalization.

In the 1960's Glashow, Weinberg and Salam formulated a renormalizable quantum field theory of the weak interactions in terms of a Yang-Mills theory. Yang-Mills theory was shown to be renormalizable by 't Hooft in 1971, a problem that was posed to him by his advisor Veltman. In 1973, Gross, Wilczek and Politzer discovered asymptotic freedom of certain Yang-Mills theories (the fact that the strong force between quarks becomes weak at high energies) and using this unique clue, they formulated (independently also Weinberg) the quantum field theory of the strong interactions. Thus, the elctro-magnetic, weak and strong forces are presently described – and very accurately so – by quantum field theory, specifically Yang-Mills theory, and this combined theory is usually referred to as *the STANDARD MODEL.* To give just one example of the power of the quantum field theory approach, one may quote the experimentally measured and theoretically calculated values of the muon magnetic dipole moment,

$$
\begin{aligned}
\frac{1}{2}g_\mu(\text{exp}) &= 1.001159652410(200) \\
\frac{1}{2}g_\mu(\text{thy}) &= 1.001159652359(282)
\end{aligned}
\tag{18.2}
$$

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revealing an astounding degree of agreement.

The gravitational force, described classically by Einstein's general relativity theory, does not seem to lend itself to a QFT description. String theory appears to provide a more appropriate description of the quantum theory of gravity. String theory is an extension of QFT, whose very formulation is built squarely on QFT and which reduces to QFT in the low energy limit.

The devlopment of quantum field theory has gone hand in hand with developments in Condensed Matter theory and Statistical Mechanics, especially critical phenomena and phase transitions.

A final remark is in order on QFT and mathematics. Contrarily to the situation with general relativity and quantum mechanics, there is no good "axiomatic formulation" of QFT, i.e. one is very hard pressed to lay down a set of simple postulates from which QFT may then be constructed in a deductive manner. For many years, physicists and mathematicians have attempted to formulate such a set of axioms, but the theories that could be fit into this framework almost always seem to miss the physically most relevant ones, such as Yang-Mills theory. Thus, to date, there is no satsifactory mathematical "definition" of a QFT.

Conversely, however, QFT has had a remarkably strong influence on mathematics over the past 25 years, with the development of Yang-Mills theory, instantons, monopoles, conformal field theory, Chern-Simons theory, topological field theory and superstring theory. Some developments is QFT have led to revolutions in mathematics, such as Seiberg-Witten theory. It is suspected by some that this is only the tip of the iceberg, and that we are only beginning to have a glimpse at the powerful applications of quantum field theory to mathematics.

# 19 Quantization of the Free Electro-magnetic Field

We shall begin by presenting a brief review of classical Maxwell theory, and then proceed to the quantization of the free Maxwell field.

## 19.1 Classical Maxwell theory

Maxwell's equations for the electric field $\mathbf{E}$ and the magnetic field $\mathbf{B}$, in the presence of an electric charge density $\rho$ and an electric charge current density $\mathbf{j}$ are usually divided into two groups. The first group of equations does not involve $\rho$ and $\mathbf{j}$ and is given as follows,

$$
\begin{aligned}
\nabla \times \mathbf{E} &= -\partial_t \mathbf{B} \\
\nabla \cdot \mathbf{B} &= 0
\end{aligned}
\tag{19.1}
$$

while the second group depends on $\rho$ and $\mathbf{j}$, and is given by

$$
\begin{aligned}
\nabla \times \mathbf{B} &= \frac{1}{c^2}\partial_t \mathbf{E} + \mu_0 \mathbf{j} \\
\nabla \cdot \mathbf{E} &= \frac{1}{\varepsilon_0}\rho
\end{aligned}
\tag{19.2}
$$

Integrability of the equations in the second group (19.2) requires (local) electric charge conservation,

$$
\nabla \cdot \mathbf{j} + \partial_t \rho = 0
\tag{19.3}
$$

Maxwell's equations are inconsistent unless this equation holds. Notice that $c^2 \varepsilon_0 \mu_0 = 1$, where $c$, $\varepsilon_0$, and $\mu_0$ are respectively the speed of light, the electric permittivity and the magnetic permeability in vacuum.

The two equations in (19.1) may be completely solved in terms of a scalar potential $A_0$, and a vector potential $\mathbf{A}$, as follows,

$$
\begin{aligned}
\mathbf{E} &= \nabla A_0 - \partial_t \mathbf{A} \\
\mathbf{B} &= \nabla \times \mathbf{A}
\end{aligned}
\tag{19.4}
$$

Note that the customary electric potential $\Phi$ is related to $A_0$ by $A_0 = -\Phi$. Given $\mathbf{E}$ and $\mathbf{B}$, the corresponding scalar and vector potentials are not unique, since $\mathbf{E}$ and $\mathbf{B}$ are invariant under the following *gauge transformations*,

$$
\begin{aligned}
A_0 &\rightarrow A_0' = A_0 + \partial_t \Lambda \\
\mathbf{A} &\rightarrow \mathbf{A}' = \mathbf{A} + \nabla \Lambda
\end{aligned}
\tag{19.5}
$$

where $\Lambda$ is an arbitrary function of $t$ and $\mathbf{x}$. This arbitrariness allows us to impose one extra scalar condition on $(A_0, \mathbf{A})$, and such a condition is referred to as a *gauge condition*, or a *gauge choice*.

For the problems of radiation which we shall be interested in here, one particularly convenient choice is the *transverse or radiation gauge*,

$$\nabla \cdot \mathbf{A} = 0 \tag{19.6}$$

Given fields $A_0$ and $\mathbf{A}$, the explicit gauge transformation $\Lambda$ that transform $\nabla \cdot \mathbf{A}$ obeys the following relation, $\nabla \cdot \mathbf{A} - \Delta\Lambda = 0$, whose general solution is given by,

$$\Lambda(t, \mathbf{x}) = \int d^3\mathbf{x}' \frac{1}{4\pi|\mathbf{x}' - \mathbf{x}|} \nabla \cdot \mathbf{A}(t, \mathbf{x}') \tag{19.7}$$

where we have used the basic Coulomb equation, $\Delta(1/|\mathbf{x}|) = -4\pi\delta^{(3)}(\mathbf{x})$. This gauge transformation is then to be carried out on both $A_0$ and $\mathbf{A}$. In transverse gauge, Gauss's law, namely $\nabla \cdot \mathbf{E} = \rho/\varepsilon_0$ allow one to solve for the electric potential $A_0$, and we find,

$$A_0(t, \mathbf{x}) = -\int d^3\mathbf{x}' \frac{1}{4\pi\varepsilon_0|\mathbf{x}' - \mathbf{x}|} \rho(t, \mathbf{x}') \tag{19.8}$$

Since, in the transverse gauge, the field $A_0$, and its time-dependence, are completely determined by the external source $\rho$, the field $A_0$ has *no dynamics*. The field $\mathbf{A}$ may be solved for in an analogous fashion. Expressing $\mathbf{E}$ and $\mathbf{B}$ in terms of $A_0$ and $\mathbf{A}$, using (19.4), the general relation

$$\nabla \times (\nabla \times \mathbf{A}) = -\Delta\mathbf{A} - \nabla(\nabla \cdot \mathbf{A}) \tag{19.9}$$

as well as the transverse gauge condition (19.6), we find that $\mathbf{A}$ obeys the following wave-like equation,

$$\frac{1}{c^2}\partial_t^2\mathbf{A} - \Delta\mathbf{A} = \mu_0\mathbf{j} - \frac{1}{c^2}\partial_t\nabla A_0 \tag{19.10}$$

where $A_0$ is now viewed as given in terms of $\rho$ by (19.8). Because in $\partial_t\nabla A_0$, only the $t$-derivative of $\rho$ enters, we are free to use the charge conservation equation (19.3), and replace $\partial_t\rho$ by $-\nabla \cdot \mathbf{j}$. The result may be expressed as follows,

$$\frac{1}{c^2}\partial_t^2\mathbf{A} - \Delta\mathbf{A} = \mu_0\mathbf{j}_\perp \tag{19.11}$$

where $\mathbf{j}_\perp$ is given by

$$\mathbf{j}_\perp(t, \mathbf{x}) = \mathbf{j}(t, \mathbf{x}) - \nabla \int d^3\mathbf{x}' \frac{1}{4\pi|\mathbf{x}' - \mathbf{x}|} \nabla \cdot \mathbf{j}(t, \mathbf{x}') \tag{19.12}$$

Since Maxwell's equations, for given external sources $\rho$ and $\mathbf{j}$ are linear, they may be solved explicitly.

The Lagrangian $L$ and Hamiltonian $H$ are given as integrals over the space of the Lagrangian density $\mathcal{L}$ and Hamiltonian density $\mathcal{H}$ respectively as follows,

$$L = \int d^3\mathbf{x}\,\mathcal{L} \qquad\qquad \mathcal{L} = \frac{1}{2}\varepsilon_0\mathbf{E}^2 - \frac{1}{2\mu_0}\mathbf{B}^2 + \rho A_0 + \mathbf{A} \cdot \mathbf{j}$$

$$H = \int d^3\mathbf{x}\,\mathcal{H} \qquad\qquad \mathcal{H} = \frac{1}{2}\varepsilon_0\mathbf{E}^2 + \frac{1}{2\mu_0}\mathbf{B}^2 - \rho A_0 - \mathbf{A} \cdot \mathbf{j} \tag{19.13}$$

In the Hamiltonian formalism, the momentum $\Pi_i$ canonically conjugate to $A_i$ is given by

$$\Pi_i = \frac{\partial \mathcal{L}}{\partial \dot{A}_i} = \varepsilon_0 \dot{A}_i = -\varepsilon_0 E_i \tag{19.14}$$

Now, in general, it is an enormous nuisance to keep the quantities $\varepsilon_0$, $\mu_0$, and even $c$ explicit. Thus, henceforth, we shall set $\varepsilon_0 = \mu_0 = c = 1$. Using dimensional analysis, these constants may always be restored in a unique way.

## 19.2   Fourrier modes and radiation oscillators

We begin by considering and solving Maxwell's equations without sources, namely for $\rho = \mathbf{j} = 0$, in which case we are left to solve the following equations,

$$\begin{aligned} \partial_t^2 \mathbf{A} - \Delta \mathbf{A} &= 0 \\ \nabla \cdot \mathbf{A} &= 0 \end{aligned} \tag{19.15}$$

Both are linear partial differential equations with constant coefficients, and may be solved using Fourrier analysis. It will be convenient to Fourrier transform only in space, but not in time; thus we define this Fourrier transform $\mathbf{C}(t, \mathbf{k})$ by,

$$\mathbf{A}(t, \mathbf{x}) = \int \frac{d^3 \mathbf{k}}{(2\pi)^3}\, \mathbf{C}(t, \mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{x}} \tag{19.16}$$

so that (19.15) reduce to,

$$\begin{aligned} (\partial_t^2 + \mathbf{k}^2)\mathbf{C}(t, \mathbf{k}) &= 0 \\ \mathbf{k} \cdot \mathbf{C}(t, \mathbf{k}) &= 0 \end{aligned} \tag{19.17}$$

The Fourrier transform $\mathbf{C}(t, \mathbf{k})$ is a complex function. Thus, the reality of the field $\mathbf{A}$ requires a complex conjugation relation on $\mathbf{C}$,

$$\mathbf{C}(t, -\mathbf{k})^* = \mathbf{C}(t, \mathbf{k}) \tag{19.18}$$

The last equation of (19.17) implies that for any given $\mathbf{k}$, the Fourrier transform $\mathbf{C}(t, \mathbf{k})$ is perpendicular, or *transverse*, to the momentum $\mathbf{k}$, whence the name for this gauge condition. Thus, for given $\mathbf{k}$, $\mathbf{C}(t, \mathbf{k})$ takes values in the 2-dimensional space orthogonal to $\mathbf{k}$. It will be convenient to choose a basis of two orthonormal vectors $\varepsilon_\alpha(\mathbf{k})$ for this transverse space,

$$\begin{aligned} \mathbf{k} \cdot \varepsilon_\alpha(\mathbf{k}) &= 0 \\ \varepsilon_\alpha^*(\mathbf{k}) \cdot \varepsilon_\beta(\mathbf{k}) &= \delta_{\alpha,\beta} \qquad\qquad \alpha, \beta = 1, 2 \end{aligned} \tag{19.19}$$

The first equation of (19.17) on $\mathbf{C}$ is a harmonic oscillator with frequency

$$\omega = \omega_{\mathbf{k}} = |\mathbf{k}| \tag{19.20}$$

whose general solution is a linear combination of $e^{i\omega t}$ and $e^{-i\omega t}$. Combining now the solution for all equations on $\mathbf{C}$, we have

$$\mathbf{C}(t, \mathbf{k}) = \frac{1}{\sqrt{2\omega}} \sum_{\alpha=1,2} \left( \varepsilon_\alpha(\mathbf{k}) a_\alpha(\mathbf{k}) e^{-i\omega t} + \varepsilon'_\alpha(\mathbf{k}) a'_\alpha(\mathbf{k}) e^{+i\omega t} \right) \tag{19.21}$$

where $a_\alpha(\mathbf{k})$ and $\alpha'_\alpha(\mathbf{k})$ are arbitrary complex coefficients. The overall normalization factor $1/\sqrt{2\omega}$ is not fixed by the Maxwell's equations, but has been introduced for later convenience. By construction, this expression automatically solves both equations in (19.15). It remains to enforce the complex conjugation condition. To this end, we compute,

$$\mathbf{C}(t, -\mathbf{k})^* = \frac{1}{\sqrt{2\omega}} \sum_{\alpha=1,2} \left( \varepsilon_\alpha(-\mathbf{k})^* a_\alpha(-\mathbf{k})^* e^{+i\omega t} + \varepsilon'_\alpha(-\mathbf{k})^* a'_\alpha(-\mathbf{k})^* e^{-i\omega t} \right) \tag{19.22}$$

Equating with $\mathbf{C}(t, \mathbf{k})$, as required by (19.18) requires that $\varepsilon'_\alpha(\mathbf{k}) a'_\alpha(\mathbf{k}) = \varepsilon_\alpha(-\mathbf{k})^* a_\alpha(-\mathbf{k})^*$ for all $\mathbf{k}$. Next, we make use of the fact that the basis $\varepsilon'_\alpha(\mathbf{k})$ may be related to the basis $\varepsilon_\alpha(bk)$, as long as both obey the equations of (19.19). Thus, we have,

$$\begin{aligned} \varepsilon'_\alpha(\mathbf{k}) &= \varepsilon_\alpha(-\mathbf{k})^* \\ a_\alpha(\mathbf{k})' &= a_\alpha(-\mathbf{k})^* \end{aligned} \tag{19.23}$$

Putting all together, we have,

$$\mathbf{C}(t, \mathbf{k}) = \frac{1}{\sqrt{2\omega}} \sum_{\alpha=1,2} \left( \varepsilon_\alpha(\mathbf{k}) a_\alpha(\mathbf{k}) e^{-i\omega t} + \varepsilon_\alpha(-\mathbf{k})^* a_\alpha(-\mathbf{k})^* e^{+i\omega t} \right) \tag{19.24}$$

To complete our solution, we substitute this result into the Fourrier transform of (19.16),

$$\mathbf{A}(t, \mathbf{x}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{1}{\sqrt{2\omega}} \sum_{\alpha=1,2} \left( \varepsilon_\alpha(\mathbf{k}) a_\alpha(\mathbf{k}) e^{-ik\cdot x} + \varepsilon_\alpha(\mathbf{k})^* a_\alpha(\mathbf{k})^* e^{+ik\cdot x} \right) \tag{19.25}$$

Here, we have started to use relativity notation for the inner product of the two 4-vectors $k$ and $x$,

$$k \cdot x \equiv \omega t - \mathbf{k} \cdot \mathbf{x} \tag{19.26}$$

The expression (19.25) provides a complete solution for the vector potential to Maxwell's equations in transverse gauge.

## 19.3   The Hamiltonian in terms of radiation oscillators

In the absence of electric charge density and current, the Maxwell Hamiltonian is simply,

$$H = \int d^3\mathbf{x} \left( \frac{1}{2}\mathbf{E}^2 + \frac{1}{2}\mathbf{B}^2 \right) \tag{19.27}$$

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To evaluate $H$ in terms of the vector potential, in transverse gauge, we use the expressions $\mathbf{E} = -\partial_t \mathbf{A}$ and $\mathbf{B} = \nabla \times \mathbf{A}$, which themselves may be expressed in terms of the oscillator variables $a_\alpha(\mathbf{k})$ as follows,

$$\mathbf{E}(t,\mathbf{x}) = -\int \frac{d^3\mathbf{k}}{(2\pi)^3} \partial_t \mathbf{C}(t,\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{x}}$$

$$\mathbf{B}(t,\mathbf{x}) = i\int \frac{d^3\mathbf{k}}{(2\pi)^3} \mathbf{k} \times \mathbf{C}(t,\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{x}} \tag{19.28}$$

The electric contribution to the Hamiltonian is calculated as follows,

$$\int d^3\mathbf{x}\, \mathbf{E}^2 = \int d^3\mathbf{x} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \partial_t \mathbf{C}(t,\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} \int \frac{d^3\mathbf{k}'}{(2\pi)^3} \partial_t \mathbf{C}(t,\mathbf{k}')e^{i\mathbf{k}'\cdot\mathbf{x}} \tag{19.29}$$

The use of the Fourrier equation

$$\int d^3\mathbf{x}\, e^{i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{x}} = (2\pi)^3 \delta^{(3)}(\mathbf{k}+\mathbf{k}') \tag{19.30}$$

implies that the $\mathbf{k}'$-integral can be carried out explicitly, and results in the following expression for the electric part of the Hamiltonian,

$$\frac{1}{2}\int d^3\mathbf{x}\, \mathbf{E}^2 = \frac{1}{2}\int \frac{d^3\mathbf{k}}{(2\pi)^3} \partial_t \mathbf{C}(t,\mathbf{k}) \cdot \partial_t \mathbf{C}(t,-\mathbf{k})$$

$$= \frac{1}{2}\int \frac{d^3\mathbf{k}}{(2\pi)^3} \partial_t \mathbf{C}(t,\mathbf{k}) \cdot \partial_t \mathbf{C}(t,\mathbf{k})^* \tag{19.31}$$

The magnetic part is computed analogously, and we find,

$$\frac{1}{2}\int d^3\mathbf{x}\, \mathbf{B}^2 = \frac{1}{2}\int \frac{d^3\mathbf{k}}{(2\pi)^3} \mathbf{k}^2 \mathbf{C}(t,\mathbf{k}) \cdot \mathbf{C}(t,\mathbf{k})^* \tag{19.32}$$

As a result, the full Hamiltonian is given by

$$H = \frac{1}{2}\int \frac{d^3\mathbf{k}}{(2\pi)^3}\left(\partial_t \mathbf{C}(t,\mathbf{k}) \cdot \partial_t \mathbf{C}(t,\mathbf{k})^* + \mathbf{k}^2 \mathbf{C}(t,\mathbf{k}) \cdot \mathbf{C}(t,\mathbf{k})^*\right) \tag{19.33}$$

Next, we proceed to express $H$ in terms of the oscillator degrees of freedom $a_\alpha(\mathbf{k})$, with the help of (19.24). First, evaluate

$$\partial_t \mathbf{C}(t,\mathbf{k}) \cdot \partial_t \mathbf{C}(t,\mathbf{k})^* + \mathbf{k}^2 \mathbf{C}(t,\mathbf{k}) \cdot \mathbf{C}(t,\mathbf{k})^*$$
$$= |\mathbf{k}|\sum_{\alpha,\beta}\left(\varepsilon_\alpha(\mathbf{k}) \cdot \varepsilon_\beta(\mathbf{k})^* \, a_\alpha(\mathbf{k})\alpha_\beta(\mathbf{k})^* + \varepsilon_\alpha^* \cdot \varepsilon_\beta \, a_\alpha(-\mathbf{k})^*\alpha_\beta(-\mathbf{k})\right) \tag{19.34}$$

Using orthogonality $\varepsilon_\alpha \cdot \varepsilon_\beta^* = \delta_{\alpha\beta}$, we find,

$$\partial_t \mathbf{C}(t,\mathbf{k}) \cdot \partial_t \mathbf{C}(t,\mathbf{k})^* + \mathbf{k}^2 \mathbf{C}(t,\mathbf{k}) \cdot \mathbf{C}(t,\mathbf{k})^*$$
$$= |\mathbf{k}|\sum_{\alpha}\left(a_\alpha(\mathbf{k})\alpha_\alpha(\mathbf{k})^* + a_\alpha(-\mathbf{k})^*\alpha_\alpha(-\mathbf{k})\right) \tag{19.35}$$

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so that we have the following expression for the full Hamiltonian,

$$H = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \sum_\alpha |\mathbf{k}| \, a_\alpha(\mathbf{k})^* \alpha_\alpha(\mathbf{k}) \tag{19.36}$$

The Poisson brackets of $a_\alpha(\mathbf{k})$ with $a_\alpha(\mathbf{k}')$ and with $a_\alpha(\mathbf{k}')^*$ may be induced from the time evolution equations for these oscillators, which are already available to us, namely,

$$a_\alpha(t, \mathbf{k}) = a_\alpha(0, \mathbf{k}) \, e^{-i|\mathbf{k}|t} \tag{19.37}$$

As a result, we have

$$\partial_t a_\alpha(t, \mathbf{k}) = -i|\mathbf{k}| a_\alpha(t, \mathbf{k}) = \{H, a_\alpha(t, \mathbf{k})\} \tag{19.38}$$

which is naturally realized in terms of

$$\begin{aligned}
\{a_\alpha(\mathbf{k}), \alpha_\beta(\mathbf{k}')\} &= 0 \\
\{a_\alpha(\mathbf{k}), \alpha_\beta(\mathbf{k}')^*\} &= i\delta_{\alpha\beta}\delta^{(3)}(\mathbf{k}' - \mathbf{k})
\end{aligned} \tag{19.39}$$

One recognizes this Hamiltonian, and associated Poisson brackets as those corresponding to an infinite number of independent harmonic oscillators $a_\alpha(\mathbf{k})$, labelled by the combined index $(\alpha, \mathbf{k})$. One may pass, formally, to a more familiar notation for the harmonic oscillators in terms of real degrees of freedom $x_\alpha(\mathbf{k})$ and $p_\alpha(\mathbf{k})$,

$$\begin{aligned}
a_\alpha(\mathbf{k}) &= \frac{1}{\sqrt{2\omega}}\left( + ip_\alpha(\mathbf{k}) + \omega x_\alpha(\mathbf{k}) \right) \\
a_\alpha(\mathbf{k})^* &= \frac{1}{\sqrt{2\omega}}\left( - ip_\alpha(\mathbf{k}) + \omega x_\alpha(\mathbf{k}) \right)
\end{aligned} \tag{19.40}$$

in terms of which the Hamiltonian takes the form

$$H = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \sum_\alpha \left( \frac{1}{2} p_\alpha(\mathbf{k})^2 + \frac{1}{2}\omega^2 \, x_\alpha(\mathbf{k})^2 \right) \tag{19.41}$$

where the Poisson brackets take the form,

$$\begin{aligned}
\{x_\alpha(\mathbf{k}), p_\alpha(\mathbf{k}')\} &= \delta_{\alpha\beta}\delta^{(3)}(\mathbf{k}' - \mathbf{k}) \\
\{x_\alpha(\mathbf{k}), x_\alpha(\mathbf{k}')\} &= 0 \\
\{p_\alpha(\mathbf{k}), p_\alpha(\mathbf{k}')\} &= 0
\end{aligned} \tag{19.42}$$

Of course, it must be pointed out that $x_\alpha$ and $p_\alpha$ are not actual positions and momentum operators of the photon. They are formal devices without direct physical meaning.

## 19.4    Momentum in terms of radiation oscillators

The classical electro-magnetic field carries momentum, which may be expressed in terms of the Poynting vector,

$$\mathbf{P} = \int d^2\mathbf{x}\, \mathbf{E}(t,\mathbf{x}) \times \mathbf{B}(t,\mathbf{x}) \tag{19.43}$$

This qunatity may be similarly expressed in terms of the radiation oscillators $a_\alpha$, in a manner analogous to energy, and we have

$$\mathbf{P} = i \int \frac{d^3\mathbf{k}}{(2\pi)^3} \partial_t \mathbf{C}(t,\mathbf{k}) \times \Big(\mathbf{k} \times \mathbf{C}(t,\mathbf{k})\Big) \tag{19.44}$$

Expressing $\mathbf{C}$ in terms of $a_\alpha$ and $a_\alpha^*$, using the algebraic identity

$$\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = \mathbf{B}(\mathbf{A} \cdot \mathbf{C}) - \mathbf{C}(\mathbf{A} \cdot \mathbf{B}) \tag{19.45}$$

applied to the problem at hand yields

$$\varepsilon_\alpha(\mathbf{k}) \times \Big(\mathbf{k} \times \varepsilon_\beta(-\mathbf{k})\Big) = \mathbf{k}\, \varepsilon_\alpha(\mathbf{k}) \cdot \varepsilon_\beta(-\mathbf{k}) \tag{19.46}$$

The integral of (19.44) contains a part in $e^{-2i\omega t}$, one in $e^{2i\omega t}$, and finally one independent of $t$. The first one of these is proportional to

$$\sum_{\alpha,\beta} \mathbf{k}\, \varepsilon_\alpha(\mathbf{k}) \cdot \varepsilon_\beta(-\mathbf{k}) \alpha_\alpha(\mathbf{k}) \alpha_\beta(-\mathbf{k}) \tag{19.47}$$

which is odd in $\mathbf{k}$, and whose integral over $\mathbf{k}$ thus vanishes. The second term similarly vanishes. The $t$-independent term is the only one that contributes, and we have

$$\mathbf{P} = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \mathbf{k} \sum_\alpha \alpha_\alpha(\mathbf{k})^* \alpha_\alpha(\mathbf{k}) \tag{19.48}$$

## 19.5    Canonical quantization of electro-magnetic fields

From the above classical discussion of the electro-magnetic fields, it is manifest that their dynamics is equivalent to that of an infinite number of harmonic oscillators

$$a_\alpha(\mathbf{k}) \qquad\qquad a_\alpha(\mathbf{k})^* \qquad\qquad \alpha = 1,2 \qquad \mathbf{k} \in \mathbf{R}^3 \tag{19.49}$$

We shall now *quantize the electro-magnetic field* by canonically quantizing each of the harmonic oscillators which build up the field. Thus, $a_\alpha(\mathbf{k})$ is to be viewed as an operator on (an until now undetermined) Hilbert space. Together with its adjoint $a_\alpha^\dagger(\mathbf{k})$, the oscillators satisfy the following canonical commutation relations,

$$
\begin{aligned}
{[a_\alpha(\mathbf{k}), a_\beta(\mathbf{k}')]} &= 0 \\
{[a_\alpha^\dagger(\mathbf{k}), a_\beta^\dagger(\mathbf{k}')]} &= 0 \\
{[a_\alpha(\mathbf{k}), a_\beta^\dagger(\mathbf{k}')]} &= (2\pi)^3 \delta_{\alpha\beta} \delta^{(3)}(\mathbf{k} - \mathbf{k}')
\end{aligned}
\tag{19.50}
$$

The only novelty here, as compared with systems of finite numbers of harmonic oscillators, is that here, the oscillators are indexed by a continuous variable $\mathbf{k}$, and the Kronecker $\delta$ in the commutation relations is replaced by a Dirac $\delta$-function.

The Hamiltonian and momentum operators take the following values,

$$
\begin{aligned}
H &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} \, \omega \sum_\alpha a_\alpha^\dagger(\mathbf{k}) a_\alpha(\mathbf{k}) \\
\mathbf{P} &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} \, \mathbf{k} \sum_\alpha a_\alpha^\dagger(\mathbf{k}) a_\alpha(\mathbf{k})
\end{aligned}
\tag{19.51}
$$

Note that the Hamiltonian, given above, involves a choice. The classical Hamiltonian was expressed in terms of $a_\alpha(\mathbf{k})^* a_\alpha(\mathbf{k})$, a quantity whose translation into an operator via the correspondence principle, is ambiguous. In general, either ordering of the operators might have occurred, or any linear combination of the two orderings, such as

$$
H_\lambda = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \, \omega \sum_\alpha \left( (1-\lambda) a_\alpha^\dagger(\mathbf{k}) a_\alpha(\mathbf{k}) + \lambda a_\alpha(\mathbf{k}) a_\alpha^\dagger(\mathbf{k}) \right)
\tag{19.52}
$$

so that the original Hamiltonian $H$ corresponds to $H = H_0$. Using the canonical commutations, the difference between two Hamiltonians may be deduced from

$$
H_\lambda - H = \lambda \int \frac{d^3\mathbf{k}}{(2\pi)^3} \, \omega \sum_\alpha [a_\alpha(\mathbf{k}), a_\alpha^\dagger(\mathbf{k})] = 2\lambda \int d^3\mathbf{k} \, \omega \, \delta^{(3)}(0)
\tag{19.53}
$$

This energy shift is infinite due to the space-volume infinity $\delta^{(3)}(0)$, as well as due to the momentum volume space infinity resulting from the integration over $\mathbf{k}$ extending out to $\infty$ values of $\mathbf{k}$. More importantly, however, the shift is a constant independent of $a_\alpha(\mathbf{k})$ and $a_\alpha^\dagger(\mathbf{k})$, which is unobservable (only differences in energy are observable). For the momentum, the analogous shift involves an integral over $\mathbf{k}$, which is odd and vanishes.

## 19.6 Photons – the Hilbert space of states

It remains to construct the Hilbert space of states. We have identified the observables $x_\alpha(\mathbf{k})$ and $p_\alpha(\mathbf{k})$, and their non-self-adjoint equivalents $a_\alpha(\mathbf{k})$ and $a_\alpha(\mathbf{k})^\dagger$, as the fundamental mutually independent quantities to which the electro-magnetic fields are equivalent. Thus, the Hilbert space may be faithfully constructed in terms of these harmonic oscillators.

### 19.6.1 The ground state or *vacuum*

The ground state, or *the vacuum*, is defined to be the state of lowest energy of the total system. Thus it must be the lowest energy state for each one of the harmonic oscillators, which requires that this state must be annihilated by the operators $a_\alpha(\mathbf{k})$ for all $\alpha = 1, 2$ and for all $\mathbf{k} \in \mathbf{R}^3$,

$$
a_\alpha(\mathbf{k})|\emptyset\rangle = 0
\tag{19.54}
$$

It will be assumed throughout that this state is unique and normalized as follows,

$$\| |\emptyset\rangle \lambda = \langle \emptyset | \emptyset \rangle = 1 \tag{19.55}$$

As an immediate result of the expressions for the hamiltonian and momentum operators (19.51), it follows that the ground state has zero energy and zero momentum,

$$H|\emptyset\rangle = \mathbf{P}|\emptyset\rangle = 0 \tag{19.56}$$

A different convention for the ordering of the oscillators in $H$ might have resulted in a non-zero energy of the ground state.

### 19.6.2 One-photon states

Applying any raising operator $a_\alpha^\dagger(\mathbf{k})$ to the vacuum will raise the energy above zero. We define these states as follows,

$$|\mathbf{k}, \alpha\rangle \equiv a_\alpha^\dagger(\mathbf{k})|\emptyset\rangle \tag{19.57}$$

The total energy and momentum of such states may be computed by applying the operators $H$ and $\mathbf{P}$ thereto, and we find,

$$H|\mathbf{k}, \alpha\rangle = \int \frac{d^3\mathbf{k'}}{(2\pi)^3} |\mathbf{k'}| \sum_\beta a_\beta^\dagger(\mathbf{k'})[a_\beta(\mathbf{k'}), a_\alpha^\dagger(\mathbf{k})]|\emptyset\rangle \tag{19.58}$$

where we have used the relation $a_\beta(\mathbf{k'})|\emptyset\rangle = 0$ in exhibiting the commutator. Using now the canonical commutator, we find,

$$
\begin{aligned}
H|\mathbf{k}, \alpha\rangle &= |\mathbf{k}| \, |\mathbf{k}, \alpha\rangle \\
\mathbf{P}|\mathbf{k}, \alpha\rangle &= \mathbf{k} \, |\mathbf{k}, \alpha\rangle
\end{aligned} \tag{19.59}
$$

The normalization of the one-particle states is that of the continuum, as is suitable for states indexed by the continuous momentum $\mathbf{k}$,

$$\langle \mathbf{k}, \alpha | \mathbf{k'}, \beta\rangle = (2\pi)^3 \delta^{(3)}(\mathbf{k'} - \mathbf{k})\delta_{\alpha\beta} \tag{19.60}$$

Given the fact that the state $|\mathbf{k}, \alpha\rangle$ has total energy $E = \hbar|\mathbf{k}|$ and momentum $\mathbf{p} = \hbar\mathbf{k}$, its relativistic invariant mass vanishes. We interpret these states as containing a *single photon*, of energy $\hbar|\mathbf{k}|$ and momentum $\hbar\mathbf{k}$. We shall see below what the nature is of states with higher numbers of photons. They cannot, in general, have vanishing mass.

### 19.6.3 Multi-photon states

Applying now several raising operators to $|0\rangle$, we obtain the following types of states,

$$|\psi\rangle = |\mathbf{k}_1, \alpha_1; \cdots; \mathbf{k}_n, \alpha_n\rangle \equiv a_{\alpha_1}^\dagger(\mathbf{k}_1) \cdots a_{\alpha_n}^\dagger(\mathbf{k}_n)|\emptyset\rangle \tag{19.61}$$

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whose energy and momentum is readily computed, and we have,

$$H|\psi\rangle = E|\psi\rangle \qquad\qquad E = |\mathbf{k}_1| + \cdots + |\mathbf{k}_n|$$
$$\mathbf{P}|\psi\rangle = \mathbf{p}|\psi\rangle \qquad\qquad \mathbf{p} = \mathbf{k}_1 + \cdots + \mathbf{k}_n \qquad (19.62)$$

Energy and momentum are simply the sums of the $n$ one-particle energy and momentum values, a superposition relation characteristic of non-interacting, or *free* particles. It is instructive to calculate the relativistic invariant mass of a system of two free photons, for example. We find,

$$m^2 = (|\mathbf{k}_1| + |\mathbf{k}_2|)^2 - (\mathbf{k}_1 + \mathbf{k}_2)^2 = 2|\mathbf{k}_1|\,|\mathbf{k}_2|(1 - \cos\theta) \qquad (19.63)$$

where $\theta$ is the angle between $\mathbf{k}_1$ and $\mathbf{k}_2$. For generic values of $\theta$, we have $m^2 \neq 0$, signaling that they form a genuine two-state system. For $\theta = 0$, we have collinear photons, with $m^2 = 0$. It may seem that the state with two parallel photons or with one photon with exactly the same total energy are really one and the same thing. But this is not so, because there exists in fact an operator whose eigenvalues distinguish between these two cases. This is the photon number operator, defined by

$$N = \int \frac{d^3\mathbf{k}'}{(2\pi)^3} \sum_\alpha a_\alpha^\dagger(\mathbf{k}) a_\alpha(\mathbf{k}) \qquad (19.64)$$

Its eigenvalue on a general state is given by,

$$N|\mathbf{k}_1, \alpha_1; \cdots; \mathbf{k}_n, \alpha_n\rangle = n|\mathbf{k}_1, \alpha_1; \cdots; \mathbf{k}_n, \alpha_n\rangle \qquad (19.65)$$

and thus distinguished between states with identical energy and momentum but different numbers of photons. Note that, for free photons, we have

$$[N, H] = [N, \mathbf{P}] = 0 \qquad (19.66)$$

so that the number of free photons is conserved during time evolution. Of course, once photons interact, such as with charges particles or dipoles, then the number of photons will no longer remain conserved and $H$ will no longer commute with $N$.

Finally, we have seen how the operator $a_\alpha^\dagger(\mathbf{k})$ *creates a photon* with momentum $\mathbf{k}$ and polarization $\alpha$. But similarly, the operator $a_\alpha(\mathbf{k})$ *annihilates a photon* with momentum $\mathbf{k}$ and polarization $\alpha$ out of any state. If the state contains no such photon, then the operator $a_\alpha(\mathbf{k})$ produces 0. More generally, we have

$$a_\alpha(\mathbf{k})|\mathbf{k}_1, \alpha_1; \cdots; \mathbf{k}_n, \alpha_n\rangle = \sum_{i=1}^{n} (2\pi)^3 \delta_{\alpha,\alpha_i} \delta^{(3)}(\mathbf{k} - \mathbf{k}_i)|\mathbf{k}_1, \alpha_1; \cdots; \widehat{\mathbf{k}_i, \alpha_i}; \cdots; \mathbf{k}_n, \alpha_n\rangle \qquad (19.67)$$

where the wide hat over $\mathbf{k}_i, \alpha_i$ gives the instruction of deleting the entry $\mathbf{k}_i, \alpha_i$ in the state description.

## 19.7   Bose-Einstein and Fermi-Dirac statistics

In classical mechanics, particles are *distinguishable*, namely each particle may be tagged and this tagging survives throughout time evolution since particle identities are conserved.

In quantum mechanics, *particles of the same species are indistinguishable*, and cannot be tagged individually. They can only be characterized by the quantum numbers of the state of the system. Therefore, the operation of interchange of any two particles of the same species must be a symmetry of the quantum system. The square of the interchange operation is the identity.[17]  As a result, the quantum states must have definite symmetry properties under the interchange of two particles.

All particles in Nature are either bosons or fermions;

- BOSONS : the quantum state is symmetric under the interchange of any pair of particles and obey *Bose-Einstein statistics*. Bosons have *integer spin*. For example, photons, $W^{\pm}$, $Z^0$, gluons and gravitons are bosonic elementary particles, while the Hydrogen atom, the $He_4$ and deuterium nuclei are composite bosons.

- FERMIONS : the quantum state is anti-symmetric under the interchange of any pair of particles and obey *Fermi-Dirac statistics*. Fermions have *integer plus half spin*. For example, all quarks and leptons are fermionic elementary particles, while the proton, neutron and $He_3$ nucleus are composite fermions.

Remarkably, the quantization of free scalars and free photons carried out in the preceeding subsections has Bose-Einstein statistics built in. The bosonic creation and annihilation operators are denoted by $a_\sigma^\dagger(\vec{k})$ and $a_\sigma(\vec{k})$ for each species $\sigma$. The canonical commutation relations inform us that all creation operators commute with one another $[a_\sigma^\dagger(\vec{k}), a_{\sigma'}^\dagger(\vec{k}')] = 0$. As a result, two states differening only by the interchange of two particle of the same species are identical quantum mechanically,

$$a_{\sigma_1}^\dagger(\vec{k}_1) \cdots a_{\sigma_i}^\dagger(\vec{k}_i) \cdots a_{\sigma_j}^\dagger(\vec{k}_j) \cdots a_{\sigma_n}^\dagger(\vec{k}_n)|\emptyset\rangle \tag{19.68}$$

$$= a_{\sigma_1}^\dagger(\vec{k}_1) \cdots a_{\sigma_j}^\dagger(\vec{k}_j) \cdots a_{\sigma_i}^\dagger(\vec{k}_i) \cdots a_{\sigma_n}^\dagger(\vec{k}_n)|\emptyset\rangle \tag{19.69}$$

The famous *CPT Theorem* states that upon the quantization of a Poincaré and CPT invariant Lagrangian, integer spin fields will always produce particle states that obey Bose-Einstein statistics, while integer plus half fields always produce states that obey Fermi-Dirac statistics.

- **Fermi-Dirac Statistics**

It remains to establish how integer plus half spin fields are to be quantized. This will be the subject of the subsection on the Dirac equation. Here, we shall take a very simple approach whose point of departure is the fact that fermions obey Fermi-Dirac statistics.

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[17]This statement holds in 4 space-time dimensions but it does not hold generally. In 3 space-time dimensions, the topology associated with the interchange of two particles allows for *braiding* and the square of this operation is not 1. The corresponding particles are *anyons*.

First of all, a free fermion may be expected to be equivalent to a collection of oscillators, just as bosonic free fields were. But they cannot quite be the usual harmonic oscillators, because we have just shown above that harmonic operators produce Bose-Einstein statistics. Instead, the *Pauli exclusion principle* states that only a single fermion is allowed to occupy a given quantum state. This means that a fermion creation operator $b^\dagger$ for given quantum numbers must square to 0. Then, its repeated application to any state (which would create a quantum state with more than one fermion particle with that species) will produce 0.

The smallest set of operators that can characterize a fermion state is given by the *fermionic oscillators* $b$ and $b^\dagger$, obeying the algebra

$$\{b, b\} = \{b^\dagger, b^\dagger\} = 0 \qquad\qquad \{b, b^\dagger\} = 1 \tag{19.70}$$

In analogy with the bosonic oscillator, we consider the following simple Hamiltonian,

$$H = \frac{\omega}{2}\left(b^\dagger b - bb^\dagger\right) = \omega\left(b^\dagger b - \frac{1}{2}\right) \tag{19.71}$$

Naturally, the ground state is defined by $b|0\rangle = 0$ and there are just two quantum states in this system, namely $|0\rangle$ and $b^\dagger|0\rangle$ with energies $-\frac{1}{2}\omega$ and $+\frac{1}{2}\omega$ respectively. A simple representation of this algebra may be found by noticing that it is equivalent to the algebra of Pauli matrices or Clifford-Dirac algebra in 2 dimensions,

$$\sigma^1 = b + b^\dagger \qquad\qquad \sigma^2 = ib - ib^\dagger \qquad\qquad H = \frac{\omega}{2}\sigma^3 \tag{19.72}$$

Vice-versa, the $\gamma$-matrices in 4 dimensions are equivalent to two sets of fermionic oscillators $b_\alpha$ and $b_\alpha^\dagger$, $\alpha = 1, 2$. The above argumentation demonstrates that its only irreducible representation is 4-dimensional, and spanned by the states $|\emptyset\rangle$, $b_1^\dagger|\emptyset\rangle$, $b_2^\dagger|\emptyset\rangle$, $b_1^\dagger b_2^\dagger|\emptyset\rangle$.

In terms of particles, we should affix the quantum number of momentum $\vec{k}$, so that we now have oscillators $b_\sigma(\vec{k})$ and $b_\sigma^\dagger(\vec{k})$, for some possible species index $\sigma$. Postulating anti-commutation relations, we have

$$\{b_\sigma(\vec{k}), b_{\sigma'}(\vec{k}')\} = \{b_\sigma^\dagger(\vec{k}), b_{\sigma'}^\dagger(\vec{k}')\} = 0$$
$$\{b_\sigma(\vec{k}), b_{\sigma'}^\dagger(\vec{k}')\} = 2\omega_k \delta_{\sigma\sigma'}(2\pi)^3\delta^{(3)}(\vec{k} - \vec{k}') \tag{19.73}$$

where again $\omega_k = \sqrt{\vec{k}^2 + m^2}$. The Hamiltonian and momentum operators are naturally

$$H = \int \frac{d^3k}{(2\pi)^3 2\omega_k}\, \omega_k \sum_\sigma b_\sigma^\dagger(\vec{k})b_\sigma(\vec{k})$$

$$\vec{P} = \int \frac{d^3k}{(2\pi)^3 2\omega_k}\, \vec{k} \sum_\sigma b_\sigma^\dagger(\vec{k})b_\sigma(\vec{k}) \tag{19.74}$$

The vacuum state $|\emptyset\rangle$ is defined by $b_\sigma(\vec{k})|\emptyset\rangle = 0$ and multiparticle states are obtained by applying creation operators to the vacuum,

$$b_{\sigma_1}^\dagger(\vec{k}_1)\cdots b_{\sigma_n}^\dagger(\vec{k}_n)|0\rangle \tag{19.75}$$

Using the fact that creation operators always anti-commute with one another, it is straightforward to show that

$$b_{\sigma_1}^\dagger(\vec{k}_1)\cdots b_{\sigma_i}^\dagger(\vec{k}_i)\cdots b_{\sigma_j}^\dagger(\vec{k}_j)\cdots b_{\sigma_n}^\dagger(\vec{k}_n)|\emptyset\rangle \tag{19.76}$$

$$= -\, b_{\sigma_1}^\dagger(\vec{k}_1)\cdots b_{\sigma_j}^\dagger(\vec{k}_j)\cdots b_{\sigma_i}^\dagger(\vec{k}_i)\cdots b_{\sigma_n}^\dagger(\vec{k}_n)|\emptyset\rangle \tag{19.77}$$

so that the state obeys Fermi-Dirac statistics.

## 19.8   The photon spin and helicity

Just as we constructed the electro-magnetic momentum in terms of the Poynting vectors, so we may also construct its total angular momentum,

$$\mathbf{J} = \int d^3\mathbf{x}\left(\mathbf{x}\times(\mathbf{E}\times\mathbf{B})\right) \tag{19.78}$$

Total angular momentum actually receives contributions from an orbital part $\mathbf{L}$ as well as from an intrinsic photon spin part $\mathbf{S}$, with the usual addition relation, $\mathbf{J} = \mathbf{L} + \mathbf{S}$. We are concerned with the spin part, and seek to separate it from $\mathbf{L}$. This separation cannot in fact be achieved in a gauge invariant way. The *helicity of the photon*, i.e. the projection of spin onto the photon momentum is the only part of the spin which can be isolated in a gauge invariant way.

We begin by producing a gauge dependent construction of $\mathbf{L}$ and $\mathbf{S}$, and we shall then extract from these the gauge invariant helicity. Using $\mathbf{B} = \nabla \times \mathbf{A}$ and the double cross product formula, we have

$$\begin{aligned}
\mathbf{E}\times\mathbf{B} &= \sum_i\left(E_i(\nabla A_i) - (\nabla_i\mathbf{A})E_i\right) \\
&= \sum_i\left(E_i(\nabla A_i) - \nabla_i(\mathbf{A}E_i)\right)
\end{aligned} \tag{19.79}$$

where we have used $\nabla \cdot \mathbf{E} = 0$ in going from the first to the second line. Next, we evaluate

$$\mathbf{x}\times\left(\mathbf{E}\times\mathbf{B}\right) = \sum_i\left(E_i(\mathbf{x}\times\nabla)A_i - \nabla_i(\mathbf{x}\times\mathbf{A}E_i) + \mathbf{E}\times\mathbf{A}\right) \tag{19.80}$$

The second term is clearly a surface term, and does not contribute to the integral when evaluating $\mathbf{J}$. The first term involves the orbital angular momentum operator $\mathbf{x}\times\nabla$, and naturally is associated with orbital angular momentum, though it is not gauge invariant. Thus, we define,

$$\begin{aligned}
\mathbf{L} &= \int d^3\mathbf{x}\sum_i E_i\left(\mathbf{x}\times\nabla\right)A_i \\
\mathbf{S} &= \int d^3\mathbf{x}\,\mathbf{E}\times\mathbf{A}
\end{aligned} \tag{19.81}$$

In transverse gauge, $\nabla \cdot \mathbf{A} = 0$, the orbital part is automatically transverse to momentum, so we shall use this gauge to evaluate spin. Expressing $\mathbf{S}$ in terms of $\mathbf{C}(t, \mathbf{k})$,

$$\mathbf{S} = \int \frac{d^3\mathbf{k}}{(2\pi)^3}\,\mathbf{C}(t,\mathbf{k})\times\partial_t\mathbf{C}(t,\mathbf{k}) \tag{19.82}$$

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Expressing $\mathbf{C}$ in terms of the oscillator modes, we obtain $t$-dependent terms and $t$-independent terms. The former vanish upon integration, as they are odd in $\mathbf{k}$. The $t$-independent terms combine as follows,

$$\mathbf{S} = i \int \frac{d^3\mathbf{k}}{(2\pi)^3} \sum_{\alpha,\beta} \left( \varepsilon_\alpha(\mathbf{k}) \times \varepsilon_\beta^*(\mathbf{k}) \right) a_\alpha(\mathbf{k}) a_\beta^\dagger(\mathbf{k}) \tag{19.83}$$

Note that the combination $\varepsilon_\alpha(\mathbf{k}) \times \varepsilon_\beta^*(\mathbf{k})$ is automatically anti-symmetric in $\alpha$ and $\beta$, and thus parallel to $\mathbf{k}$.

It is instructive to work out the Hilbert space of one-photon states at fixed value of their momentum. To do so, we choose the momentum along the $z$-axis, so that

$$\mathbf{k} = (0,0,k) \qquad\qquad \begin{aligned} \varepsilon_1(\mathbf{k}) &= (1,0,0) \\ \varepsilon_2(\mathbf{k}) &= (0,1,0) \end{aligned} \tag{19.84}$$

The polarization states may be denoted by

$$\begin{aligned} |\mathbf{k},1\rangle &= a_1^\dagger(\mathbf{k})|\emptyset\rangle \\ |\mathbf{k},2\rangle &= a_2^\dagger(\mathbf{k})|\emptyset\rangle \end{aligned} \tag{19.85}$$

Measuring the $z$-component of spin (which is equivalent to helicity, since $\mathbf{k}$ points in the $z$-direction), gives the following,

$$\begin{aligned} S_z|\mathbf{k},\gamma\rangle &= i \sum_\beta \left( \varepsilon_\gamma(\mathbf{k}) \times \varepsilon_\beta^*(\mathbf{k}) \right)_z a_\beta^\dagger(\mathbf{k})|\emptyset\rangle \\ &= i \sum_\beta \left( \varepsilon_\gamma(\mathbf{k}) \times \varepsilon_\beta^*(\mathbf{k}) \right)_z |\mathbf{k},\beta\rangle \end{aligned} \tag{19.86}$$

Working this out separately for the cases $\gamma = 1,2$, we obtain,

$$\begin{aligned} S_z|\mathbf{k},1\rangle &= i \left( \varepsilon_1(\mathbf{k}) \times \varepsilon_2^*(\mathbf{k}) \right)_z |\mathbf{k},2\rangle = +i|\mathbf{k},2\rangle \\ S_z|\mathbf{k},2\rangle &= i \left( \varepsilon_2(\mathbf{k}) \times \varepsilon_1^*(\mathbf{k}) \right)_z |\mathbf{k},1\rangle = -i|\mathbf{k},2\rangle \end{aligned} \tag{19.87}$$

Forming the combinations with circular polarization gives the eigenstates of $S_z$, as follows,

$$S_z|\mathbf{k},\pm\rangle = \pm|\mathbf{k},\pm\rangle \qquad\qquad |\mathbf{k},\pm\rangle = \frac{1}{\sqrt{2}} \left( |\mathbf{k},1\rangle \pm i|\mathbf{k},2\rangle \right) \tag{19.88}$$

As a result, the photon states contains just two spin states, with eigenvalues $\pm\hbar$, and we conclude that the photon is spin 1.

## 19.9   The Casimir Effect on parallel plates

Thus far, we have dealt with the quantization of the free electromagnetic fields $\vec{E}$ and $\vec{B}$, Already at this stage, it is possible to infer measurable predictions, such as the Casimir effect. The Casimir effect is a purely quantum field theory phenomenon in which the quantization of the electromagnetic fields in the presence of a electric conductors results in a net force between these conductors. The most famous example involves two conducting parallel plates, separated by a distance $a$, as represented in Fig18(a).
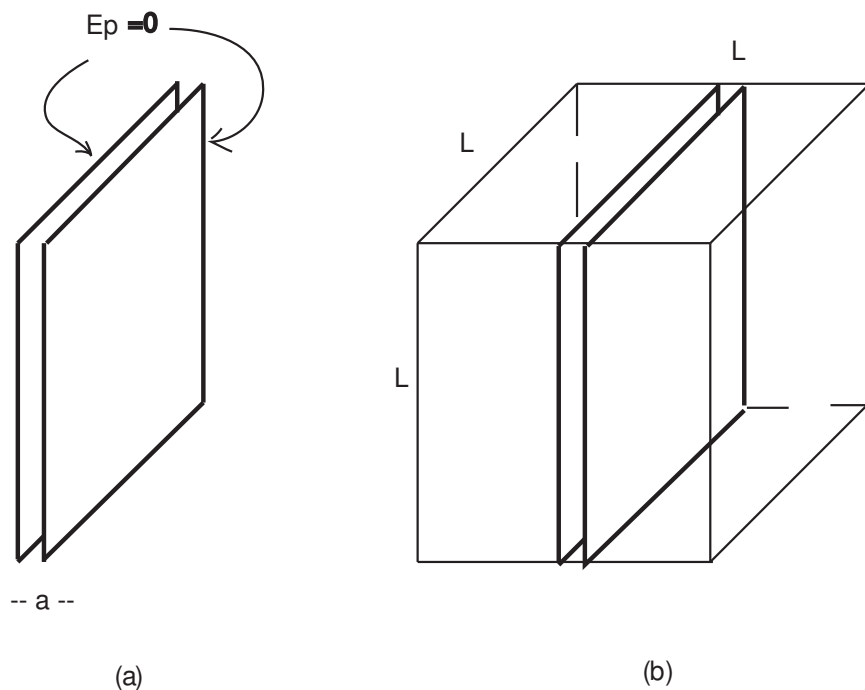


Figure 18: The Casimir effect : (a) electromagnetic vacuum fluctuations produce a force between two parallel plates; (b) the problem in a space box.

   The assumptions entering the set-up are as follows.

1. For a physical conductor, the electric field $\vec{E}_p$ parallel to the plates will vanish for frequencies much lower than the typical atomic scale $\omega_c$. At frequencies much higher than the atomic scale, the conductor effectively becomes transparent and no constraint is to be imposed on the electric field. In the frequency region comparable to the atomic scale $\omega_c$, the conductivity is a complicated function of frequency, which we shall simply approximate by a step function $\theta(\omega_c - \omega)$.

2. The separation $a$ should be taken much larger than interatomic distances, or $a\omega_c \gg 1$.

3. In order to regularize the problems associated with infinite volume, we study the problem in a square box in the form of a cube, with periodic boundary conditions, as depicted in

Fig18(b).

## • Calculation of the frequencies

There are three distinct regimes in which the frequencies of the quantum oscillators need to be computed. The momenta parallel to the plates are always of the following form,

$$k_x = \frac{2\pi n_x}{L} \qquad k_y = \frac{2\pi n_y}{L} \qquad n_x, n_y \in \mathbf{Z} \tag{19.89}$$

Along the third direction, we distinguish three different regimes, so that the frequency has three different branches,

$$\omega^{(i)} = \sqrt{k_x^2 + k_y^2 + (k_z^{(i)})^2} \qquad i = 1, 2, 3 \tag{19.90}$$

The three regimes are as follows,

1. $\omega > \omega_c$ : the frequencies are the same as in the absence of the plates, since the plates are acting as transparent objects,

$$k_z^{(1)} = \frac{2\pi n_z}{L} \qquad n_z \in \mathbf{Z}$$

2. $\omega < \omega_c$ & between the two plates.

$$k_z^{(2)} = \frac{\pi n_z}{a} \qquad 0 \le n_z \in \mathbf{Z}$$

3. $\omega < \omega_c$ & outside the two plates.

$$k_z^{(3)} = \frac{\pi n_z}{L - a} \qquad 0 \le n_z \in \mathbf{Z}$$

## • Summing up the contributions of all frequencies

Finally, we are not interested in the total energy, but rather in the enrgy in the presence of the plates minus the energy in the absence of the plates. Thus, when the frequencies exceed $\omega_c$, all contributions to the enrgy cancel since the plates act as transparent bodies. Thus, we have

$$E(a) - E_0 = \sum_{n_x, n_y, n_z} \left( \frac{1}{2} \omega^{(2)}(n_x, n_y, n_z) + \frac{1}{2} \omega^{(3)}(n_x, n_y, n_z) - \frac{1}{2} \omega^{(1)}(n_x, n_y, n_z) \right) \tag{19.91}$$

When $n_z \ne 0$, two polarization modes have $\vec{E}$ with 2 components along the plates, while for $n_z = 0$, $n_x, n_y \ne 0$, there is only one. Therefore, we isolate $n_z = 0$,

$$E(a) - E_0 \;=\; \frac{1}{2} \sum_{n_x, n_y} \omega(n_x, n_y, 0) \tag{19.92}$$

$$+ \sum_{n_x, n_y} \sum_{n_z=1}^{\infty} \left( \omega^{(2)}(n_x, n_y, n_z) + \omega^{(3)}(n_x, n_y, n_z) - 2\omega^{(1)}(n_x, n_y, n_z) \right)$$

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Next, we are interested in taking the size of the box $L$ very large compared to all other scales in the problem. The levels in $n_x$ and $n_y$ then become very closely spaced and the sums over $n_x$ and $n_y$ may be well-approximated by integrals, with the help of the following conversion process,

$$dn_x = \frac{L dk_x}{2\pi} \qquad dn_y = \frac{L k_y}{2\pi} \tag{19.93}$$

so that

$$E(a) - E_0 = \frac{L^2}{4\pi^2} \int_{-\infty}^{+\infty} dk_x \int_{-\infty}^{+\infty} dk_y \left[ \frac{1}{2}\omega\theta(\omega_c - \omega) \right. \tag{19.94}$$

$$\left. + \sum_{n_z=1}^{\infty} \left( \omega^{(2)}\theta(\omega_c - \omega^{(2)}) + \omega^{(3)}\theta(\omega_c - \omega^{(3)}) - 2\omega^{(1)}\theta(\omega_c - \omega^{(1)}) \right) \right] \tag{19.95}$$

Now, for $\omega^{(1)}$ and $\omega^{(3)}$, the frequency levels are also close together and the sum over $n_z$ may also be approximated by an integral,

$$\sum_{n_z=1}^{\infty} \omega^{(2)}\theta(\omega_c - \omega^{(2)}) = \frac{L-a}{\pi} \int_0^{\infty} dk_z \sqrt{k_x^2 + k_y^2 + k_z^2} \; \theta(\omega_c - \sqrt{k_x^2 + k_y^2 + k_z^2})$$

$$\sum_{n_z=1}^{\infty} 2\omega^{(1)} \theta(\omega_c - \omega^{(1)}) = \frac{L}{2\pi} 2 \int_0^{\infty} dk_z \sqrt{k_x^2 + k_y^2 + k_z^2} \; \theta(\omega_c - \sqrt{k_x^2 + k_y^2 + k_z^2})$$

Introducing $k^2 = k_x^2 + k_y^2$, and in the last integral the continuous variable $n = ak_z/\pi$, we have

$$E(a) - E_0 = \frac{L^2}{2\pi} \int_0^{\infty} dk \; k \left[ \frac{1}{2}k\theta(\omega_c - k) + \sum_{n=1}^{\infty} \sqrt{k^2 + \frac{\pi^2 n^2}{a^2}} \; \theta(\omega_c^2 - k^2 - \frac{\pi^2 n^2}{a^2}) \right.$$

$$\left. - \int_0^{\infty} dn \sqrt{k^2 + \frac{\pi^2 n^2}{a^2}} \; \theta(\omega_c^2 - k^2 - \frac{\pi^2 n^2}{a^2}) \right]$$

Introducing the function

$$f(n) \equiv \int_0^{\infty} \frac{dk}{2\pi} k \sqrt{k^2 + \frac{\pi^2 n^2}{a^2}} \; \theta(\omega_c^2 - k^2 - \frac{\pi^2 n^2}{a^2}) \tag{19.96}$$

we have

$$\frac{E(a) - E_0}{L^2} = \frac{1}{2}f(0) + \sum_{n=1}^{\infty} f(n) - \int_0^{\infty} dn f(n) \tag{19.97}$$

Now, there is a famous formula that relates a sum of the values of a function at integers to the integral of this function,

$$\int_0^{\infty} dn f(n) = \frac{1}{2}f(0) + \sum_{n=1}^{\infty} f(n) + \sum_{p=1}^{\infty} \frac{B_{2p}}{(2p)!} f^{(2p-1)}(0) \tag{19.98}$$

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where the Bernoulli numbers are defined by

$$\frac{x}{e^x - 1} = \sum_{n=0}^{\infty} B_n \frac{x^n}{n!} \qquad B_2 = -\frac{1}{6}, \quad B_4 = -\frac{1}{30}, \cdots \tag{19.99}$$

Assuming a sharp cutoff, so that $\theta$ is a step function, we easily compute $f(n)$,

$$f(n) = \frac{1}{6\pi} \left( \omega_c^3 - \frac{\pi^3 n^3}{a^3} \right) \tag{19.100}$$

Thus, $f^{(2p-1)}(0) = 0$ as soon as $p > 2$, while $f^{(3)}(0) = -\pi^2/a^3$, and thus we have

$$\frac{E(a) - E_0}{L^2} = \frac{\pi^2}{a^3} \frac{B_4}{4!} = -\frac{\pi^2}{720} \hbar c \frac{L^2}{a^3} \tag{19.101}$$

This represents a universal, attractive force proportional to $1/a^4$. To make their dependence explicit, we have restored the factors of $\hbar$ and $c$.

# 20  Photon Emission and Absorption

In this chapter, we couple the quantized electro-magnetic field to quantized matter, such as electrons, protons, atoms and molecules. The matter is assumed to be non-relativistic, and thus described by the usual Hamiltonians where the number of matter particles is fixed. We shall set up the general problem of photon emission and absorption from matter, calculate the rate for a single photon, apply this calculation to the case of the 2p state of atomic Hydrogen, and extend the problem to black body radiation.

## 20.1  Setting up the general problem of photon emission/absorption

For simplicity, we shall consider here a pure matter Hamiltonian $H_m$ for just a single particle of mass is $m$, subject to a potential $V$,

$$H_m = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) \tag{20.1}$$

Concretely, one may think of $H_m$ as describing an electron bound to an atom or to an ion by the potential $V$. We shall denote the Hilbert space of states for the pure matter system by $\mathcal{H}_m$, and denote its states by $|\psi\rangle_m$. Typically, we shall be interested in the system being initially in the pure matter state $|\psi_i\rangle_m$, which is an eigenstate of $H_m$, and finally in the pure matter state $|\psi_f\rangle_m$ plus photons.

The quantized photons are governed by the Maxwell Hamiltonian $H_{EM}$ which was studied in the preceding chapter. It is given by,

$$H_{EM} = \int d^3\mathbf{x} \left( \frac{1}{2}\mathbf{E}^2 + \frac{1}{2}\mathbf{B}^2 \right) \tag{20.2}$$

The Hilbert space of all photon states will be denoted by $\mathcal{H}_{EM}$. The photon states are labelled by the momenta and the polarizations of the photons. For example, a state with one-photon of momentum $\mathbf{k}$ and polarization $\alpha$ is labeled by $|\mathbf{k}, \alpha\rangle$.

The full Hamiltonian is not just the sum of $H_m$ and $H_{EM}$, but requires the inclusion of the couplings between matter and radiation. These interactions are accounted for by including an interaction Hamiltonian $H_I$,

$$H_I = \frac{e}{2m}(\mathbf{A} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{A}) + \frac{e^2}{2m}\mathbf{A}^2 + \mu\mathbf{B} \cdot \mathbf{S} \tag{20.3}$$

For spin 1/2 particles, the $\mathbf{B} \cdot \mathbf{S}$ term naturally arises from the non-relativistic approximation to the Dirac equation, as we shall establish later. The full hamiltonian $H = H_m + H_{EM} + H_I$ then takes the form,

$$H = \frac{1}{2m}(\mathbf{p} + e\mathbf{A})^2 + V(\mathbf{x}) + \mu\mathbf{B} \cdot \mathbf{S} + \int d^3\mathbf{x} \left( \frac{1}{2}\mathbf{E}^2 + \frac{1}{2}\mathbf{B}^2 \right) \tag{20.4}$$

We recognize the first three terms in $H$ as identical to the Hamiltonian for a charged particle in the presence of an external electro-magnetic field. Thus, the coupling to the quantized fields is

obtained by simply promoting the classical $\mathbf{A}$ field to a quantum operator. The Hilbert space $\mathcal{H}$ of the full system is the tensor product of the Hilbert spaces of the matter and free radiation parts, and given by $\mathcal{H} = \mathcal{H}_m \otimes \mathcal{H}_{EM}$.

## 20.2 Single Photon Emission/Absorption

Having developed the general set-up of the matter-radiation system, we shall now apply it to the emission/absorption of a single photon. The initial state is assumed to correspond to a pure matter state $|\psi_i\rangle_m$ of $\mathcal{H}_m$, and to have no photons. We shall denote this total state by $|\psi_i; \emptyset\rangle = |\psi_i\rangle_m \otimes |\emptyset\rangle_{EM}$. We shall assume that $|\psi_i\rangle_m$ is an eigenstate of $H_m$. This condition often constitutes a good approximation to the situation in a real physical problem, in view of the fact that the electromagnetic coupling $\alpha = e^2/\hbar c$ is small. The final state corresponds to a pure matter state $|\psi_f\rangle_m$, but now has an extra photon. We shall denote this state by $|\psi_f; \mathbf{k}, \alpha\rangle = |\psi_f\rangle_m \otimes |\mathbf{k}, \alpha\rangle_{EM}$, and assume that also $|\psi_f\rangle_m$ is an eigenstate of $H_m$. Since the coupling is weak, we shall use first order perturbation theory to evaluate the transition rate. To do so, the full Hamiltonian is separated into a "free part" $H_0 = H_m + H_{EM}$ and an interacting part $H_I$. The initial states are eigenstates of $H_0$,

$$
\begin{aligned}
H_0|\psi_i; \emptyset\rangle &= E_i^{(0)}|\psi_i; \emptyset\rangle \\
H_0|\psi_f; \mathbf{k}, \alpha\rangle &= (E_f^{(0)} + \omega_k)|\psi_f; \mathbf{k}, \alpha\rangle
\end{aligned}
\tag{20.5}
$$

where $E_i^{(0)}$ and $E_f^{(0)}$ are the energies of $|\psi_i\rangle_m$ and $|\psi_f\rangle_m$ respectively, and $\omega_k = |\mathbf{k}|$.

First order perturbation theory allows us to compute the transition rate $\Gamma_{i \to f}$ from the initial state $|i\rangle = |\psi_i; \emptyset\rangle$ to the final state $|f\rangle = |\psi_f; \mathbf{k}, \alpha\rangle$, under the time evolution governed by the full Hamiltonian $H = H_0 + H_1$. The rate is given by Fermi's golden rule formula,

$$
\Gamma_{i \to f} = 2\pi \Big| \langle f|H_1|\imath\rangle \Big|^2 \delta(E_f - E_i)
\tag{20.6}
$$

where $E_f$ and $E_i$ are the total energies of the final and initial states respectively, and given by $E_i = E_i^{(0)}$ and $E_f = E_f^{(0)} + \omega_k$. The rate $\Gamma_{i \to f}$ is often referred to as the *exclusive* rate because the final state is specified to be a photon with specific momentum $\mathbf{k}$ and polarization $\alpha$. It is often useful to consider the *includive* or *total rate*, obtained by summing over the contributions to all possible final states, obtained here by summing over all photon momenta and polarizations. The total rate is given by

$$
\Gamma = \sum_f \Gamma_{i \to f}
\tag{20.7}
$$

To evaluate the rate in practice, we have to calculate the matrix element of $H_1$ between the state without photon and the state with one photon. As a result, the $\mathbf{A}^2$ term in $H_1$ does not contribute, since it has vanishing matrix elements. The term involving the electron magnetic moment is typically much smaller than the contribution from the orbital term, and will be neglected here. (Of

course, in cases where the orbital term gives vanishing contribution, the electron magnetic moment term may become important, and will have to be included.) Hence, the sole remaining contribution to the matrix element is given by,

$$\langle f|H_1|i\rangle = \left(\langle\psi_f|_m \otimes \langle\emptyset|_{EM} a_\alpha(\mathbf{k})\right)\frac{e}{2m}\left(\mathbf{A}\cdot\mathbf{p}+\mathbf{p}\cdot\mathbf{A}\right)\left(|\psi_i\rangle_m \otimes |\emptyset\rangle_{EM}\right) \tag{20.8}$$

We begin by evaluating the matrix element in $\mathcal{H}_{EM}$, with the help of the free electro-magnetic field $\mathbf{A}$, in transverse gauge,

$$\mathbf{A}(t,\mathbf{x}) = \int \frac{d^3k'}{(2\pi)^3}\,\frac{1}{\sqrt{2|\mathbf{k}'|}}\sum_\beta\left(\varepsilon_\beta(\mathbf{k}')a_\beta(\mathbf{k}')e^{-ik'\cdot x}+\varepsilon_\beta^*(\mathbf{k})a_\beta^\dagger(\mathbf{k}')e^{ik'\cdot x}\right) \tag{20.9}$$

where $\mathbf{k}'\cdot x = |\mathbf{k}'|t - \mathbf{k}'\cdot\mathbf{x}$. Using the canonical commutation relations of the radiation oscillators, we readily find that,

$$\langle\emptyset|a_\alpha(\mathbf{k})\,\mathbf{A}(t,\mathbf{x})|\emptyset\rangle = \frac{1}{\sqrt{2|\mathbf{k}|}}\varepsilon_a^*(\mathbf{k})e^{-ik\cdot x} \tag{20.10}$$

Note that the ordering between $\mathbf{A}$ and $\mathbf{p}$ is immaterial here, since the commutator of the two terms is proportional to $\nabla\cdot\mathbf{A} = 0$ in transverse gauge. As a result, the full matrix element takes the form,

$$\langle f|H_1|i\rangle = \frac{e}{m\sqrt{2\omega}}\,e^{i\omega t}\langle\psi_f|\varepsilon_\alpha^*(\mathbf{k})\cdot\mathbf{p}\,e^{-i\mathbf{k}\cdot\mathbf{x}}|\psi_i\rangle \tag{20.11}$$

Upon taking the norm square, as needed to compute the rate, we have,

$$|\langle f|H_1|i\rangle|^2 = \frac{e^2}{2m\omega}\left|\langle\psi_f|\varepsilon_\alpha^*(\mathbf{k})\cdot\mathbf{p}\,e^{-i\mathbf{k}\cdot\mathbf{x}}|\psi_i\rangle\right|^2 \tag{20.12}$$

Finally, the summation over all final states, required to derive the total rate, amounts to an integration over all photon momenta and summation over both photon polarizations. This gives,

$$\Gamma = 2\pi\int\frac{d^3k}{(2\pi)^3}\frac{e^2}{2m\omega}\sum_\alpha\left|\langle\psi_f|\varepsilon_\alpha^*(\mathbf{k})\cdot\mathbf{p}\,e^{-i\mathbf{k}\cdot\mathbf{x}}|\psi_i\rangle\right|^2\delta\left(E_i^{(0)}-E_f^{(0)}-\omega_k\right) \tag{20.13}$$

The radial part of the $\mathbf{k}$-integration may be easily carried out in view of the presence of the $\delta$-function on $\omega_k = |\mathbf{k}|$, and we have $d^3k = \omega^2 d\omega\,d\Omega$, where $d\Omega$ is the solid angle volume element for the direction $\mathbf{k}/|\mathbf{k}|$. Carrying out the $\omega$ integration gives,

$$\Gamma = \frac{e^2}{8\pi^2 m}\left(E_i^{(0)}-E_f^{(0)}\right)\sum_\alpha\int d\Omega\left|\langle\psi_f|\varepsilon_\alpha^*(\mathbf{k})\cdot\mathbf{p}\,e^{-i\mathbf{k}\cdot\mathbf{x}}|\psi_i\rangle\right|^2 \tag{20.14}$$

We simplify this formula one more step. If the rate is to correspond to the decay of an excited atomic state to a lower energy state or the ground state, then the energy differences are of order $mc^2\alpha^2 \sim c|\mathbf{k}|$. The typical size of the atom is the Bohr radius, which is given by $|\mathbf{x}| \sim a_0 = \hbar/(mc\alpha)$.

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As a result, the product $\mathbf{k} \cdot \mathbf{x} \sim \alpha$ is small compare to 1, and the exponential may be approximated by 1, at the same order of approximation that we use when we neglected two photon exchanges. The resulting formula for the total rate is,

$$\Gamma = \frac{e^2}{8\pi^2 m} \left( E_i^{(0)} - E_f^{(0)} \right) \sum_\alpha \int d\Omega \left| \langle \psi_f | \varepsilon_\alpha^*(\mathbf{k}) \cdot \mathbf{p} | \psi_i \rangle \right|^2 \tag{20.15}$$

Finally, we shall perform the summation over polarizations, and the integral over directions, as follows,

$$\sum_\alpha \int d\Omega \left| \langle \psi_f | \varepsilon_\alpha^*(\mathbf{k}) \cdot \mathbf{p} | \psi_i \rangle \right|^2 = \sum_\alpha \int d\Omega \, \varepsilon_a^*(\mathbf{k})^i \varepsilon_a(\mathbf{k})^j \, \langle \psi_f | p^i | \psi_i \rangle \langle \psi_f | p^j | \psi_i \rangle^* \tag{20.16}$$

Let $\mathbf{n} = \mathbf{k}/|\mathbf{k}|$, so that $\mathbf{n}^2 = 1$, then we have

$$\sum_\alpha \varepsilon_a^*(\mathbf{k})^i \varepsilon_a(\mathbf{k})^j = \delta^{ij} - n^i n^j \tag{20.17}$$

Note that this formula is in agreement with the fact that $\varepsilon_\alpha(\mathbf{k})$ is transverse to $\mathbf{k}$ and that this space is 2-dimensional. The integration over $\Omega$ may be evaluated as follows. The the result of the integral must be, by construction, a rank 2 symmetric tensor in $i, j$ which is rotation invariant (since we integrate over all directions $\mathbf{n}$ with a rotation invariant measure). There is only one such tensor, namely $\delta^{ij}$ up to an overall multiplicative factor $\ell$, so that

$$\int d\Omega \left( \delta^{ij} - n^i n^j \right) = \ell \, \delta^{ij} \tag{20.18}$$

The value of $\ell$ is determined by taking the trace over $i, j$, which gives $8\pi = 3\ell$. Putting all together, we find,

$$\Gamma = \frac{e^2}{6\pi m^2} \left( E_i^{(0)} - E_f^{(0)} \right) \left| \langle \psi_f | \mathbf{p} | \psi_i \rangle \right|^2 \tag{20.19}$$

Finally, it is customary to recast the atomic matrix element in terms of the position operator $\mathbf{x}$ instead of momentum. This may be achieved by noticing that

$$\frac{i\hbar}{m} \mathbf{p} = [\mathbf{x}, H_m] \tag{20.20}$$

so that

$$\Gamma = \frac{e^2}{6\pi \hbar^2} \left( E_i^{(0)} - E_f^{(0)} \right)^3 \left| \langle \psi_f | \mathbf{x} | \psi_i \rangle \right|^2 \tag{20.21}$$

## 20.3  Application to the decay rate of 2p state of atomic Hydrogen

The simplest application of the above general formulation of single photon decay is to the decay of the 2p state of atomic Hydrogen to its 1s ground state, $|\psi_i\rangle = |2p\rangle$, and $|\psi_f\rangle = |1s\rangle$. We have,

$$
\begin{aligned}
|\langle 1s|z|2p\rangle|^2 &= \left(\frac{8}{9}\right)^5 \frac{1}{m^2\alpha^2} \\
E_{2p}^{(0)} - E_{1s}^{(0)} &= \frac{3}{8}mc^2\alpha^2
\end{aligned}
\tag{20.22}
$$

Combining these partial results, we find,

$$
\Gamma = mc^2\alpha^5 \qquad\qquad \tau = \frac{\hbar}{\Gamma} = 1.6 \times 10^{-9}\text{sec} \tag{20.23}
$$

where $\tau$ stands for the life-time.

This is one instance where the rules of the Wigner-Eckart theorem come in handy. The position operator $\mathbf{x}$ is a vector or $j = 1$ operator, and thus we know that the initial and final total angular momenta, respectively $j_i$ and $j_f$, must obey,

$$
\left|j_i - j_f\right| \leq 1 \tag{20.24}
$$

In addition, there is a selection rule on the conservation of magnetic quantum number,

$$
m_i = m_f \pm 1 \tag{20.25}
$$

What happens for initial and final states for which these conditions are not satisfied ? Is the state $|\psi_i\rangle$ then stable ?

The answer to these questions can be gathered by realizing that in the above calculation, we have made various approximations to the real situation. We considered only single photon decay, and neglected the electron magnetic moment coupling.

When two or more photons are exchanged, the difference in total angular momentum is pretty much arbitrary. Every additional photon produced, however, will require an extra factor of $e$ in the amplitude and thus an extra factor of $\alpha$ in the rate. Since $\alpha \sim 1/137$, the production of multiple photons will be suppressed. Also, for multiple photons, less phase space becomes available, and in general a suppression will result from phase space considerations as well. In summary, when the above selection rules for single photon decay are not satisfied, the rate will be suppressed, and the life-time of the 2p state will be prolonged.

## 20.4  Absorption and emission of photons in a cavity

By a *cavity*, we mean an enclosure whose walls are built of solid material, such as a metal or a porcelain. The atoms and molecules of the cavity wall vibrate (increasingly so when the temperature increases), and emit and absorb photons. At equilibrium, a balance is achieved where photons are being absorbed and emitted in a steady state process. The spectrum of photons (including the

spectrum of visible light) inside the cavity depends on the temperature. We know from experience with ovens and flames that at moderate temperatures a red glow is visible, while at higher temperature colors move to the yellow, green and blue, namely to higher frequencies. In the present section, we shall calculate the *absorption rate of photons in the cavity* from first principles. The emission rate may be calculated analogously.

We shall work in a cavity, thus in a spatial box of finite extent, so that photon momenta may be labeled by discrete vectors $\mathbf{k}$, and their number can be counted in a discrete manner. The corresponding radiation oscillators satisfy the canonical commutation relations,

$$[a_\alpha(\mathbf{k}), a_\beta^\dagger(\mathbf{k}')] = \delta_{\alpha,\beta}\delta_{\mathbf{k},\mathbf{k}'} \tag{20.26}$$

The rates for the different possible values of the wave-vector $\mathbf{k}$ decouple from one another, and may be treated separately. Thus, we concentrate on photons with a single value of the wave vector $\mathbf{k}$. We shall denote by $|n_\alpha(\mathbf{k}); \alpha, \mathbf{k}\rangle$ the state with $n_\alpha(\mathbf{k})$ photons of polarization $\alpha$ and wave number $\mathbf{k}$; these states are given by,

$$|n_\alpha(\mathbf{k}); \alpha, \mathbf{k}\rangle = \frac{1}{\sqrt{n_\alpha(\mathbf{k})!}}\left(a_\alpha^\dagger(\mathbf{k})\right)^{n_\alpha(\mathbf{k})}|\emptyset\rangle \tag{20.27}$$

The number $n_\alpha(\mathbf{k})$ is referred to as the *occupation number* of the state of photon momentum $\mathbf{k}$ and polarization $\alpha$.

Absorption will send the atomic state $|\psi_i\rangle$ (which is often the ground state of the atomic part of the system) to an excited atomic state $|\psi_f\rangle$, and will diminish the number of photons. Considering here the simplest case where absorption occurs of a single photon, we shall be interested in transitions between the following total states,

$$\begin{aligned}
|i\rangle &= |\psi_i; n_\alpha(\mathbf{k}), \alpha, \mathbf{k}\rangle &\equiv& \ |\psi_i\rangle \otimes |n_\alpha(\mathbf{k}), \alpha\mathbf{k}\rangle \\
|f\rangle &= |\psi_f; n_\alpha(\mathbf{k}) - 1, \alpha, \mathbf{k}\rangle &\equiv& \ |\psi_f\rangle \otimes |n_\alpha(\mathbf{k}) - 1, \alpha\mathbf{k}\rangle
\end{aligned} \tag{20.28}$$

Using again the Fermi golden rule formula for the rate,

$$\Gamma = 2\pi\left|\langle\varphi|H_1|i\rangle\right|^2\delta(E_f - E_i) \tag{20.29}$$

where we use the same approximation for the photon-matter coupling that we used for the single photon emission calculation,

$$H_1 = \frac{e}{m}\mathbf{A}\cdot\mathbf{p} \tag{20.30}$$

where the electro-magnetic field $\mathbf{A}$ is in the transverse gauge. The first part of the calculation consists again in evaluating the matrix elements of the $\mathbf{A}$-field, but this time between two states with multiple photons. To evaluate it, we need the following relation,

$$a_\beta(\mathbf{k}')|n_\alpha(\mathbf{k}), \alpha, \mathbf{k}\rangle = (n_\alpha(\mathbf{k}))^{\frac{1}{2}}|n_\alpha(\mathbf{k}) - 1, \alpha, \mathbf{k}\rangle\delta_{\alpha,\beta}\delta^{(3)}(\mathbf{k}' - bk) \tag{20.31}$$

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and we find the following formulas for respectively absorption and emission,

$$\langle n_\alpha(\mathbf{k}) - 1, \alpha, \mathbf{k}|\mathbf{A}(t, \mathbf{x})|n_\alpha(\mathbf{k}), \alpha, \mathbf{k}\rangle = (n_\alpha(\mathbf{k}))^{\frac{1}{2}} \, \varepsilon_\alpha^*(\mathbf{k}) \, e^{ik\cdot x}$$

$$\langle n_\alpha(\mathbf{k}) + 1, \alpha, \mathbf{k}|\mathbf{A}(t, \mathbf{x})|n_\alpha(\mathbf{k}), \alpha, \mathbf{k}\rangle = (n_\alpha(\mathbf{k}) + 1)^{\frac{1}{2}} \, \varepsilon_\alpha(\mathbf{k}) \, e^{-ik\cdot x} \qquad (20.32)$$

The extra factor of $(n_\alpha(\mathbf{k}))^{1/2}$ is the key difference with the calculation of the single-photon emission rate. The differential rate for the absorption of a single photon is then,

$$d\Gamma_{abs} = \frac{8\pi^2}{L^3} \, n_\alpha(\mathbf{k}) \, \frac{\alpha}{2\omega_k m^2} \left|\langle \psi_f|\varepsilon_\alpha(\mathbf{k}) \cdot \mathbf{p} \, e^{i\mathbf{k}\cdot\mathbf{x}}|\psi_i\rangle\right|^2 \delta(E_f - E_i - \omega_k)d\omega_k \qquad (20.33)$$

while the rate for the emission of a photon is given by,

$$d\Gamma_{emi} = \frac{8\pi^2}{L^3} \, (n_\alpha(\mathbf{k}) + 1) \, \frac{\alpha}{2\omega_k m^2} \left|\langle \psi_f|\varepsilon_\alpha^*(\mathbf{k}) \cdot \mathbf{p} \, e^{-i\mathbf{k}\cdot\mathbf{x}}|\psi_i\rangle\right|^2 \delta(E_f - E_i + \omega_k)d\omega_k \qquad (20.34)$$

## 20.5 Black-body radiation

Black body radiation assumes thermodynamic equilibrium between the emitted and absorbed photons and the cavity wall. The process responsible for this thermalization may be depicted as follows,

$$\psi_A \leftrightarrow \psi_B + \gamma \qquad (20.35)$$

The absorption and emissions rates, calculated previously, may be applied to this process alternatively with the initial state $|\psi_i\rangle$ being $|\psi_A\rangle$ (for emission), and $|\psi_B\rangle$ for absorption, and the final state $|\psi_f\rangle$ being $|\psi_A\rangle$ for absorption, and $|\psi_B\rangle$ for emission.

The corresponding emission and absorption rates for the above process are then given by

$$w_{emi}(\alpha, \mathbf{k}) = (n_\alpha(\mathbf{k}) + 1) \left|\langle \psi_B|\varepsilon_\alpha^*(\mathbf{k}) \cdot \mathbf{p} \, e^{-i\mathbf{k}\cdot\mathbf{x}}|\psi_A\rangle\right|^2$$

$$w_{abs}(\alpha, \mathbf{k}) = n_\alpha(\mathbf{k}) \left|\langle \psi_A|\varepsilon_\alpha(\mathbf{k}) \cdot \mathbf{p} \, e^{i\mathbf{k}\cdot\mathbf{x}}|\psi_B\rangle\right|^2 \qquad (20.36)$$

The matrix elements are related by complex conjugation,

$$\langle \psi_B|\varepsilon_\alpha^*(\mathbf{k}) \cdot \mathbf{p} \, e^{-i\mathbf{k}\cdot\mathbf{x}}|\psi_A\rangle = \langle \psi_A|\varepsilon_\alpha(\mathbf{k}) \cdot \mathbf{p} \, e^{i\mathbf{k}\cdot\mathbf{x}}|\psi_B\rangle^* \qquad (20.37)$$

This relation requires commuting $\mathbf{p}$ with the exponential; since the commutator $[\mathbf{p}, e^{i\mathbf{k}\cdot\mathbf{x}}] = \hbar\mathbf{k}$, and $\varepsilon_\alpha(\mathbf{k}) \cdot \mathbf{k} = 0$, this commutator does not contribute. Since the rates involve the absolute value square of these quantities, we find that

$$\frac{w_{emi}(\alpha, \mathbf{k})}{n_\alpha(\mathbf{k}) + 1} = \frac{w_{abs}(\alpha, \mathbf{k})}{n_\alpha(\mathbf{k})} \qquad (20.38)$$

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This is clearly a very powerful relation, because it implies that the details of the absorption and emission process, encoded in the detailed common matrix elements, are irrelevant in determining the photon occupation numbers $n_\alpha(\mathbf{k})$.

Next, we denote the population numbers of the states $\psi_A$ and $\psi_B$ by $N(A)$ and $N(B)$ respectively. Thermodynamic equilibrium requires that the detailed balance equation for the process,

$$N(A)\, w_{emi}(\alpha, \mathbf{k}) = N(B)\, w_{abs}(\alpha, \mathbf{k}) \tag{20.39}$$

The ratio of these population numbers is given by the Boltzmann distribution formula,

$$\frac{N(A)}{N(B)} = e^{-(E_A - E_B)/(k_B T)} = e^{-\hbar\omega/(k_B T)} \tag{20.40}$$

here $k_B$ is the Boltzmann constant, $T$ is the temperature at equilibrium, and $\omega = c|\mathbf{k}|$. Combining (20.39) and (20.40), and eliminating the ratios $N(A)/N(B)$, and $w_{emi}/w_{abs}$, we find,

$$\frac{N(A)}{N(B)} = \frac{w_{abs}(\alpha, \mathbf{k})}{w_{emi}(\alpha, \mathbf{k})} = \frac{n_\alpha(\mathbf{k})}{n_\alpha(\mathbf{k}) + 1} = e^{-\hbar\omega/(k_B T)} \tag{20.41}$$

The last equality may be readily solved for $n_\alpha(\mathbf{k})$, and we find,

$$n_\alpha(\mathbf{k}) = \frac{1}{e^{\hbar\omega/(k_B T)} - 1} \tag{20.42}$$

This formula is an example of the occupation numbers for particles obeying Bose-Einstein statistics.

From this formula, it is a small extra step to derive the Planck formula for the black body radiation spectrum as a function of temperature. The contribution $U(\omega)d\omega$ to the internal energy density of the distribution of photons in an infinitesimal interval $[\omega, \omega + d\omega]$ is given by

$$U(\omega)d\omega = \frac{1}{L^3} \times 2 \times \hbar\omega \times \frac{1}{e^{\hbar\omega/(k_B T)} - 1} \times \left[\left(\frac{L}{2\pi}\right)^3 4\pi k^2 dk\right] \tag{20.43}$$

The factor $1/L^3$ results from considering the energy density; the factor of 2 results from the sum over both polarizations of the photon; the factor $\hbar\omega$ is the energy contribution of a single photon with wave number $\mathbf{k}$; the denominator is the photon occupation number. Finally, the last factor, in brackets, is the phase space factor giving the number of states in a spherical shell in wave-number space of thickness $dk$. It may be evaluated as follows. The allowed wave numbers in a cubic box of size $L$, with periodic boundary conditions, are

$$k_x = 2\pi n_x \qquad k_y = 2\pi n_y \qquad k_z = 2\pi n_z \tag{20.44}$$

The number of states in an infinitesimal volume element are then,

$$dn_x \, dn_y \, dn_z = \left(\frac{L}{2\pi}\right)^3 dk_x \, dk_y \, dk_z = \left(\frac{L}{2\pi}\right)^3 4\pi \, k^2 \, dk \tag{20.45}$$

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After some simplifications, the internal energy density per unit frequency is given by

$$U(\omega) = \frac{8\pi\hbar}{c^3} \left(\frac{\omega}{2\pi}\right)^3 \frac{1}{e^{\hbar\omega/(k_B T)} - 1} \tag{20.46}$$

Expressing the formula alternatively in terms of frequency $\nu = \omega/(2\pi)$, and "Planck's constant" $h = 2\pi\hbar$, we have

$$U(\omega) = W(\nu) = \frac{4h\nu^3}{c^3} \frac{1}{e^{h\nu/(k_B T)} - 1} \tag{20.47}$$

which is the original Planck black body radiation formula.

# 21  Relativistic Field Equations

In the preceding chapters matter, such as electrons and nuclei, was treated as non-relativistic and distinguishable, while electro-magnetic radiation, in the form of emissions and absorptions, is relativistic and was treated field theoretically. Indeed, in field theory, the number of particles, such as photons, does not have to be conserved, while the number of non-relativistic electrons and nuclei was conserved. Relativity, especially through its equivalence of matter and energy, makes it impossible for the number of particles to be conserved, whether they be photons, electrons, protons, neutrons or nuclei. For example, electrons and positrons can collide and annihilate one another by producing photons, and leaving no charged particles behind. The same can happen to protons and anti-protons, and even the collision of two protons at high energy can produce new particles, including protons, electrons and positrons. Thus, the dynamics of electrons (and later on of all particles) will have to be formulated field theoretically, so that the number of electrons need not be conserved throughout physical processes.

In this chapter, we shall begin by reviewing those aspects of special relativity that will be needed here, and then proceed to constructing relativistic invariant field theory equations in a systematic manner, including Maxwell's equations. The field equations for electrons, namely the Dirac equation, will be constructed in the subsequent chapter.

## 21.1  A brief review of special relativity

Special relativity is based on two basic postulates

1. The laws of Nature and the results of all experiments in any two inertial frames with relative velocity $\mathbf{v}$ are the same.

2. The speed of light is independent of the relative speed $\mathbf{v}$.

To make the consequences of these postulates explicit, we spell out the properties of inertial frames and the relations between two such frames.

An inertial frame in special relativity is a coordinate system $\mathcal{R}(t, \mathbf{x})$ in which Maxwell's equations *in the absence of matter* hold true. The coordinates of two inertial frames $\mathcal{R}(t, \mathbf{x})$ and $\mathcal{R}'(t', \mathbf{x}')$ are related to one another by affine transformations, which include translations (the affine part), rotations and boosts the linear part).

To make this more precise, we define the Minkowski distance $s^2$ between two events $(t_1, \mathbf{x}_1)$ and $(t_2, \mathbf{x}_2)$,

$$s^2 = -c^2(t_1 - t_2)^2 + (\mathbf{x}_1 - \mathbf{x}_2)^2 \tag{21.1}$$

The physical interpretation of $ds^2$ depends upon its sign;

- $s^2 = 0$, the events are causally related by the propagation of light;

- $s^2 > 0$, the events are causally unrelated;

- $s^2 < 0$, the events are causally related by the propagation of particles of any mass; one may view $\tau$, defined by $\tau^2 = -s^2/c^2$, as the proper time between the two events.

The coordinates of two inertial frames $\mathcal{R}(t, \mathbf{x})$ and $\mathcal{R}'(t', \mathbf{x}')$ are related by an affine transformation which leaves the Minkowski distance $s^2$ between any two events invariant,

$$-c^2(t_1 - t_2)^2 + (\mathbf{x}_1 - \mathbf{x}_2)^2 = -c^2(t'_1 - t'_2)^2 + (\mathbf{x}'_1 - \mathbf{x}'_2)^2 \tag{21.2}$$

It is immediate that this construction automatically implies the second postulate that the speed of light is $c$ in all inertial frames. It is also immediate that space and time translations leave the Minkowski distance invariant. Amongst the linear transformations, rotations leave $s^2$ invariant as well. The remaining transformations are boosts, which act linearly. Using rotation symmetry, any boost may be rotated to the $x$-direction, leaving $y$ and $z$-coordinates untransformed. We may then parametrize a boost as follows,

$$
\begin{aligned}
ct' &= Act + Bx \\
x' &= Cct + Dx \\
y' &= y \\
z' &= z
\end{aligned}
\tag{21.3}
$$

Choosing two events as follows $(t_1, \mathbf{x}_1) = (t, x, 0, 0)$ and $(t_2, \mathbf{x}_2) = (0, 0, 0, 0)$, and requiring invariance of the Minkowski distance between them, gives

$$
\begin{aligned}
-c^2t^2 + x^2 &= -c^2(t')^2 + (x')^2 \\
&= -(Act + Bx)^2 + (Cct + Dx)^2
\end{aligned}
\tag{21.4}
$$

Since this relation must hold for all possible events, it must hold for all $t, x$, which requires

$$
\begin{aligned}
1 &= A^2 - C^2 \\
1 &= -B^2 + D^2 \\
0 &= -AB + CD
\end{aligned}
\tag{21.5}
$$

Parametrizing $A = \mathrm{ch}\phi$, $C = \mathrm{sh}\phi$, $B = \mathrm{sh}\psi$, and $D = \mathrm{ch}\psi$ solves the first two equations. The third equation is solved by having $\psi = \phi$. To gain better physical insight into the transformation, we set

$$B = C = -\beta\gamma \qquad\qquad A = D = \gamma \equiv \frac{1}{\sqrt{1 - \beta^2}} \tag{21.6}$$

where $\beta$ is viewed as the parameter taking all possible real values $|\beta| < 1$. The transformations of (21.7) take the following form in this parametrization,

$$
\begin{aligned}
ct' &= \gamma(ct - \beta x) \\
x' &= \gamma(x - \beta ct) \\
y' &= y \\
z' &= z
\end{aligned}
\tag{21.7}
$$

From this it is clear that $\beta c$ must be interpreted as the relative velocity between the two frames. Indeed, the point $x' = 0$, which is fixed in frame $\mathcal{R}'$, travels with velocity $v = x/t = \beta c$ from the point of view of frame $\mathcal{R}$, which is one way we may define the relative velocity between the frames.

The relativistic transformation properties of momentum, energy, mass, and of the electromagnetic fields may be derived analogously. It is much more efficient, however, to obtain such relations using the Lorentz vector and tensor notation, which we shall provide first.

## 21.2   Lorentz vector and tensor notation

Just as we use vector notation in 3-dimensional space to collect the three coordinates $(x, y, z)$ into a vector $\mathbf{x}$, so we use also 4-vector notation to collect the four coordinates of an event $(ct, x, y, z) = (ct, \mathbf{x})$ into a 4-vector $x$, denoted *without bold face or arrow embellishment*. Actually, one mostly uses a slight variant of the 4-vector notation, with an index added,

$$ x^\mu \equiv (x^0, x^1, x^2, x^3) = (ct, x, y, z) \qquad\qquad \mu = 0, 1, 2, 3 \qquad (21.8) $$

The time direction being special through its special signature in the Minkowski distance, one reserves the index "0" to denote it. The Minkowski distance may be easily cast in this notation,

$$ s^2 = \sum_{\mu,\nu=0,1,2,3} \eta_{\mu\nu}(x_1^\mu - x_2^\mu)(x_1^\nu - x_2^\nu) \qquad (21.9) $$

where the Minkowski metric $\eta_{\mu\nu}$ is defined as follows,

$$ \eta_{\mu\nu} \equiv \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}_{\mu\nu} \qquad (21.10) $$

Einstein introduced the *repeated index summation convention*, which instructs one to sum over one repeated upper and one repeated lower index. With the Einstein index convention, we thus have,

$$ s^2 = \eta_{\mu\nu}(x_1^\mu - x_2^\mu)(x_1^\nu - x_2^\nu) \qquad (21.11) $$

The precise distinction between upper and lower indices and their separate roles will be spelled out later.

A relativistic transformation may be expressed in 4-index notation as well. A general affine transformation between the coordinates $x^\mu$ and $x'^\mu$ may be parametrized as follows,

$$ x^\mu \rightarrow x'^\mu = \Lambda^\mu{}_\nu x^\nu + a^\mu \qquad (21.12) $$

Here, $\Lambda$ is a $4 \times 4$ matrix with real entries, and the repeated $\nu$-index is to be summed over. The 4-vector $a^\mu$ is real, and parametrizes translations in time and space. Invariance of the Minkowski distance $s^2$ is tantamount to

$$ \begin{aligned} \eta_{\mu\nu}x^\mu x^\nu &= \eta_{\mu\nu}x'^\mu x'^\nu \\ &= \eta_{\mu\nu}\Lambda^\mu{}_\rho x^\rho \, \Lambda^\nu{}_\sigma x^\sigma \\ &= \eta_{\rho\sigma}\Lambda^\rho{}_\mu x^\mu \, \Lambda^\sigma{}_\nu x^\nu \end{aligned} \qquad (21.13) $$

In passing from the second to the third line, we have relabeled the summation indices so that as to expose the combination $x^\mu x^\nu$ in both cases. This relation has to hold for all $x^\mu$, so that we must have

$$\eta_{\mu\nu} = \eta_{\rho\sigma} \Lambda^\rho{}_\mu \Lambda^\sigma{}_\nu \tag{21.14}$$

This relation defines all Lorentz transformations. It is instructive to count their number of independent parameters. The matrix $\Lambda$ has 16 real components, but obeys 16 relations expressed through the equation of two matrices which are both automatically symmetric. A real symmetric $4 \times 4$ matrix has 10 real independent components, so $16 - 10 = 6$ independent parameters, which precisely accounts for 3 rotations and 3 boosts.

## 21.3 General Lorentz vectors and tensors

The starting point for introducing 4-vector notation in the preceding section was the quantity $x^\mu$, which, under a Lorentz transformation $\Lambda$ behaves linearly in $x^\mu$,

$$x^\mu \to x'^\mu = \Lambda^\mu{}_\nu x^\nu \tag{21.15}$$

One refers to any object $V^\mu = (V^0, V^1, V^2, V^3)$ which transforms under $\Lambda$ by

$$A^\mu \to A'^\mu = \Lambda^\mu{}_\nu A^\nu \tag{21.16}$$

as a *Lorentz vector*. To be more precise, one sometimes refers to $A^\mu$ as a *Lorentz vector with upper index*, or a *contravariant vector*.

### 21.3.1 Contravariant tensors

The transformation law of the product of $n$ vectors $x_i^{\mu_i}$ with $i = 1, 2, \cdots, n$ follows from the transformation law of each vector, $x_i^\mu \to x_i'^\mu = \Lambda^\mu{}_\nu x_i^\nu$, and we have,

$$x_1^{\mu_1} \cdots x_n^{\mu_n} \to x_1'^{\mu_1} \cdots x_n'^{\mu_n} = \left( \Lambda^{\mu_1}{}_{\nu_1} \cdots \Lambda^{\mu_n}{}_{\nu_n} \right) x_1^{\nu_1} \cdots x_n^{\nu_n} \tag{21.17}$$

The product $x_1^{\mu_1} \cdots x_n^{\mu_n}$ is a *tensor of rank $n$*. One refers to any object $A^{\mu_1 \cdots \mu_n}$ which transforms under $\Lambda$ by

$$A^{\mu_1 \cdots \mu_n} \to A'^{\mu_1 \cdots \mu_n} = \left( \Lambda^{\mu_1}{}_{\nu_1} \cdots \Lambda^{\mu_n}{}_{\nu_n} \right) A^{\nu_1 \cdots \nu_n} \tag{21.18}$$

as a Lorentz tensor of rank $n$, or more precisely as a Lorentz tensor with upper indices or a contravariant tensor of rank $n$. A special case is when $n = 0$, where we obtain,

$$A \to A' = A \tag{21.19}$$

namely a tensor of rank 0, more commonly referred to as a *Lorentz scalar*.

### 21.3.2 Covariant tensors

Every contravariant vector and tensor naturally has an associated *covariant vector* or tensor of the same rank, which is obtained by *lowering all upper indices* using the Minkowski metric $\eta_{\mu\nu}$. The simplest case is for a contravariant vector $A^\mu$, where we define the associated covariant vector by

$$A_\mu \equiv \eta_{\mu\nu} A^\nu \qquad \Leftrightarrow \qquad A^\mu = \eta^{\mu\nu} A_\nu \tag{21.20}$$

Under a Lorentz transformation $\Lambda$, the covariant vector $A_\mu$ is mapped as follows,

$$
\begin{aligned}
A_\mu \to A'_\mu &= \eta_{\mu\nu} A'^\nu \\
&= \eta_{\mu\nu} \Lambda^\nu{}_\rho A^\rho \\
&= \eta_{\mu\nu} \Lambda^\nu{}_\rho \eta^{\rho\sigma} A_\sigma
\end{aligned}
\tag{21.21}
$$

By our standard conventions of raising and lowering indices, we adopt the following notation,

$$\eta_{\mu\nu} \Lambda^\nu{}_\rho \eta^{\rho\sigma} = \Lambda_\mu{}^\sigma \tag{21.22}$$

Using the defining relations of Lorentz transformations, $\eta_{\mu\nu} = \eta_{\rho\sigma}\Lambda^\rho{}_\mu\Lambda^\sigma{}_\nu$, we may reinterpret this matrix as follows. contract the defining relation with $\eta^{\mu\tau}$ gives,

$$\delta^\tau{}_\nu = \eta_{\rho\sigma}\Lambda^\rho{}_\mu\eta^{\mu\tau}\Lambda^\sigma{}_\nu = \Lambda_\sigma{}^\tau\Lambda^\sigma{}_\nu \tag{21.23}$$

Hence, $\Lambda_\mu{}^\nu$ is the inverse of the matrix $\Lambda^\mu{}_\nu$. Thus, another way of expressing the transofmration law for a covariant vector is in terms of the inverse of $\Lambda$,

$$A_\mu \to A'_\mu = \Lambda_\mu{}^\nu A_\nu \tag{21.24}$$

Analogously, one refers to any object $A_{\mu_1\cdots\mu_n}$ which transforms under $\Lambda$ by

$$A_{\mu_1\cdots\mu_n} \to A'_{\mu_1\cdots\mu_n} = \left(\Lambda_{\mu_1}{}^{\nu_1}\cdots\Lambda_{\mu_n}{}^{\nu_n}\right) A_{\nu_1\cdots\nu_n} \tag{21.25}$$

as a Lorentz tensor of rank $n$, or more precisely as a Lorentz tensor with lower indices or a covariant tensor of rank $n$.

One very important example of a covariant vector is provided by the 4-derivative,

$$\partial_\mu \equiv \frac{\partial}{\partial x^\mu} \tag{21.26}$$

In view of its defining relation, $[\partial_\mu, x^\nu] = \delta_\mu{}^\nu$, it is clear that $\partial_\mu$ transforms as a covariant vector,

$$\partial'_\mu = \frac{\partial}{\partial x'^\mu} = \Lambda_\mu{}^\nu \frac{\partial}{\partial x^\nu} = \Lambda_\mu{}^\nu \partial_\nu \tag{21.27}$$

### 21.3.3 Contraction and trace

Two vectors $A^\mu, B^\mu$ may be *contracted* to form their Minkowski inner product,

$$A \cdot B \equiv \eta_{\mu\nu} A^\mu B^\nu = A_\mu B^\mu = A^\mu B_\mu \qquad (21.28)$$

We have already encountered this inner product of two 4-vectors, one of position $x^\mu = (ct, \mathbf{x})$, and one of momentum $k^\mu = (\omega/c, \mathbf{k})$, which is given explicitly by,

$$k \cdot x = -\omega t + \mathbf{k} \cdot \mathbf{x} \qquad (21.29)$$

This inner product is invariant under Lorentz transformations. More generally, two tensors $A^{\mu_1 \cdots \mu_n}$, $B^{\mu_1 \cdots \mu_n}$ of the same rank $n$ may be contracted to form a scalar,

$$A \cdot B = A_{\mu_1 \cdots \mu_n} B^{\mu_1 \cdots \mu_n} \qquad (21.30)$$

One may also contract two tensors $A$, and $B$, of ranks $m + p$ and $n + p$ respectively over $p$ indices to yield a tensor of rank $m + n$,

$$A_{\mu_1 \cdots \mu_m \rho_1 \cdots \rho_p} B^{\nu_1 \cdots \nu_n \rho_1 \cdots \rho_p} = C_{\mu_1 \cdots \mu_m}{}^{\nu_1 \cdots \nu_n} \qquad (21.31)$$

A particularly important contraction of this type consists in taking a trace by contracting a tensor $A$ of rank $m+2$ with the Minkowski metric tensor $\eta$ (note that the pair of indices has to be specified) to yield a tensor of rank $m$,

$$A_{\mu_1 \cdots \mu_i \cdots \mu_j \cdots \mu_m} \eta^{\mu_i \mu_j} = B_{\mu_1 \cdots \widehat{\mu_i} \cdots \widehat{\mu_j} \cdots \mu_m} \qquad (21.32)$$

Later on, we shall describe further linear operations on tensors, namely symmetrization and anti-symmetrizations, with the help of which general tensors may be decomposed into their irreducible components.

## 21.4  Classical relativistic kinematics and dynamics

In non-relativistic mechanics, the relation between energy $E$, mass $m$, velocity $\mathbf{v}$ and momentum $\mathbf{p}$ is given by

$$E = \frac{1}{2} m \mathbf{v}^2 = \frac{\mathbf{p}^2}{2m} \qquad (21.33)$$

To obtain the relativistic invariant modification of these relations, we begin by identifying the relevant Lorentz 4-vectors of the problem. It turns out that the correct 4-vector which generalizes the 3-dimensional momentum vector $\mathbf{p}$ is

$$p^\mu = (E/c, \mathbf{p}) \qquad (21.34)$$

Under a Lorentz transformation $\Lambda$, $p^\mu$ indeed transforms as a contravariant vector,

$$p^\mu \to p'^\mu = \Lambda^\mu{}_\nu p^\nu \qquad (21.35)$$

The transformation under rotations is standard, since $\mathbf{p}$ is a vector, while $E$ is rotation-invariant. Under a boost in the 1-direction, by a velocity $v$, we have

$$
\begin{aligned}
E' &= \gamma\left(E - vp^1\right) \\
p'^1 &= \gamma\left(p^1 - vE/c^2\right) \\
p'^2 &= p^2 \\
p'^3 &= p^3
\end{aligned}
\tag{21.36}
$$

where $\gamma = (1 - v^2/c^2)^{-1/2}$. If this result is to agree with the non-relativistic limit where $|v| \ll c$, and $\gamma \sim 1$, we must have $p'^1 = p^1 - mv$, and this requires that as $v \to 0$, the energy of the particle remain finite, and given by its rest mass,

$$
E = mc^2
\tag{21.37}
$$

which is Einstein's famous relation.

A fully relativistic relation between energy and momentum is obtained by using the fact that $p^\mu$ is a 4-vector, and hence the "square" $p_\mu p^\mu$ must be Lorentz invariant. Since its value is independent of the frame where it is being evaluated, we may evaluate it in the frame where the particle is at rest, i.e. its momentum is zero, and its energy is $mc^2$. This gives,

$$
p_\mu p^\mu = -E^2/c^2 + \mathbf{p}^2 = -m^2 c^2
\tag{21.38}
$$

or alternatively written as a formula for energy,

$$
E^2 = m^2 c^4 + \mathbf{p}^2 c^2
\tag{21.39}
$$

Energy-omentum conservation is then simply the statement that the 4-vector $p^\mu$ is conserved.

## 21.5 Particle collider versus fixed target experiments

Suppose we have two possible experimental set-ups for the collisions of particle os mass $m$ onto one another;

- *Fixed target*: one incoming particle has energy $E$, the other is at rest.

- *Collider*: the particles have opposite momenta, and each has energy $E/2$.

The question is now in which experiment one gets the most "bang for the buck". Translated into scientific terms, what this amounts to is the largest total energy in the rest frame.

For the Collider, the center of mass energy available is simply $E$, the sum of the energies of the two particles.

To compute the center of mass energy $E_{cm}$ for the fixed target experiment, we use the fact that the total momentum $p^\mu$ has the same square in the fixed target frame as in the center of mass frame where, by definition, its momentum vanishes. This reads as follows,

$$
p_\mu p^\mu = -(E/c + mc)^2 - p^2 c^2 = -(E_{cm}/c)^2
\tag{21.40}
$$

Here, $p$ is the momentum of the incoming particle, which is related to the energy by $E^2 = p^2c^2 + m^2c^4$. Eliminating $p^2$ between these two equations gives a formula for $E_{cm}$ directly in terms of $E$ and $m$,

$$E_{cm} = \sqrt{2m^2c^4 + 2mc^2E} \tag{21.41}$$

We see that for large energy ($mc^2 \ll E$), the center of mass energy in the collider experiment gros like $E$, while in the fixed target experiment, it grows only like $\sqrt{E}$. Thus, the collider provides much more bang for the buck !

## 21.6   A physical application of time dilation

There are all the funny applications of time dilation in relativity related to space-travel and the twin paradox. But there are also very important and directly observable applications to particle physics. Here, we shall provide one such example in terms of the observed life-time of unstable particles.

For definiteness, we consider the example of a muon $\mu^-$ particle; it is very similar to the electron, but it is 200 times heavier, namely $mc^2 \sim 100 MeV$, and unstable against weak interactions, with a life-time of approximately $2 \times 10^{-6}$ sec. Muons are observed in cosmic ray showers. How far can the muons travel since they were first created ? Without taking time-dilation into account, they can travel at most a distance $2 \times 10^{-6}$ sec $\times c = 600\,m$, certainly not enough to travel intergalactically.

But if the energy of the muon is actually $E = mc^2\gamma$ in the frame of observation, then they can travel a distance $\gamma$ times than 600. For a muon of energy $E \sim 10^6\,GeV$, this comes to approximately a distance of $10^7 km$, more in the range of intergalactic traveling distances.

## 21.7   Relativistic invariance of the wave equation

In the preceding sections, we have introduced scalars, vectors and tensors. Now we shall be interested in *scalar fields*, *vector fields*, and only rarely also in *tensor fields*. A function $\phi(x)$, where $x^\mu = (ct, \mathbf{x})$, is said to be a scalar field is it behaves as follows under a Lorentz transformation,

$$\phi(x) \to \phi'(x') = \phi(x) \qquad\qquad x'^\mu = \Lambda^\mu{}_\nu x^\nu \tag{21.42}$$

In English, this means that the field $\phi'$ in the new frame with coordinates $x'$ equals to old field $\phi$ in the old frame with coordinates $x$.

A suitable Lorentz-invariant equation for the propagation of a scalar field is given by the wave equation,

$$\left( -\frac{1}{c^2}\frac{\partial^2}{\partial t^2} + \Delta \right) \phi(x) = \partial^\mu \partial_\mu \phi(x) = 0 \tag{21.43}$$

Note that there is no suitable Lorentz invarinat 1-st order differential equation for a scalar field, since $\partial_\mu \phi = 0$ would imply that $\phi$ is constant. An important generalization of the wave equation

is obtained by including a *mass term*,

$$\left(\hbar^2 \partial_\mu \partial^\mu - m^2 c^2\right) \phi(x) = 0 \tag{21.44}$$

This equation for a massive scalar field may be solved by Fourrier analysis, and we have

$$\phi_k(x) = e^{ik \cdot x} \qquad\qquad \hbar^2 k_\mu k^\mu + m^2 c^2 = 0 \tag{21.45}$$

Since $p^\mu = \hbar k^\mu$, we see that this relation gives the energy - momentum relation for a relativistic particle (or wave) with mass $m$. A further Lorentz-invariant generalization of the scalar field wave equation is obtained by adding an arbitrary function $V'(\phi)$,

$$\hbar^2 \partial_\mu \partial^\mu \phi - m^2 c^2 \phi - V'(\phi) = 0 \tag{21.46}$$

The latter may be derived via the action principle from the invariant Lagrangian density,

$$\mathcal{L} = -\frac{1}{2}\hbar^2 \partial_\mu \phi \partial^\mu \phi - \frac{1}{2}m^2 c^2 \phi^2 - V(\phi) \tag{21.47}$$

The Higgs particle, for example, is an elementary scalar particle, which is described by a real scalar field $\phi$, with a quartic potential $V(\phi)$. Of course, the Higgs particle couples to many other particles, such as electrons, quarks and neutrinos, and this description will require additional fields in the Lagrangian density.

## 21.8 Relativistic invariance of Maxwell equations

The prime example of a vector field under Lorentz transformations is provided by Maxwell theory of electro-magnetism. A general (covariant) vector field $V_\mu(x)$ is a collection of 4 fields $V_0(x), V_1(x), V_2(x), V_3(x)$ which behave as follows under a Lorentz transformation $\Lambda$,

$$V_\mu(x) \ \rightarrow \ V'_\mu(x') = \Lambda_\mu{}^\nu V_\nu(x) \tag{21.48}$$

and analogously for a contravariant vector field.

### 21.8.1 The gauge field and field strength

In electro-magnetism, we encounter two vector fields, the gauge potential $A_\mu = (-\Phi/c, \mathbf{A})$, and the electric current density $j^\mu = (\rho c, \mathbf{j})$, where $\Phi$ is the electric potential, $\mathbf{A}$ the usual 3-dimensional vector potential, $\rho$ the charge density, and $\mathbf{j}$ the 3-dimensional electric current density. Consistency of Maxwell's equations requires the current density to be conserved,

$$\partial_\mu j^\mu = \frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0 \tag{21.49}$$

Maxwell's equations are invariant under gauge transformations on the vector potential,

$$A_\mu \ \rightarrow \ A'_\mu = A_\mu + \partial_\mu \theta \tag{21.50}$$

for any scalar function $\theta$. The electric and magnetic fields are first order time and space-dervatives of the electric potential and of the vector potential, and bot are gauge invariant. The most systematic way to construct the electric and magnetic field is to precisely take advantage of these two properties. Computing the general first order derivatives gives $\partial_\mu A_\nu$, which behaves as follows under a gauge transformation of $A_\mu$,

$$\partial_\mu A_\nu \rightarrow \partial_\mu A'_\nu = \partial_\mu A_\nu + \partial_\mu \partial_\nu \theta \tag{21.51}$$

Thus, the most general first order derivative of $A_\mu$ is not gauge invariant. The gauge term $\partial_\mu \partial_\nu \theta$, however, is always symmetric under the interchange of $\mu$ and $\nu$. Therefore, we are guaranteed that *anti-symmetric* part of the derivative will be gauge invariant. The corresponding *field strength* is defined by

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \tag{21.52}$$

Counting the number of independent fields in the rank 2 anti-symmetric tensor $F_{\mu\nu} = -F_{\nu\mu}$ gives $4 \times 3/2 = 6$, which is precisely the correct number to incorporate the 3 components of $\mathbf{E}$ and the three components of $\mathbf{B}$. Decomposing $F_{\mu\nu}$ according to its space and time indices, and using anti-symmetry, we find the following parts,

$$\begin{aligned} F_{0i} &= \partial_0 A_i - \partial_i A_0 \\ F_{ij} &= \partial_i A_j - \partial_j A_i \end{aligned} \qquad i,j = 1,2,3 \tag{21.53}$$

The standard electric and magnetic fields may now be identified as follows,

$$\begin{aligned} F_{i0} &= E_i \\ F_{ij} &= \sum_{k=1}^{3} \varepsilon_{ijk} B_k \end{aligned} \tag{21.54}$$

As a matrix, the field strength tensor has the following entries,

$$F_{\mu\nu} = \begin{pmatrix} 0 & -E_1 & -E_2 & -E_3 \\ E_1 & 0 & B_3 & -B_2 \\ E_2 & -B_3 & 0 & B_1 \\ E_3 & B_2 & -B_1 & 0 \end{pmatrix}_{\mu\nu} \tag{21.55}$$

### 21.8.2 Maxwell's equations in Lorentz covariant form

Lorentz invariance of the equations dictates, to a large extent, the structure of the possible equations we may have for the gauge field $A_\mu$, and its gauge invariant field strength tensor $F_{\mu\nu}$. Maxwell's equations emerge in two groups; a first set independent of the external electric current density $j^\mu$, and a second set which does involve $j^\mu$.

The first group of Maxwell's equations results directly from the fact that $F_{\mu\nu}$ is a "curl" in the 4-dimensional sense. From $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$, it readily follows that

$$\varepsilon^{\mu\nu\rho\sigma} \partial_\rho F_{\mu\nu} = 2\varepsilon^{\mu\nu\rho\sigma} \partial_\rho \partial_\mu A_\nu = 0 \tag{21.56}$$

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since the derivative $\partial_\rho \partial_\mu A_\nu$ is symmetric in $\rho, \mu$, while the $\varepsilon^{\mu\nu\rho\sigma}$ is antisymmetric in all its indices, and may be normalized to $\varepsilon^{0123} = 1$ (note that because of the Minkowski signature of the metric, this implies that $\varepsilon_{0123} = -1$. Expressed in terms of $\mathbf{E}$ and $\mathbf{B}$, this yields the first group of Maxwell's equations, by considering separately the cases where $\sigma = 0$ and $\sigma = i$ with $i = 1, 2, 3$,

$$
\begin{aligned}
\varepsilon^{\mu\nu\rho 0} \partial_\rho F_{\mu\nu} = 0 \qquad &\Leftrightarrow \qquad \nabla \cdot \mathbf{B} = 0 \\
\varepsilon^{\mu\nu\rho i} \partial_\rho F_{\mu\nu} = 0 \qquad &\Leftrightarrow \qquad \partial_0 \mathbf{B} + \nabla \times \mathbf{E} = 0
\end{aligned}
\tag{21.57}
$$

It is instructive to give the derivation of these formulas. On the first line, the last index on $\varepsilon$ is a time-index, namely 0, so that the other three indices on $\varepsilon$ must be space-indices, which we shall rebaptize $i, j, k$. Thus, the first line becomes $\varepsilon^{ijk0} \partial_k F_{ij} = 0$. Using the definition of the magnetic field $F_{ij} = \sum_m \varepsilon_{ijm} B_m$, the fact that, with our conventions, $\varepsilon^{ijk0} = -\varepsilon^{ijk}$, and the double contraction

$$
\varepsilon^{ijk} \varepsilon_{ijm} = 2\delta^k_m
\tag{21.58}
$$

we find $\varepsilon^{ijk0} \partial_k F_{ij} = 2\partial_k B^k = 2\nabla \cdot \mathbf{B}$. On the second line, the last index is $i$, which is space-like. Thus, one and only one of the indices $\mu, \nu, \rho$ must be 0. Collecting all possibilities gives $\varepsilon^{jk0i} \partial_0 F_{jk} + 2\varepsilon^{0jki} \partial_k F_{0j} = 0$. Using the definitions of the electric and magnetic fields, ad the above double contraction formula, we obtain $\partial_0 B^i + \varepsilon^{ijk} \partial_j E_k = 0$, which gives the formula quoted.

The second group of Maxwell equations are also linear and involve first derivatives of the electric and magnetic fields and are sourced by the current density. There is only one Lorentz-invariant combination with these properties, up to an overall constant factor, namely

$$
\partial_\mu F^{\mu\nu} = -j^\nu
\tag{21.59}
$$

Note that, because $F_{\mu\nu}$ is antisymmetric in $\mu$ and $\nu$, the current density must be conserved, $\partial_\nu \partial_\mu F^{\mu\nu} = \partial_\nu j^\nu = 0$. There are actually 4 equations encoded in (21.59), one for each of the possible values of $\nu$.

$$
\begin{aligned}
\partial_\mu F^{\mu 0} = -j^0 \qquad &\Leftrightarrow \qquad \nabla \cdot \mathbf{E} = \rho \\
\partial_\mu F^{\mu i} = -j^i \qquad &\Leftrightarrow \qquad \partial_0 \mathbf{E} - \nabla \times \mathbf{B} = \mathbf{j}
\end{aligned}
\tag{21.60}
$$

In summary, the relativistic form of the two groups of Maxwell's equations reduce to,

$$
\begin{aligned}
\varepsilon^{\mu\nu\rho\sigma} \partial_\rho F_{\mu\nu} &= 0 \\
\partial_\mu F^{\mu\nu} &= -j^\nu
\end{aligned}
\tag{21.61}
$$

These equations may be derived from an action principle. Considering $A_\mu$ as the fundamental variable, and defining $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$, then a suitable action is given by,

$$
S[A] = \int d^4x \left( -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + A_\mu j^\mu \right)
\tag{21.62}
$$

A variation $\delta A_\mu$ of $A_\mu$ then yields the following variation of the action,

$$
\begin{aligned}
\delta S[A] &= \int d^4x \left(-\frac{1}{2}F^{\mu\nu}\delta F_{\mu\nu} + \delta A_\mu j^\mu\right) \\
&= \int d^4x \left(F^{\mu\nu}\partial_\nu \delta A_\mu + \delta A_\mu j^\mu\right)
\end{aligned}
\tag{21.63}
$$

Integration by part of the first term gives (surface terms vanish for variations $\delta A_\mu$ with compact support, and will be omitted here),

$$
\delta S[A] = \int d^4x \, \delta A_\mu \left(-\partial_\nu F^{\mu\nu} + j^\mu\right)
\tag{21.64}
$$

Its vanishing for all $\delta A_\mu$ requires the second group of Maxwell equations.

Maxwell's equations may also be viewed directly as differential equations for $A_\mu$ with source $j^\mu$. This is achieved by eliminating $F_{\mu\nu}$ in terms of $A_\mu$, so that

$$
\partial_\mu \left(\partial^\mu A^\nu - \partial^\nu A^\mu\right) = -j^\nu
\tag{21.65}
$$

In a relativistic framework, it is more convenient to choose a relativistic gauge condition than it would be to choose the transverse gauge $\nabla \cdot \mathbf{A} = 0$, which is not Lorentz invariant. A convenient gauge is the *Landau gauge*, $\partial_\mu A^\mu = 0$, in terms of which the field equation for $A_\mu$ becomes the wave equation with a source,

$$
\partial_\mu \partial^\mu A^\nu = -j^\nu
\tag{21.66}
$$

and current density conservation now holds in view of the gauge choice.

## 21.9 Structure of the Poincaré and Lorentz algebras

The Lorentz algebra forms a 6-dimensional Lie algebra, parametrized by 3 rotations and 3 boosts. The Poincaré algebra is the semi-direct sum of the Lorentz algebra with the 4 translations of time and space, so that the Poincaré algebra is 10-dimensional. We begin by determining the structure of the Lorentz algebra, by expanding the defining relation of finite Lorentz transformations,

$$
\eta_{\mu\nu} = \Lambda_\mu{}^\rho \Lambda_\nu{}^\sigma \eta_{\rho\sigma}
\tag{21.67}
$$

around the identity,

$$
\lambda_\mu{}^\rho = \delta_\mu{}^\rho + \omega_\mu{}^\rho + \mathcal{O}(\omega^2)
\tag{21.68}
$$

This relation implies the requirement that

$$
\omega_{\nu\mu} = -\omega_{\mu\nu}
\tag{21.69}
$$

Next, we determine the structure relations of the Lorentz algebra. To this end, we consider an arbitrary representation $D(\Lambda)$ of the Lorentz group, satisfying $D(\Lambda_1\Lambda_2) = D(\Lambda_1)D(\Lambda_2)$ by definition of a representation. Let $L_{\mu\nu}$ be the representation matrices of the corresponding Lie algebra, related to $D(\Lambda)$ for $\Lambda$ close to the identity in the following way,

$$D(\Lambda) = I + \frac{1}{2}\omega^{\mu\nu}L_{\mu\nu} + \mathcal{O}(\omega^2) \tag{21.70}$$

By construction, we have $L_{\nu\mu} = -L_{\mu\nu}$. The structure relations of the Lorentz algebra are deduced by considering the following combination,

$$\begin{aligned} D(\Lambda)D(I + \omega_1)D(\Lambda)^{-1} &= D(I + \tilde{\omega}_1) + \mathcal{O}(\omega^2) \\ \tilde{\omega}_1^{\mu\nu} &= \Lambda^{\mu}{}_{\rho}\Lambda^{\nu}{}_{\sigma}\omega_1^{\rho\sigma} \end{aligned} \tag{21.71}$$

Identifying terms of order $\omega$, for all finite values of $\Lambda$, we find the transformation law for the generators $L_{\mu\nu}$ under a Lorentz transformation $\Lambda$,

$$D(\Lambda)L_{\mu\nu}D(\Lambda)^{-1} = \Lambda^{\rho}{}_{\mu}\Lambda^{\sigma}{}_{\nu}L_{\rho\sigma} \tag{21.72}$$

Taking now the special case where $\Lambda$ is infinitesimally close to the identity, $\Lambda^{\rho}{}_{\mu} = \delta^{\rho}{}_{\mu} + \omega^{\rho}{}_{\mu} + \mathcal{O}(\omega^2)$, and retaining the terms to first order in $\omega$, we derive the structure constants of $L_{\mu\nu}$,

$$[L_{\kappa\lambda}, L_{\mu\nu}] = +\eta_{\lambda\mu}L_{\kappa\nu} - \eta_{\kappa\mu}L_{\lambda\nu} + \eta_{\lambda\nu}L_{\mu\kappa} - \eta_{\kappa\nu}L_{\mu\lambda} \tag{21.73}$$

Alternatively, we may express the algebra in terms of rotations $J_k$, and boosts $K_k$, for $i = 1, 2, 3$, where $L_{ij}$ corresponds to rotations $J_k$, provided we include a factor of $i$ in its definition, and $L_{k0}$ corresponds to boosts $K_k$, for which we shall also include a factor of $i$,

$$\begin{aligned} J_1 &= -iL_{23} & K_1 &= iL_{10} \\ J_2 &= -iL_{31} & K_2 &= iL_{20} \\ J_3 &= -iL_{12} & K_3 &= iL_{30} \end{aligned} \tag{21.74}$$

The commutation relation $[L_{23}, L_{31}] = -L_{12}$ corresponds to the following commutator of the $J_k$, $[J_1, J_2] = iJ_3$, giving indeed the standard normalization of the commutation relations. Putting together all structure relations in terms of $J_k$ and $K_k$, we have,

$$\begin{aligned} [J_i, J_j] &= i\varepsilon_{ijk}J_k \\ [J_i, K_j] &= i\varepsilon_{ijk}K_k \\ [K_i, K_j] &= -i\varepsilon_{ijk}J_k \end{aligned} \tag{21.75}$$

A further change of variables of the basic generators reveals that the Lorentz algebra is actually a direct sum of two algebras, provided we *complexify the Lorentz algebra*. Complexifing means that we consider the same generators as we had in the original algebra, but we allow linear combinations with *complex* coefficients. The resulting algebra no longer acts on real objects such as the real

coordinates of space-time, but usually, we may ultimately restrict to its real subalgebra when needed. The relevant linear complexified combinations of $J_k$ and $K_k$ are given as follows,

$$A_k \equiv \frac{1}{2}(J_k - iK_k) \qquad\qquad J_k = A_k + B_k$$

$$B_k \equiv \frac{1}{2}(J_k + iK_k) \qquad\qquad K_k = i(A_k - B_k) \qquad\qquad (21.76)$$

Their commutation relations are as follows,

$$\begin{aligned}
[A_i, B_j] &= 0 \\
[A_i, A_j] &= i\varepsilon_{ijk}A_k \\
[B_i, B_j] &= i\varepsilon_{ijk}B_k
\end{aligned} \qquad\qquad (21.77)$$

The relation on the top line signifies that the sets of generators $\mathcal{A} = \{A_1, A_2, A_3\}$ and $\mathcal{B} = \{B_1, B_2, B_3\}$ mutually commute, so that the full *complexified* Lorentz algebra is a direct sum of two $SU(2)$ algebras, considered with complex coefficients.

Finally, the representations of the Lorentz algebra have certain reality properties. If the finite-dimensional representation, given by the generators $L_{\mu\nu}$ is *real*, so that the matrices $L_{\mu\nu}$ are real, and $D(\Lambda)$ is real for all $\Lambda$, then, the rotation and boost generators, $J_k, K_k$ must be purely imaginary. As a result of the standard commutation relations of angular momentum, the generators $J_k$ must be (equivalent to) Hermitian matrices. For boosts, however, the structure relations allow for either anti-Hermitian $K_k$ or Hermitian $K_k$. Hermitian $K_k$ corresponds to the rotation algebra in 4 dimensions, not the Lorentz algebra. The Lorentz algebra corresponds to the other alternative : Hermitian $K_k$. As a result, we then have the following complex conjugation relation,

$$A_k^\dagger = B_k \qquad\qquad (21.78)$$

Thus, the operation of complex conjugation interchanges the subalgebras $\mathcal{A}$ and $\mathcal{B}$.

## 21.10 Representations of the Lorentz algebra

We have already encountered several representations of the Lorentz algebra,

| | | |
|---|---|---|
| scalar | dimension 1 | $\phi$ |
| vector | dimension 4 | $x^\mu$, $\partial_\mu$, $A_\mu$ |
| anti − symmetric rank 2 tensor | dimension 6 | $F_{\mu\nu}$, $L_{\mu\nu}$ |

$$(21.79)$$

Here, we wish to construct all finite-dimensional representations of the Lorentz algebra in a systematic way. This problem is greatly simplified by the observation that the complexified Lorentz algebra is a direct sum of two complexified $SU(2)$ algebras. Thus, our procedure will consist in first constructing all *complex* finite-dimensional representations of the complexified Lorentz algebra, and then restrict those complex representations to real ones, when possible. Note that, as a

result of the complexification, the finite-dimensional representations we will obtain this way may not be unitary.

The finite-dimensional representations of the algebras $\mathcal{A}$ and $\mathcal{B}$ are perfectly well-known. Each is labeled by a non-negative integer or half-integer, which we shall denote by $a$ for the algebra $\mathcal{A}$, and $b$ for the algebra $\mathcal{B}$. The corresponding magnetic quantum numbers will be denoted $m_a$ and $m_b$, and have the customary ranges,

$$
\begin{array}{ll}
-a \leq m_a \leq +a & a - m_a \ \text{integer} \\
-b \leq m_b \leq +b & b - m_b \ \text{integer}
\end{array}
\tag{21.80}
$$

The states may be labeled by $a$ and $m_a$, as follows, $|a, m_a\rangle$, and the quantum numbers are defined by

$$
\begin{aligned}
\vec{A}^2 |a, m_a\rangle &= a(a+1)|a, m_a\rangle \\
\vec{B}^2 |b, m_b\rangle &= b(b+1)|b, m_b\rangle \\
A_3 |a, m_a\rangle &= m_a |a, m_a\rangle \\
B_3 |b, m_b\rangle &= m_b |b, m_b\rangle
\end{aligned}
\tag{21.81}
$$

Thus, we may label the finite-dimensional representations of the Lorentz algebra by a pair of non-negative integers or half-integers,

$$
(a, b) \qquad\qquad a, b \geq 0, \qquad , 2a, 2b \in \mathbf{Z}
\tag{21.82}
$$

Since $\vec{A}$ and $\vec{B}$ are neither Hermitian conjugates of one another, and not necessarily Hermitian themselves, the representation $(a, b)$ will in general be complex. However, the complex conjugate of the representation $(a, b)$ is effectively obtained by interchanging $\vec{A}$ and $\vec{B}$, and thus transforms under the representation $(b, a)$. One may thus identify these two representations,

$$
(a, b)^* = (b, a)
\tag{21.83}
$$

In particular, this means that the following representations,

$$
(a, a) \qquad\qquad (a, b) + (b, a)
\tag{21.84}
$$

are always real, for any $a, b$. The dimension of a representation $(a, b)$ is given by

$$
\dim(a, b) = (2a + 1)(2b + 1)
\tag{21.85}
$$

The representations $(a, b)$ are genuine single-valued if $a + b$ is integer, and they are double valued when $a + b$ is a half-integer, so that

$$
\begin{array}{lll}
\text{bosons} & (a, b) & a + b \ \text{integer} \ +\dfrac{1}{2} \\[2mm]
\text{fermions} & (a, b) & a + b \ \text{integer}
\end{array}
\tag{21.86}
$$

The lowest dimensional representations play an ubiquitous role in physics,

$$
\begin{array}{llll}
(0,0) & \dim = 1 & \text{real} & \text{scalar} \\
(\tfrac{1}{2},0) & \dim = 2 & \text{complex} & \text{left Weyl spinor} \\
(0,\tfrac{1}{2}) & \dim = 2 & \text{complex} & \text{right Weyl spinor} \\
(\tfrac{1}{2},\tfrac{1}{2}) & \dim = 4 & \text{real} & \text{vector} \\
(1,0) & \dim = 3 & \text{complex} & \text{self} - \text{dual antisymmetric tensor} \\
(0,1) & \dim = 3 & \text{complex} & \text{anti} - \text{self} - \text{dual antisymmetric tensor} \\
(\tfrac{1}{2},1) & \dim = 6 & \text{complex} & \text{left gravitino} \\
(1,\tfrac{1}{2}) & \dim = 6 & \text{complex} & \text{right gravitino} \\
(1,1) & \dim = 9 & \text{real} & \text{graviton}
\end{array}
\tag{21.87}
$$

In this course, we shall only need the scalar, the Weyl spinors, and the vector. Note that the combination

$$
(\tfrac{1}{2},0) \oplus (0,\tfrac{1}{2})
\tag{21.88}
$$

corresponds to a 4-dimensional (complex) Dirac spinor if the two component representations are unrelated, while it corresponds to a Majorana spinor if the representations are complex conjugates of one another.

# 22   The Dirac Field and the Dirac Equation

Among the relativistic wave equations, we have not yet obtained one suitable for spin 1/2, doing so is the object of the present chapter. From the preceding discussion, there are 3 cases,

$$\left(\frac{1}{2}, 0\right) \qquad\qquad\qquad \text{left Weyl spinor}$$

$$\left(0, \frac{1}{2}\right) \qquad\qquad\qquad \text{right Weyl spinor}$$

$$\left(\frac{1}{2}, 0\right) \oplus \left(0, \frac{1}{2}\right) \qquad\qquad\qquad \text{Dirac spinor} \tag{22.1}$$

(The case of a Majorana spinor will turn out to be equivalent to that of a Weyl spinor, and will not be discussed further here.) It is actually convenient to treat all cases at once by concentrating on the reducible case of the Dirac spinor. Historically, this is also what Dirac did.

The representation $(\frac{1}{2}, 0)$ is well-known: it can be obtained in terms of the Pauli matrices. Similarly, the case of the representation $(0, \frac{1}{2})$ may be given in terms of the Pauli matrices as well; (here and below, $k = 1, 2, 3$),

$$D_L(A_k) = \frac{\sigma_k}{2} \qquad\qquad\qquad D_L(B_k) = 0$$

$$D_R(A_k) = 0 \qquad\qquad\qquad D_L(B_k) = \frac{\sigma_k}{2} \tag{22.2}$$

Of course, $D_L$ and $D_R$ act on two different two-dimensional representation spaces, and so do the corresponding Pauli matrices. To make this crystal clear, it is preferable to work on the direct sum representation $D = D_L \oplus D_R$ of the two spinors, so that the representation matrices are given as follows,

$$D(A_k) = \begin{pmatrix} \frac{1}{2}\sigma_k & 0 \\ 0 & 0 \end{pmatrix} \qquad\qquad D(B_k) = \begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{2}\sigma_k \end{pmatrix} \tag{22.3}$$

or in terms of the original rotation and boost generators,

$$D(J_k) = \begin{pmatrix} \frac{1}{2}\sigma_k & 0 \\ 0 & \frac{1}{2}\sigma_k \end{pmatrix} \qquad\qquad D(K_k) = \begin{pmatrix} \frac{1}{2}\sigma_k & 0 \\ 0 & -\frac{1}{2}\sigma_k \end{pmatrix} \tag{22.4}$$

It is not à priori so easy to write down a Lorentz-covariant equation because the generators are not labeled by Lorentz vector indices (such as tensors were), but rather by a novel type of spinor index. To circumvent these problems, we introduce the Dirac matrices.

## 22.1   The Dirac-Clifford algebra

One defines the Dirac-Clifford algebra in space-time dimension 4 as an algebra of Dirac matrices $\gamma^\mu$, where $\mu = 0, 1, 2, 3$, which satisfy the following defining equation,

$$\{\gamma^\mu, \gamma^\nu\} = \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2\eta^{\mu\nu} I \tag{22.5}$$

where $I$ is the unit matrix in the Dirac representation space. Given the Dirac matrices, which we shall realize shortly in explicit form, one automatically constructs the Dirac spinor representation of the Lorentz algebra,

$$D(L_{\mu\nu}) \equiv S_{\mu\nu} = \frac{1}{4}[\gamma^\mu, \gamma^\nu] \tag{22.6}$$

To show that $S_{\mu\nu}$ indeed forms a representation of the Lorentz algebra, all we need to do is to show that it satisfies the structure constants of (21.73). To do so, it will be useful to recast $S_{\mu\nu} = \frac{1}{2}\gamma_\mu\gamma_\nu - \frac{1}{2}\eta_{\mu\nu}I$, since the term proportional to $I$ will cancel out in the argument of the commutator. Thus, we have

$$
\begin{aligned}
[S_{\kappa\lambda}, S_{\mu\nu}] &= \frac{1}{4}[\gamma_\kappa\gamma_\lambda, \gamma_\mu\gamma_\nu] = \frac{1}{4}\left(\gamma_\kappa\gamma_\lambda\gamma_\mu\gamma_\nu - \gamma_\mu\gamma_\nu\gamma_\kappa\gamma_\lambda\right) \\
&= \frac{1}{4}\gamma_\kappa\left(-\gamma_\mu\gamma_\lambda + 2\eta_{\mu\lambda}\right)\gamma_\nu - \frac{1}{4}\gamma_\mu\left(-\gamma_\kappa\gamma_\nu + 2\eta_{\kappa\nu}\right)\gamma_\lambda \\
&= \frac{1}{2}\eta_{\mu\lambda}\gamma_\kappa\gamma_\nu - \frac{1}{2}\eta_{\kappa\nu}\gamma_\mu\gamma_\lambda - \frac{1}{4}(2\eta_{\kappa\mu} - \gamma_\mu\gamma_\kappa)\gamma_\lambda\gamma_\nu + \frac{1}{4}\gamma_\mu\gamma_\kappa(2\eta_{\nu\lambda} - \gamma_\lambda\gamma_\nu)
\end{aligned} \tag{22.7}
$$

The terms quartic in $\gamma$-matrices cancel on the last line, and we are left with terms quadratic in $\gamma$ only. They become,

$$
\begin{aligned}
[S_{\kappa\lambda}, S_{\mu\nu}] &= \frac{1}{2}\eta_{\mu\lambda}\gamma_\kappa\gamma_\nu - \frac{1}{2}\eta_{\kappa\nu}\gamma_\mu\gamma_\lambda - \frac{1}{2}\eta_{\kappa\mu}\gamma_\lambda\gamma_\nu + \frac{1}{2}\eta_{\nu\lambda}\gamma_\mu\gamma_\kappa \\
&= \frac{1}{4}\eta_{\mu\lambda}[\gamma_\kappa, \gamma_\nu] - \frac{1}{4}\eta_{\kappa\nu}[\gamma_\mu, \gamma_\lambda] - \frac{1}{4}\eta_{\kappa\mu}[\gamma_\lambda, \gamma_\nu] + \frac{1}{4}\eta_{\nu\lambda}[\gamma_\mu, \gamma_\kappa] \\
&= \eta_{\mu\lambda}S_{\kappa\nu} - \eta_{\kappa\nu}S_{\mu\lambda} - \eta_{\kappa\mu}S_{\lambda\nu} + \eta_{\nu\lambda}S_{\mu\kappa}
\end{aligned} \tag{22.8}
$$

which is precisely the structure relation of the Lorentz algebra.

The representation $S_{\mu\nu}$ obtained this way is always reducible. This may be established by constructing the famous chirality, or $\gamma^5$-matrix, which is given by the product of all $\gamma$-matrices, up to an overall complex multiple. We shall make the choice

$$\gamma^5 \equiv -i\gamma^0\gamma^1\gamma^2\gamma^3 \tag{22.9}$$

so that its square equals the identity matrix,

$$\left(\gamma^5\right)^2 = -\gamma^0\gamma^1\gamma^2\gamma^3\gamma^0\gamma^1\gamma^2\gamma^3 = \gamma^0\gamma^1\gamma^2\gamma^0\gamma^1\gamma^2 = \gamma^0\gamma^1\gamma^0\gamma^1 = -\gamma^0\gamma^0 = I \tag{22.10}$$

Furthermore, $\gamma^5$ anti-commutes with all $\gamma^\mu$,

$$\{\gamma^5, \gamma^\mu\} = 0 \qquad\qquad \mu = 0, 1, 2, 3 \tag{22.11}$$

and therefore must commute with the generators of the Lorentz algebra,

$$[\gamma^5, S_{\mu\nu}] = 0 \qquad\qquad \mu, \nu = 0, 1, 2, 3 \tag{22.12}$$

Since $\{\gamma^5, \gamma^\mu\} = 0$, the matrix $\gamma^5$ cannot simply be proportional to the identity matrix. Thus, we have a non-trivial matrix $\gamma^5$ commuting with the entire representation $S_{\mu\nu}$, which implies that the representation $S_{\mu\nu}$ of the Lorentz algebra is a *reducible representation*. Note that, although the representation of the Lorentz algebra is reduced by $\gamma^5$, the Clifford algebra of the $\gamma$-matrices is irreducible.

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## 22.2 Explicit representation of the Dirac algebra

From the definition of $\gamma^5$, we have, $\mathrm{tr}(\gamma^5) = -i\mathrm{tr}(\gamma^0\gamma^1\gamma^2\gamma^3)$. By using the cyclic property of the trace, this quantity equals $-i\mathrm{tr}(\gamma^1\gamma^2\gamma^3\gamma^0)$. On the other hand, by anti-commuting $\gamma^0$ through the matrices $\gamma^1\gamma^2\gamma^3$, it also equals $+i\mathrm{tr}(\gamma^1\gamma^2\gamma^3\gamma^0)$, and thus must vanish,

$$\mathrm{tr}\left(\gamma^5\right) = 0 \tag{22.13}$$

Since we also have $(\gamma^5)^2 = I$, it follows that $\gamma^5$ must have equal numbers of eigenvalues $+1$ and $-1$. Thus, the representation space must have even dimension $2n$, for $n$ integer. In a basis where $\gamma^5$ is diagonal, we thus have

$$\gamma^5 = \begin{pmatrix} I_n & 0 \\ 0 & -I_n \end{pmatrix} \tag{22.14}$$

The matrix $\gamma^0$ anti-commutes with $\gamma^5$, and squares to $-I_{2n}$; it may be chosen as follows,

$$\gamma^0 = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix} \tag{22.15}$$

Finally, the combinations $\gamma^0\gamma^i$ for $i = 1, 2, 3$ commute with $\gamma^5$, and must thus be block-diagonal in the basis where $\gamma^5$ is diagonal,

$$\gamma^0\gamma^i = \begin{pmatrix} a^i_+ & 0 \\ 0 & a^i_- \end{pmatrix} \tag{22.16}$$

From the Clifford algebra relations, we also have

$$\left\{\gamma^0\gamma^i, \gamma^0\gamma^j\right\} = 2\delta^{ij} I_{2n} \tag{22.17}$$

so that

$$\left\{a^i_\pm, a^j_\pm\right\} = 2\delta^{ij} I_n \tag{22.18}$$

But this last relation is the defining equation for the Pauli matrices, of which the lowest-dimensional representation has $n = 2$, and $a^i_\pm = \varepsilon_\pm \sigma^i$, with $(\varepsilon_\pm)^2 = 1$. We may choose $\varepsilon_+ = 1$ without loss of generality. The value $\varepsilon_- = +1$ then makes $a^i_+ = a^i_-$ and results in $[\gamma^0, \gamma^i] = 0$, which is unacceptable. Thus, we are left with the unique solution $\varepsilon_- = -1$. The $\gamma^\mu$-matrices now take the following explicit form in this basis,

$$\gamma^0 = \begin{pmatrix} 0 & I_2 \\ -I_2 & 0 \end{pmatrix} \qquad\qquad \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix} \tag{22.19}$$

We check that

$$\gamma^5 = -i\gamma^0\gamma^1\gamma^2\gamma^3 = -i\begin{pmatrix} \sigma^1\sigma^2\sigma^3 & 0 \\ 0 & -\sigma^1\sigma^2\sigma^3 \end{pmatrix} = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix} \tag{22.20}$$

The generators of the Lorentz algebra in this basis are given by

$$
\begin{aligned}
S_{0i} &= \frac{1}{2}\gamma_0\gamma_i = -\frac{1}{2}\gamma^0\gamma^i = \frac{1}{2}\begin{pmatrix} -\sigma^i & 0 \\ 0 & \sigma^i \end{pmatrix} \\
S_{ij} &= S^{ij} = \frac{1}{4}\begin{pmatrix} [\sigma^i,\sigma^j] & 0 \\ 0 & [\sigma^i,\sigma^j] \end{pmatrix} = \frac{i}{2}\varepsilon_{ijk}\begin{pmatrix} \sigma^k & 0 \\ 0 & \sigma^k \end{pmatrix}
\end{aligned}
\tag{22.21}
$$

We may use these expressions to find also the representations of the generators $J_k$ and $K_k$ in this basis,

$$
J_k = \frac{1}{2}\begin{pmatrix} \sigma^k & 0 \\ 0 & \sigma^k \end{pmatrix} \qquad\qquad K_k = \frac{i}{2}\begin{pmatrix} \sigma^k & 0 \\ 0 & -\sigma^k \end{pmatrix}
\tag{22.22}
$$

and from these we get

$$
A_k = \frac{1}{2}\begin{pmatrix} \sigma^k & 0 \\ 0 & 0 \end{pmatrix} \qquad\qquad B_k = \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & \sigma^k \end{pmatrix}
\tag{22.23}
$$

These expressions reveal that the subalgebras $\mathcal{A}$ and $\mathcal{B}$ indeed correspond to the reducibility of the spinor representation.

## 22.3 Action of Lorentz transformations on $\gamma$-matrices

The Lorentz algebra in the Dirac spinor representation acts by the following infinitesimal transformations,

$$
\begin{aligned}
\Lambda^\mu{}_\nu &= \delta^\mu{}_\nu + \omega^\mu{}_\nu + \mathcal{O}(\omega^2) \\
D(\Lambda) &= I + \frac{1}{2}\omega^{\mu\nu}S_{\mu\nu} + \mathcal{O}(\omega^2)
\end{aligned}
\tag{22.24}
$$

which allows us to compute the action of the Lorentz algebra on the $\gamma$-matrices,

$$
\begin{aligned}
D(\Lambda)\gamma_\kappa D(\Lambda)^{-1} &= \left(I + \frac{1}{2}\omega^{\mu\nu}S_{\mu\nu}\right)\gamma_\kappa\left(I - \frac{1}{2}\omega^{\mu\nu}S_{\mu\nu}\right) + \mathcal{O}(\omega^2) \\
&= \gamma_\kappa + \frac{1}{2}\omega^{\mu\nu}[S_{\mu,\nu},\gamma_\kappa] + \mathcal{O}(\omega^2)
\end{aligned}
\tag{22.25}
$$

The commutator may be evaluated using only the Clifford algebra relations, and we find,

$$
[S_{\mu,\nu},\gamma_\kappa] = \eta_{\kappa\nu}\gamma_\mu - \eta_{\kappa\mu}\gamma_\nu
\tag{22.26}
$$

Asa result, we have

$$
\begin{aligned}
D(\Lambda)\gamma_\kappa D(\Lambda)^{-1} &= \gamma_\kappa + \omega^\mu{}_\kappa\gamma_\mu + \mathcal{O}(\omega^2) \\
&= \Lambda^\mu{}_\kappa\gamma_\mu
\end{aligned}
\tag{22.27}
$$

The relation, as it was derived above, holds for $\Lambda$ close to the identity. Given the overall covariance of the tensors of the last line, this relation must now be valid for finite $\Lambda$ as well. Another way of writing this relation is by contracting both sides with $\Lambda_\kappa{}^\lambda$, so that we get

$$\lambda_\kappa{}^\lambda D(\Lambda)\gamma_\kappa D(\Lambda)^{-1} = \gamma^\lambda \tag{22.28}$$

This relation signifies that the $\gamma$-matrices are *constants* provided that we transform both their vector index and their spinor indices. The Lorentz transformation property of the generators $S_{\mu\nu}$ themselves follows from that of the $\gamma$-matrices, and we have,

$$D(\Lambda)S_{\kappa\lambda}D(\Lambda)^{-1} = \Lambda^\mu{}_\kappa \Lambda^\nu{}_\lambda S_{\mu\nu} \tag{22.29}$$

The structure relations may be recovered from this relation.

## 22.4   The Dirac equation and its relativistic invariance

We now have all the tools ready to construct relativistic invariant equations for fields which are spinors of the Lorentz algebra. We shall work in the (reducible) Dirac representation, leaving the Weyl and Majorana cases as a special case of the Dirac spinors.

The basic Dirac field $\psi(x)$ transforms as a 4-component representation of the form $(\frac{1}{2},0)\oplus(0,\frac{1}{2})$, for which we have just constructed the representation matrices. The field transforms as follows,

$$\psi(x) \;\rightarrow\; \psi'(x') = D(\Lambda)\psi(x) \tag{22.30}$$

where the infinitesimal transformations were given in (22.24). We begin by constructing an equation for a *free field*, namely a linear equation for $\psi$. Of course, we could write down the free Klein-Gordon equation for $\psi$,

$$(\partial^\mu\partial_\mu - m^2)\psi(x) = 0 \tag{22.31}$$

and this is a perfectly fine free wave equation for a spinor. The correct equation, however, turns out to be a first order equation, namely the *free Dirac equation*,

$$(\gamma^\mu\partial_\mu - m)\,\psi(x) = 0 \tag{22.32}$$

Note that the free Dirac equation implies the free Klein-Gordon equation. This may be seen by multiplying the Dirac equation to the left by the operator $(\gamma^\nu\partial_\nu + m)$, which gives,

$$\left(\gamma^\nu\partial_\nu\gamma^\mu\partial_\mu - m^2\right)\psi = 0 \tag{22.33}$$

Using the fact that the derivatives are symmetric under interchange of $\mu$ and $\nu$, and using the Clifford relation, it is immediate that this equation coincides with the Klein-Gordon equation. The converse is, however, not true, as a field $\psi$ satisfying (22.31) may be decomposed into solutions of $(\gamma^\mu\partial_\mu \pm m)\psi = 0$, with either $\pm$ sign. In fact, the Dirac equation has only half the number of solutions of the Klein-Gordon equation (both for 4-component spinors).

We begin by checking that the free Dirac equation is indeed Lorentz invariant. We shall show that

$$\left(\gamma^\mu \partial'_\mu - m\right)\psi'(x') = D(\Lambda)\left(\gamma^\mu \partial_\mu - m\right)\psi(x) \tag{22.34}$$

To establish this relation, it suffices to compute the left hand side, using the following transformation results,

$$
\begin{aligned}
\psi'(x') &= D(\Lambda)\psi(x) \\
\partial'_\mu &= \Lambda_\mu{}^\nu \partial_\nu \\
\gamma^\mu \Lambda_\mu{}^\nu &= D(\Lambda)\gamma^\nu D(\Lambda)^{-1}
\end{aligned}
\tag{22.35}
$$

If now $(\gamma^\mu \partial_\mu - m)\psi(x) = 0$, then it follows that also $\left(\gamma^\mu \partial'_\mu - m\right)\psi'(x') = 0$, and the equation is covariant.

Group theoretically, the structure of the Dirac equation is organized as follows,

$$
\begin{aligned}
\psi &\sim \left(\frac{1}{2},0\right) \oplus \left(0,\frac{1}{2}\right) \\
\partial &\sim \left(\frac{1}{2},\frac{1}{2}\right) \\
\partial\psi &\sim \left(\frac{1}{2},\frac{1}{2}\right) \otimes \left[\left(\frac{1}{2},0\right) \oplus \left(0,\frac{1}{2}\right)\right] \\
&= \left(0,\frac{1}{2}\right) \oplus \left(1,\frac{1}{2}\right) \oplus \left(\frac{1}{2},0\right) \oplus \left(\frac{1}{2},1\right)
\end{aligned}
\tag{22.36}
$$

The $\gamma$-matrix is responsible for projecting out the representations $(1,\frac{1}{2}) \oplus (\frac{1}{2},1)$ and retaining only $(\frac{1}{2},0) \oplus (0,\frac{1}{2})$. In the Weyl basis, we have

$$
\gamma^0 = \begin{pmatrix} 0 & I_2 \\ -I_2 & 0 \end{pmatrix} \qquad \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix} \qquad \gamma^5 = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix} \tag{22.37}
$$

It is customary to introduce the Pauli matrices with a Lorentz index, as follows,

$$
\begin{aligned}
\sigma^\mu &\equiv (+I_2, \sigma^i) \\
\bar{\sigma}^\mu &\equiv (-I_2, \sigma^i)
\end{aligned}
\tag{22.38}
$$

The Dirac matrices may then be expressed in a manifestly Lorentz covariant way,

$$
\gamma^\mu = \begin{pmatrix} 0 & \sigma^\mu \\ \bar{\sigma}^\mu & 0 \end{pmatrix} \tag{22.39}
$$

Decomposing now also the Dirac field $\psi$ into 2-component spinors $\psi_L$ and $\psi_R$, referred to as the left and the right Weyl spinors,

$$
\psi = \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix} \tag{22.40}
$$

the free Dirac equation reads,

$$\begin{pmatrix} -m & \sigma^\mu \partial_\mu \\ \bar{\sigma}^\mu \partial_\mu & -m \end{pmatrix} \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix} = 0 \tag{22.41}$$

Separating the two components,

$$\begin{aligned} \sigma^\mu \partial_\mu \psi_R - m\psi_L &= 0 \\ \bar{\sigma}^\mu \partial_\mu \psi_L - m\psi_R &= 0 \end{aligned} \tag{22.42}$$

we see that the mass $m$ produces a coupling or a mixing between the left and right Weyl spinors.

When the mass $m$ vanishes, the equations for left and right Weyl spinors decouple, and we are left with the Dirac equation for a massless spinor,

$$\begin{aligned} \sigma^\mu \partial_\mu \psi_R &= 0 \\ \bar{\sigma}^\mu \partial_\mu \psi_L &= 0 \end{aligned} \tag{22.43}$$

It is now consistent to retain only one of these 2-component spinors, and set the other to zero. For example, setting $\psi_R = 0$ produces the left Weyl spinor equation,

$$\sigma^\mu \partial_\mu \psi_L = 0 \tag{22.44}$$

Note that, by construction, this equation is also Lorentz-invariant, just as the full Dirac equation was. When $m \neq 0$, it is of course inconsistent to set $\psi_R = 0$, since the Dirac equation then automatically implies that also $\psi_L = 0$.

## 22.5   Elementary solutions to the free Dirac equation

The free Dirac equation, $(\gamma^\mu \partial_\mu - m)\psi(x) = 0$ is a linear partial differential equation with $x$-independent coefficients, and may thus be solved by Fourrier analysis. The elementary solutions are labeled by the 4-momentum $k$,

$$\psi_k(x) = u(k)\, e^{-ik \cdot x} \tag{22.45}$$

where $u(k)$ is a 4-component spinor which satisfies the algebraic equation

$$(i\gamma^\mu k_\mu + m)u(k) = 0 \tag{22.46}$$

In the Weyl basis, we decompose $u(k)$ into $u_L(k)$ and $u_R(k)$, for which the equation reads,

$$\begin{pmatrix} m & i\sigma^\mu k_\mu \\ i\bar{\sigma}^\mu k_\mu & m \end{pmatrix} \begin{pmatrix} u_L \\ u_R \end{pmatrix} = 0 \tag{22.47}$$

or separating out space from time components,

$$\begin{aligned} i(-k_0 + \vec{k} \cdot \vec{\sigma})u_L + mu_R &= 0 \\ i(+k_0 + \vec{k} \cdot \vec{\sigma})u_R + mu_L &= 0 \end{aligned} \tag{22.48}$$

Eliminating one or the other components, gives the standard energy-momentum-mass relation, $(k_0^2 - \vec{k}^2 - m^2)u_{L,R}(\vec{k}) = 0$. To solve the Dirac equation, it is useful to separate the massless case from the massive one. When $m = 0$, we may choose the momentum as follows, $k_\mu = (k_0, 0, 0, k)$ where $k_0 = |k|$. The equations for $u_L, u_R$ then read,

$$\begin{aligned}
(k_0 - k\sigma^3)u_L &= 0 \\
(k_0 + k\sigma^3)u_R &= 0
\end{aligned} \tag{22.49}$$

The solutions depend on the sign of $k$, and we have,

$$
\begin{aligned}
k > 0 &\qquad \begin{cases} u_{L2} = 0 \\ u_{R1} = 0 \end{cases} \\
k < 0 &\qquad \begin{cases} u_{L1} = 0 \\ u_{R2} = 0 \end{cases}
\end{aligned} \tag{22.50}
$$

For a left Weyl spinor, for example, with $k > 0$, there is a 1-dimensional space of solutions, parametrized by $u_{L1}$, corresponding to the definite helicity $+1/2\hbar$. For $m \neq 0$, we have two linearly independent solutions $u^{(\ell)}$ for $\ell = 1, 2$, which may be parametrized as follows,

$$
u_R^{(\ell)} = \frac{i}{m}(k_0 - \vec{k} \cdot \vec{\sigma})u_L^{(\ell)} \qquad u_L^{(1)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad u_L^{(2)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{22.51}
$$

## 22.6 The conserved current of fermion number

The Dirac equation is invariant under phase rotations of the field $\psi$ by an $x$-independent angle $\theta$,

$$\psi(x) \to \psi'(x) = e^{i\theta}\,\psi(x) \tag{22.52}$$

and the associated conserved current is given by

$$j^\mu = \psi^\dagger \gamma^0 \gamma^\mu \psi \tag{22.53}$$

We begin by showing that $j^\mu$ indeed transforms as a 4-vector under Lorentz transformations. Group theoretically, this works as follows. We decompose $\psi$ into its Weyl components, and recast the fermion number current in terms of $\psi_{L,R}$,

$$j^\mu = \psi_L^\dagger \bar{\sigma}^\mu \psi_L + \psi_R^\dagger \sigma^\mu \psi_R \tag{22.54}$$

Since $\psi_L \sim (\frac{1}{2}, 0)$ and $\psi_R \sim (0, \frac{1}{2})$, this combination does indeed give rise to a vector, since $\psi_L^\dagger \otimes \psi_L \sim (\frac{1}{2}, \frac{1}{2})$, as well as $\psi_R^\dagger \otimes \psi_R \sim (\frac{1}{2}, \frac{1}{2})$. More precisely, we need the transformation matrices for the complex conjugate of $\psi$, which can be obtained as follows,

$$
\begin{aligned}
\psi(x) &\to \psi'(x') = D(\Lambda)\psi(x) \\
\psi(x)^\dagger &\to (\psi'(x))^\dagger = \psi(x)^\dagger D(\Lambda)^\dagger \\
\bar{\psi}(x) &\to \bar{\psi}'(x') = \psi(x)^\dagger D(\Lambda)^\dagger \gamma^0 = -\bar{\psi}(x)\gamma^0 D(\Lambda)^\dagger \gamma^0
\end{aligned} \tag{22.55}
$$

To calculate the combination $-\gamma^0 D(\Lambda)^\dagger \gamma^0$, we take $\Lambda$ infinitesimally close to the identity, so that

$$
\begin{aligned}
D(\Lambda) &= I + \frac{1}{2}\omega^{\mu\nu}S_{\mu\nu} + \mathcal{O}(\omega^2) \\
&= I + \omega^{0i}S_{0i} + \frac{1}{2}\omega^{ij}S_{ij} + \mathcal{O}(\omega^2) \\
D(\Lambda)^\dagger &= I + \omega^{0i}S_{0i}^\dagger + \frac{1}{2}\omega^{ij}S_{ij}^\dagger + \mathcal{O}(\omega^2)
\end{aligned}
\tag{22.56}
$$

From the explicit representations of $S_{\mu\nu}$, we have that

$$
\begin{aligned}
S_{0i}^\dagger &= +S_{0i} = \gamma^0 S_{0i}\gamma^0 \\
S_{ij}^\dagger &= -S_{ij} = \gamma^0 S_{ij}\gamma^0
\end{aligned}
\tag{22.57}
$$

Thus, we have

$$
\begin{aligned}
D(\Lambda)^\dagger &= I + \omega^{0i}\gamma^0 S_{i0}\gamma^0 + \frac{1}{2}\omega^{ij}\gamma^0 S_{ij}\gamma^0 + \mathcal{O}(\omega^2) \\
&= -\gamma^0 \left( I - \omega^{0i}S_{0i} - \frac{1}{2}\omega^{ij}S_{ij} + \mathcal{O}(\omega^2) \right)\gamma^0 \\
&= -\gamma^0 D(\Lambda)^{-1}\gamma^0
\end{aligned}
\tag{22.58}
$$

Using this expression in the transformation law for $\bar{\psi}$, we get

$$
\bar{\psi}(x) \to \bar{\psi}'(x') = \bar{\psi}(x)D(\Lambda)^{-1}
\tag{22.59}
$$

It is now straightforward to derive the transformation law of the fermion current,

$$
\begin{aligned}
j^\mu(x) \to j'^\mu(x') &= \bar{\psi}'(x')\gamma^\mu \psi'(x') \\
&= \bar{\psi}(x)D(\Lambda)^{-1}\gamma^\mu D(\Lambda)\psi(x) \\
&= \Lambda^\mu{}_\nu j^\nu(x)
\end{aligned}
\tag{22.60}
$$

Finally, we check that the current is conserved,

$$
\partial_\mu j^\mu = \partial_\mu(\bar{\psi}\gamma^\mu\psi) = \bar{\psi}\gamma^\mu\partial_\mu\psi + (\partial_\mu\bar{\psi})\gamma^\mu\psi
\tag{22.61}
$$

The first term on the rhs is simplified by using the Dirac equation, $\gamma^\mu\partial_\mu\psi = m\psi$, while the second term can be handled using the conjugate of the Dirac equation,

$$
(\partial_\mu\psi)^\dagger(\gamma^\mu)^\dagger - m\psi^\dagger = 0
\tag{22.62}
$$

Using $(\gamma^\mu)^\dagger = \gamma^0\gamma^\mu\gamma^0$, this becomes,

$$
(\partial_\mu\bar{\psi})\gamma^\mu + m\bar{\psi} = 0
\tag{22.63}
$$

Combining both equations gives $\partial_\mu j^\mu = 0$.

## 22.7    The free Dirac action and Hamiltonian

The field equations $(\gamma^\mu \partial_\mu - m)\psi = 0$ may be derived from an action principle. The action involves the field $\psi$, as well as the field $\bar\psi$, which is being considered as independent from the field $\psi$, in the same sense that the complex variables $z$ and $\bar z$ are considered as being independent variables. The action is given by

$$S[\psi, \bar\psi] = \int d^4x\, \bar\psi (\gamma^\mu \partial_\mu - m)\psi \tag{22.64}$$

Varying $\bar\psi$ produces the Dirac equation, while varying $\psi$ produces its conjugate equation. The action is manifestly Lorentz invariant, since we have already shown the transformation laws of $(\gamma^\mu \partial_\mu - m)\psi$ and $\bar\psi$ to be inverse of one another.

*Note: for the time being, $\bar\psi$ should always be kept to the left of the field $\psi$ in the action. Ultimately, we shall see that $\psi$ and $\bar\psi$ in the classical action are not ordinary complex-valued fields, but rather Grassmann-valued.*

The Hamiltonian formulation of the Dirac equation is rather intricate. The momentum conjugate to $\psi$ is given by

$$\Pi_\psi = \frac{\partial \mathcal{L}}{\partial \partial_0 \psi} = -\bar\psi \gamma^0 = \psi^\dagger \tag{22.65}$$

but the momentum conjugate to $\bar\psi$ vanishes ! This is a reflection of the fact that the Dirac system is first-order in time-derivatives. The Hamiltonian becomes,

$$
\begin{aligned}
H &= \int d^3x \ (\Pi_\psi \partial_0 \psi - \mathcal{L}) \\
&= \int d^3x\, \bar\psi \left( -\gamma^i \partial_i + m \right) \psi
\end{aligned}
\tag{22.66}
$$

## 22.8    Coupling to the electro-magnetic field

We now wish to include the interactions between the Dirac field and electro-magnetism, represented by the electro-magnetic vector potential $A_\mu$, and we want the final theory to be Lorentz invariant. Recall from our discussion of Maxwell theory that $A_\mu$ must couple to a conserved electric current density. We have already identified this current in Dirac theory : it must be proportional to $\bar\psi \gamma^\mu \psi$, and the factor of proportionality $q$ gives the strength of the coupling, which is nothing but the electric charge of the unit element of the Dirac field. The corresponding action is

$$S[\psi, \bar\psi, A] = \int d^4x \left[ -\frac{1}{4} F^{\mu\nu} F_{\mu\nu} + \bar\psi \left( \gamma^\mu \partial_\mu + iq\gamma^\mu A_\mu - m \right) \psi \right] \tag{22.67}$$

This action is manifestly Lorentz-invariant. We shall now show that it is also gauge invariant. Under a gauge transformation, $\psi$ is multiplied by an $x$-dependent phase factor, while $A_\mu$ transforms as,

$$
\begin{aligned}
A_\mu(x) &\to A'_\mu(x) = A_\mu(x) + \partial_\mu \theta(x) \\
\psi(x) &\to \psi'(x) = e^{-iq\theta(x)} \psi(x)
\end{aligned}
\tag{22.68}
$$

The key property is that the *gauge covariant derivative* $D_\mu = \partial_\mu + iqA_\mu$ of $\psi$ transforms exactly as $\psi$ does under gauge transformations. Indeed, we have

$$D_\mu \psi(x) \to D'_\mu \psi'(x) = (\partial_\mu + iqA'_\mu(x))\psi'(x) = e^{-iq\theta(x)} D_\mu \psi(x) \tag{22.69}$$

The modified Dirac equation, in the presence of the electro-magnetic field is obtained by varying the action with respect to $\bar\psi$, and we find,

$$\left(\gamma^\mu \partial_\mu + iq\gamma^\mu A_\mu - m\right)\psi = 0 \tag{22.70}$$

It is very interesting to work out the non-relativistic limit of this equation. To do so, we multiply the Dirac equation by the operator $(\gamma^\mu \partial_\mu + iq\gamma^\mu A_\mu + m)$, to get a second order equation,

$$\left(\gamma^\mu \partial_\mu + iq\gamma^\mu A_\mu + m\right)\left(\gamma^\mu \partial_\mu + iq\gamma^\mu A_\mu - m\right)\psi = 0 \tag{22.71}$$

or equivalently,

$$\left(\gamma^\mu \gamma^\nu (\partial_\mu + iqA_\mu)(\partial_\nu + iqA_\nu) - m^2\right)\psi = 0 \tag{22.72}$$

Using the decomposition of the product into symmetric and anti-symmetric tensors,

$$\gamma^\mu \gamma^\nu = \eta^{\mu\nu} + 2S^{\mu\nu} \qquad\qquad S^{\mu\nu} = \frac{1}{4}[\gamma^\mu, \gamma^\nu] \tag{22.73}$$

the second order equation becomes,

$$\left((\partial_\mu + iqA_\mu)(\partial^\mu + iqA^\mu) + S^{\mu\nu}[\partial_\mu + iqA_\mu, \partial_\nu + iqA_\nu] - m^2\right)\psi = 0 \tag{22.74}$$

in view of the anti-symmetry in $\mu, \nu$ of $S^{\mu\nu}$. The commutator is easily computed, and we have,

$$[\partial_\mu + iqA_\mu, \partial_\nu + iqA_\nu] = iqF_{\mu\nu} \tag{22.75}$$

Hence, the second order equation becomes,

$$\left((\partial_\mu + iqA_\mu)(\partial^\mu + iqA^\mu) + iqF_{\mu\nu}S^{\mu\nu} - m^2\right)\psi = 0 \tag{22.76}$$

In the non-relativistic limit, we have $i\partial_0 \psi = (m + E)\psi$ with $E \ll m$. As a result, we have

$$\left(2m(E + qA_0) - (\vec{p} + q\vec{A})^2 + iqF_{\mu\nu}S^{\mu\nu}\right)\psi = 0 \tag{22.77}$$

The corresponding Schrödinger equation is then,

$$\left(\frac{1}{2m}(\vec{p} + q\vec{A})^2 - \frac{iq}{2m}F_{\mu\nu}S^{\mu\nu} - qA_0\right)\psi = E\psi \tag{22.78}$$

This gives $\vec{B} \cdot \vec{S}$ coupling $\mu_e = e/m$.

# 23　Quantization of the Dirac Field

We proceed to quantizing first the free Dirac field, and shall then motivate the quantization of the interacting field. Recall that we have,

- $\left(\gamma^\mu \partial_\mu - m\right)\psi = 0$

- $H = \displaystyle\int d^3x\, \psi^\dagger \left(-\gamma^0\gamma^i\partial_i + m\gamma^0\right)\psi$

- $Q = \displaystyle\int d^3x\, \psi^\dagger \psi$ (23.1)

Recall that the key new feature of the Dirac field is that it must describe fermions, in contrast to the scalar or electro-magnetic field which describes bosons. The Fock space of states for the Dirac field should automatically reflect the the corresponding Fermi-Dirac statistic, just as the Fock space for bosons automatically reflected Bose-Einstein statistics. While bosonic fields are decomposed into bosonic oscillators, we should expect the Dirac field to decompose into fermionic oscillators, as had already been guessed in earlier sections.

## 23.1　The basic free field solution

Recall that the general solution to the free Dirac equation is given by by a linear superposition of Fourier modes of the form,

$$
\begin{aligned}
\psi(x) &= u(k)\, e^{-ik\cdot x} \\
(ik_\mu\gamma^\mu + m)\, u(k) &= 0
\end{aligned}
\tag{23.2}
$$

with the "on-shell" condition $k^\mu k_\mu = k^2 = m^2$. The equation for $u(k)$ has solutions for both $k^0 > 0$ and $k^0 < 0$. It is conventional to reorganize the solutions with the help of the following notation,

$$
\begin{aligned}
\psi_+(x) &= u(k)\, e^{-ik\cdot x} & k^0 &> 0 \\
\psi_-(x) &= v(k)\, e^{+ik\cdot x} & k^0 &< 0
\end{aligned}
\tag{23.3}
$$

where now,

$$
\begin{aligned}
(ik_\mu\gamma^\mu + m)\, u(k) &= 0 \\
(ik_\mu\gamma^\mu - m)\, v(k) &= 0
\end{aligned}
\tag{23.4}
$$

Note that each equation actually has two linearly independent solutions, which we may label by an extra index, $s$, standing for the spin of the particle. Thus, the 4 independent solutions to the Dirac equation are $u_s(k)$ and $v_s(k)$ for $s = 1, 2$. The solutions $\psi_+$ admit the standard interpretation as particle with *positive energy*.

　　Historically, the interpretation of the solutions $\psi_-$ and $v(k)$ was at first confusing, as they seemed to correspond to particle with negative energy, which is absurd. The issue was first clarified by Feynman in 1948. The solution $\psi_-$ cab be obtained formally from $\psi_+$ by "reversing the arrow

of time", instead of reversing the sign of the energy. Let us see how this would work in practice. Creating a particle with positive energy would then be mapped into annihilating an anti-particle with positive energy. Analogously, annihilating a particle with positive energy maps to creating an anti-particle with positive energy. Thus, if the solution $u(k)$ multiplies an annihilation operator for a particle, then $v(k)$ should multiply a creation operator for an anti-particle. Thus, the Dirac field decomposes as follows,

$$
\begin{aligned}
\psi(x) &= \sum_{k,s} \left\{ u_s(k) b_s(k) e^{-ik \cdot x} + v_s(k) d_s^\dagger(k) e^{+ik \cdot x} \right\} \\
\psi^\dagger(x) &= \sum_{k,s} \left\{ u_s^\dagger(k) b_s^\dagger(k) e^{+ik \cdot x} + v_s^\dagger(k) d_s(k) e^{-ik \cdot x} \right\}
\end{aligned}
\tag{23.5}
$$

Here, we have expressed the superposition in $k$ as a sum, but an integral over $k$ should be used instead on $R^3$. The physical interpretation of the operators is as follows,

$$
\begin{array}{ll}
b_s(k) & \text{annihilation operator for a particle} \\
d_s^\dagger(k) & \text{creation operator for an anti-particle} \\
b_s^\dagger(k) & \text{creation operator for a particle} \\
d_s(k) & \text{annihilation operator for an anti-particle}
\end{array}
\tag{23.6}
$$

The Dirac spinor representation being complex, there is a priori no reality relation between the oscillators $b_s(k)$ and $d_s(k)$. We shall see later on that a Lorentz invariant reality (or Majorana) condition may be imposed consistently under certain assumptions, and in that restricted case we have $d_s(k) = b_s(k)$, so that the corresponding Majorana fermion particle coincides with its anti-particle (just as the photon did).

From the above construction, we can immediately draw a conclusion on the electric charge assignments of the particle and anti-particle. Recall that the electric charge is the Nöther charge associated to phase rotation symmetry of the Dirac field,

$$
\psi(x) \to \psi'(x) = e^{i\theta} \psi(x)
\tag{23.7}
$$

for constant phases $\theta$. We conclude that the electric charges of $b_s(k)$ and $d_s^\dagger(k)$ must be the same. This means that the change in charge due to annihilating a particle must be the same as the electric charge change due to creating an anti-particle. Thus, the electric charges of particle and anti-particle must be opposite. As a corollary, only electrically neutral particle can be their own anti-particles.

Dirac at first did not know how to interpret the extra "negative energy solutions", and neither did anybody else for some time. In fact, Dirac originally proposed that the proton would be this missing anti-particle to the electron, mainly because the electric charges of the proton and electron are exactly opposite. This is actually incorrect, since we can clearly see from the Dirac equation and its solutions that mass of the particle and anti-particle must be the same, while the masses of the proton and the electron differ by a factor of 2000.

The correct interpretation is that these "negative energy solutions" actually describe the anti-particle of the electron, i.e. the positron. Its mass is exactly equal to that of the electron, and its charge is exactly opposite. When the positron was discovered experimentally in the 1930s, Dirac's theory was immediately propelled to great fame.

We are now ready to writing the general solution of the free Dirac equation,

$$
\psi(x) = \int \frac{d^3k}{(2\pi)^3} f(k^0) \sum_{s=1,2} \left\{ u_s(k) b_s(k) e^{-ik\cdot x} + v_s(k) d_s^\dagger(k) e^{+ik\cdot x} \right\}
$$

$$
\psi^\dagger(x) = \int \frac{d^3k}{(2\pi)^3} f(k^0) \sum_{s=1,2} \left\{ u_s^\dagger(k) b_s^\dagger(k) e^{+ik\cdot x} + v_s^\dagger(k) d_s(k) e^{-ik\cdot x} \right\} \tag{23.8}
$$

where $k^\mu = (k^0, \vec{k})$ and $k^0 = +\sqrt{\vec{k}^2 + m^2}$, and exhibits only positive energy solutions. Here we have included a normalization factor $f(k^0)$ whose precise form will be fixed by standard convention later on.

Given the above expressions for the fields $\psi$ and $\psi^\dagger$, we are in a position to evaluate physical observables, such as the electric charge $Q$ and the Hamiltonian $H$ for the free Dirac field. We shall begin by working out the charge. Substituting $\psi$ and $\psi^\dagger$ given in (23.8) into the definition of electric charge in (23.1), we find,

$$
Q = \int d^3x \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} f(k^0) f(k'^0)^* \sum_{s,s'} \left\{ u_{s'}^\dagger(k') b_{s'}^\dagger(k') e^{+ik'\cdot x} + v_{s'}^\dagger(k') d_{s'}(k') e^{-ik'\cdot x} \right\}
$$

$$
\times \left\{ u_s(k) b_s(k) e^{-ik\cdot x} + v_s(k) d_s^\dagger(k) e^{+ik\cdot x} \right\} \tag{23.9}
$$

Carrying out the integration over $x$ sets $\vec{k}' = +\vec{k}$ in the direct terms, and $\vec{k}' = -\vec{k}$ in the cross terms. As a result, we have

$$
Q = \int \frac{d^3k}{(2\pi)^3} |f(k^0)|^2 \sum_{s,s'} \left\{ u_{s'}^\dagger(k) u_s(k) b_{s'}^\dagger(k) b_s(k) + v_{s'}^\dagger(k) v_s(k) d_{s'}(k) d_s^\dagger(k) \right.
$$

$$
\left. + u_{s'}^\dagger(-k) v_s(k) b_{s'}^\dagger(-k) d_s^\dagger(k) + v_{s'}^\dagger(-k) u_s(k) d_{s'}(-k) b_s(k) \right\} \tag{23.10}
$$

To simplify this expression further, we need a number of spinor identities, which we shall first develop.

## 23.2 Spinor Identities

The staring point is the defining relations for the spinors $u_s$ and $v_s$,

$$
(ik_\mu \gamma^\mu + m) u_s(k) = 0
$$

$$
(ik_\mu \gamma^\mu - m) v_s(k) = 0 \tag{23.11}
$$

It will be convenient to parametrize the corresponding solutions in a basis where the chirality matrix is diagonal. In this basis, we decompose the 4-component spinors into blocks of two-component left- and right-spinors,

$$u_s(k) = \begin{pmatrix} u_{Ls}(k) \\ u_{Rs}(k) \end{pmatrix} \qquad\qquad v_s(k) = \begin{pmatrix} v_{Ls}(k) \\ v_{Rs}(k) \end{pmatrix} \tag{23.12}$$

The equations (23.11) then reduce to

$$\begin{pmatrix} -im & k \cdot \sigma \\ k \cdot \bar{\sigma} & -im \end{pmatrix} \begin{pmatrix} u_{Ls}(k) \\ u_{Rs}(k) \end{pmatrix} = 0$$

$$\begin{pmatrix} +im & k \cdot \sigma \\ k \cdot \bar{\sigma} & +im \end{pmatrix} \begin{pmatrix} v_{Ls}(k) \\ v_{Rs}(k) \end{pmatrix} = 0 \tag{23.13}$$

or in components,

$$\begin{aligned}
(k \cdot \sigma) u_{Rs}(k) &= +i\,m\,u_{Ls}(k) \\
(k \cdot \bar{\sigma}) u_{Ls}(k) &= +i\,m\,u_{Rs}(k) \\
(k \cdot \sigma) v_{Rs}(k) &= -i\,m\,u_{Ls}(k) \\
(k \cdot \bar{\sigma}) v_{Ls}(k) &= -i\,m\,u_{Rs}(k)
\end{aligned} \tag{23.14}$$

Since we have

$$(k \cdot \sigma)(k \cdot \bar{\sigma}) = m^2 I_2 \tag{23.15}$$

the general solutions to these equations may be parametrized by two pairs of independent 2-component spinors $\xi_s$ and $\eta_s$, by,

$$u_s(k) = \begin{pmatrix} (\sqrt{k \cdot \sigma})\xi_s \\ i(\sqrt{k \cdot \bar{\sigma}})\xi_s \end{pmatrix} \qquad\qquad v_s(k) = \begin{pmatrix} (\sqrt{k \cdot \sigma})\eta_s \\ -i(\sqrt{k \cdot \bar{\sigma}})\eta_s \end{pmatrix} \tag{23.16}$$

There is no problem in defining the square roots of the matrices $k \cdot \sigma$ and $k \cdot \bar{\sigma}$, since they are Hermitian, and may be diagonalized. The spinors $\xi_s$ and $\eta_s$ are arbitrary basis vectors, and may be conveniently chosen to obey the following normalization conditions,

$$\begin{aligned}
\xi_{s'}^\dagger \xi_s = \eta_{s'}^\dagger \eta_s &= \delta_{s',s} \\
\xi_{s'}^\dagger \eta_s = \eta_{s'}^\dagger \xi_s &= 0
\end{aligned} \tag{23.17}$$

One may then choose the following explicit basis,

$$\xi_1 = \eta_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \xi_2 = \eta_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{23.18}$$

With the help of these normalizations, it is now straightforward to evaluate

$$\begin{aligned}
\bar{u}_r(k)\,u_s(k) &= +2m\delta_{rs} & \bar{u}_r(k)v_s(k) &= 0 \\
\bar{v}_r(k)\,v_s(k) &= -2m\delta_{rs} & \bar{v}_r(k)u_s(k) &= 0
\end{aligned} \tag{23.19}$$

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The calculation of the first line, for example, proceeds as follows,

$$
\begin{aligned}
\bar{u}_r(k)\, u_s(k) = u^\dagger(k)\gamma^0 v_s(k) \;\; &= \;\; \begin{pmatrix} \xi_r^\dagger(\sqrt{k\cdot\sigma}) \\ -i\xi_r^\dagger(\sqrt{k\cdot\bar{\sigma}}) \end{pmatrix}^t \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \begin{pmatrix} (\sqrt{k\cdot\sigma})\xi_s \\ i(\sqrt{k\cdot\bar{\sigma}})\xi_s \end{pmatrix} \\
&= \;\; i\xi_r^\dagger \left\{ (\sqrt{k\cdot\sigma})(\sqrt{k\cdot\bar{\sigma}}) + (\sqrt{k\cdot\bar{\sigma}})(\sqrt{k\cdot\sigma}) \right\} \xi_s \\
&= \;\; 2i\,m\xi_r^\dagger\xi_s = 2i\,m\delta_{rs} \qquad (23.20)
\end{aligned}
$$

These results may be used in turn to evaluate other spinor bilinears, such as the quantity $\bar{u}_r\gamma^\mu u_s$. This is a 4-vector, which can only depend upon $k^\mu$, so that it must be of the form,

$$
\bar{u}_r\gamma^\mu u_s = k^\mu M_{rs} \qquad (23.21)
$$

The matrix $M_{rs}$, which in principle could depend on the Lorentz-invariant quantity $m$, is actually independent of $m$ on dimensional grounds. To evaluate $M_{rs}$, we contract both sides with $k_\mu$, and obtain,

$$
m^2 M_{rs} = \bar{u}_r k_\mu \gamma^\mu u_s = -im\bar{u}_r u_s = 2m^2\delta_{rs} \qquad (23.22)
$$

where we have used the defining equation for $u_s$ for the second equality. A similar calculation may be carried out for $v_s$, and we find,

$$
\begin{aligned}
\bar{u}_r(k)\gamma^\mu u_s(k) &= 2k^\mu\delta_{rs} \\
\bar{v}_r(k)\gamma^\mu v_s(k) &= 2k^\mu\delta_{rs}
\end{aligned} \qquad (23.23)
$$

Finally, we will also need

$$
u_r^\dagger(k)v_s(-k) = v_r^\dagger(k)u_s(-k) = 0 \qquad (23.24)
$$

## 23.3 Evaluation of the electric charge operator and Hamiltonian

Using the above spinor identities, it is now straightforward to further simplify the expression for the electric charge, and we find,

$$
Q = \int \frac{d^3k}{(2\pi)^3} \sum_{s=1,2} \left\{ b_s^\dagger(k)b_s(k) + d_s(k)d_s^\dagger(k) \right\} \qquad (23.25)
$$

where we have made the following convenient choice for the normalization factor,

$$
f(k^0) = \frac{1}{\sqrt{2k^0}} \qquad (23.26)
$$

To evaluate the Hamiltonian, we use the Dirac equation to recast its expression as follows,

$$
H = \int d^3x\, \psi^\dagger \left( -\gamma^i\partial_i + m \right)\psi = \int d^3x\, i\,\psi^\dagger\partial_0\psi \qquad (23.27)
$$

Evaluating the time derivative, we find,

$$i\partial_0\psi = \int \frac{d^3k}{(2\pi)^3} \frac{1}{\sqrt{2k^0}} \sum_{s=1,2} \left\{ k^0 u_s(k) b_s(k) e^{-ik\cdot x} - k^0 v_s(k) d_s^\dagger(k) e^{+ik\cdot x} \right\} \tag{23.28}$$

and we find,

$$H = \int \frac{d^3k}{(2\pi)^3} k^0 \sum_{s=1,2} \left\{ b_s^\dagger(k) b_s(k) - d_s(k) d_s^\dagger(k) \right\} \tag{23.29}$$

## 23.4   Quantization of fermion oscillators

We are now ready to proceed with quantization. Recall that we had declared $b^\dagger$ and $d^\dagger$ to be the creation operators for particles and anti-particles, having charges $+1$ and $-1$ respectively, and both with positive energy. The oscillators $b, d, b^\dagger, d^\dagger$ have to be quantized as fermions. As we have seen earlier, this is done in terms of anti-commutation relations. It will turn out that the correct relations are,

$$\begin{aligned}
\{b_r(k), b_s(k')\} = \{d_r(k), d_s(k')\} &= 0 \\
\{b_r(k), d_s(k')\} = \{b_r(k), d_s^\dagger(k')\} &= 0 \\
\{b_r(k), b_s^\dagger(k')\} = \{d_r(k), d_s^\dagger(k')\} &= (2\pi)^3 \delta_{r,s} \delta^{(3)}(k - k')
\end{aligned} \tag{23.30}$$

as well as the adjoint relations of the first two lines. Normal ordering now the expressions for electric charge $Q$, Hamiltonian $H$, as well as the momentum $\vec{P}$, we get,

$$\begin{aligned}
Q &= \int \frac{d^3k}{(2\pi)^3} \sum_{s=1,2} \left\{ b_s^\dagger(k) b_s(k) - d_s^\dagger(k) d_s(k) \right\} \\
H &= \int \frac{d^3k}{(2\pi)^3} k^0 \sum_{s=1,2} \left\{ b_s^\dagger(k) b_s(k) + d_s^\dagger(k) d_s(k) \right\} \\
\vec{P} &= \int \frac{d^3k}{(2\pi)^3} \vec{k} \sum_{s=1,2} \left\{ b_s^\dagger(k) b_s(k) + d_s^\dagger(k) d_s(k) \right\}
\end{aligned} \tag{23.31}$$

## 23.5   Canonical anti-commutation relations for the Dirac field

From the anti-commutation relations of the oscillators $b, d, b^\dagger, d^\dagger$, we deduce those of the Dirac fields themselves. It is immediate that

$$\{\psi_\alpha(x), \psi_\beta(y)\} = \{\psi_\alpha^\dagger(x), \psi_\beta^\dagger(y)\} = 0 \tag{23.32}$$

where $\alpha, \beta$ run over the spinor components of the Dirac fields. It remains to compute

$$\begin{aligned}
\{\psi_\alpha^\dagger(x), \psi_\beta(y)\} &= \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \sum_{s,s'} \frac{1}{2\sqrt{k^0 k'^0}} \Big\{ u_{s\alpha}^\dagger(k) b_s^\dagger(k) e^{ik\cdot x} + v_{s\alpha}^\dagger(k) d_s(k) e^{-ik\cdot x}, \\
&\qquad u_{s'\beta}(k') b_{s'}(k') e^{-ik'\cdot y} + v_{s'\beta}(k') d_{s'}^\dagger(k') e^{ik'\cdot y} \Big\}
\end{aligned} \tag{23.33}$$

Using the anti-commutation relations and $b$ and $d$ oscillators, we obtain contributions of either 0 or $\delta_{s,s'}(2\pi)^3\delta(\vec{k}-\vec{k}')$. The expression thus simplifies to

$$\{\psi_\alpha^\dagger(x),\psi_\beta(y)\} = \int \frac{d^3k}{(2\pi)^3}\frac{1}{2k^0}\sum_s \left\{u_{s\alpha}^\dagger(k)u_{s\beta}(k)e^{ik\cdot(x-y)} + v_{s\alpha}^\dagger(k)v_{s\beta}(k)e^{+ik\cdot(x-y)}\right\} \quad (23.34)$$

It remains to obtain the final spinor relation we need,

$$\sum_s u_{s\alpha}^\dagger u_{s\beta} = (\gamma^\mu k_\mu + m)_{\alpha\beta}$$
$$\sum_s v_{s\alpha}^\dagger v_{s\beta} = (\gamma^\mu k_\mu - m)_{\alpha\beta} \quad (23.35)$$

Putting all together, we have

$$\{\psi_\alpha^\dagger(x),\psi_\beta(y)\} = \int \frac{d^3k}{(2\pi)^3}\frac{1}{2k^0}\left\{(\gamma^\mu k_\mu + m)\gamma^0 e^{ik\cdot(x-y)} + (\gamma^\mu k_\mu - m)\gamma^0 e^{+ik\cdot(x-y)}\right\}_{\alpha\beta} \quad (23.36)$$

Now, this is the expression for free fermions. Setting the time components equal to one another, we have a relation which is independent of dynamics, and giving the canonical anti-commutation relations of the fields,

$$\{\psi_\alpha^\dagger(x),\psi_\beta(y)\}\delta(x^0-y^0) = \delta_{\alpha\beta}\delta^{(4)}(x-y) \quad (23.37)$$

## 23.6 The fermion propagator

The free fermion propagator is the "inverse of the Dirac operator". A useful way to look at this quantity is from how it arises from the Dirac field. The two pieces of information we need are summarized as follows,

$$(\gamma^\mu\partial_\mu - m)\,\psi(x) = 0$$
$$\{\psi_\alpha^\dagger(x),\psi_\beta(y)\}\delta(x^0-y^0) = \delta_{\alpha\beta}\delta(x-y) \quad (23.38)$$

where the derivative operator acts as $\partial_\mu = \partial/\partial x^\mu$. So, the Dirac field may be viewed as a "homogeneous" solution to the Dirac equation. The Dirac propagator should thus satisfy the inhomogeneous equation,

$$(\gamma^\mu\partial_\mu - m)\,S(x,y) = I_4\delta^{(4)}(x-y) \quad (23.39)$$

where $I_4$ is the identity matrix in the 4-component Dirac spinor space. On the one hand, this equation may be solved (formally) by Fourier transform, and we find,

$$\int \frac{d^4k}{(2\pi)^4}\frac{e^{ik\cdot(x-y)}}{i\gamma^\mu k_\mu - m} \quad (23.40)$$

This is formal because the denominator will have a vanishing eigenvalue for a whole family of values of $k$, namely those that obey $k^\mu k_\mu + m^2 = 0$. This problem is familiar from the Lippmann-Schwinger

equation for potential scattering, and was solved there by the introduction of a small imaginary part. The same works here, and we replace the above formal expression by the following accurate one,

$$S(x, y) = \int \frac{d^4 k}{(2\pi)^4} \frac{e^{ik \cdot (x-y)}}{i\gamma^\mu k_\mu - m + i\varepsilon} \tag{23.41}$$

for $\varepsilon > 0$. The actual value of the integral is complicated, except for $m = 0$, but will not be needed explicitly here.

There is another way of expressing the free fermion propagator, which will be very useful in carrying out perturbative calculations. It is based on the fact that to obtain the inverse of the Dirac operator, it suffices to "patch together" two solutions to the homogeneous equation. This is done by using the time-ordering operation that we had encountered when carrying out time-depenedent perturbation theory. Consider the following object,

$$T\psi_\alpha(x)\bar{\psi}_\beta(y) \equiv \theta(x^0 - y^0)\psi_\alpha(x)\bar{\psi}_\beta(y) - \theta(y^0 - x^0)\psi_\beta(y)\bar{\psi}_\alpha(x) \tag{23.42}$$

Note the minus sign used in the time-ordering of fermion operators. Applying now the Dirac operator in the coordinate $x$ to both sides, we see that when the operator lands on the field $\psi_a(x)$, the corresponding contribution cancels, in view of the fact that $\psi_\alpha(x)$ satisfies the Dirac equation. So, the only non-zero contribution arises from when the time-derivative in the Dirac equation hits the $\theta$-function, and this contribution gives,

$$\begin{aligned}
(\gamma^\mu \partial_\mu - m)_{\gamma\alpha} \left(T\psi_\alpha(x)\bar{\psi}_\beta(y)\right) &= \delta(x^0 - y^0)(\gamma^0)_{\gamma\alpha}(\gamma^0)_{\delta\beta}\{\psi_\alpha(x), \psi_\delta^\dagger(y)\} \\
&= (\gamma^0)_{\gamma\alpha}(\gamma^0)_{\delta\beta}\delta_{\alpha\delta}\delta^{(4)}(x - y) \\
&= \delta_{\gamma\beta}\delta^{(4)}(x - y)
\end{aligned} \tag{23.43}$$

Of course, $T\psi_\alpha(x)\bar{\psi}_\beta(y)$ is an operator, not a number, but we can easily extract from it a pure number, so that we find,

$$S_{\alpha\beta}(x - y) = \langle \emptyset | T\psi_\alpha(x)\bar{\psi}_\beta(y) | \emptyset \rangle \tag{23.44}$$

where $|\emptyset\rangle$ is the free-fermion vacuum state.

## 23.7  The concept of vacuum polarization

We are now ready to study one of the most basic effects in interacting quantum field theory, namely vacuum polarization. We all know what a regular polarized medium is. For example, water molecules exhibit an asymmetrical geometry, with the two Hydrogen atoms being on one side, and the Oxygen atom being at the other side of the molecule.

$$- \quad O < \begin{array}{c} H \\ H \end{array} \quad + \tag{23.45}$$

This gives the molecule an electric dipole moment. An electric charge $q$ inserted into water vapor, will experience screening. A positive charge $q > 0$ located at a point $P$ will preferentially orient the water molecules so that their negative ends (the Oxygen) point towards the point $P$, while their positive ends point away from $P$. The collective effect produced by the systematic orientations of the water molecules results in the screening of the charge $q$, so that the effective charge observed some distance away from $q$ will be smaller than $q$.

Now introduce the electric charge $q$ in the *vacuum*. At first sight, it will seem that there is no material available to screen this charge, since naively the vacuum is empty. In fact, we know already from the Casimir effect that vacuum fluctuations of the quantum electro-magnetic field induces physically observable effects. Here, it is the vacuum fluctuations of the Dirac field of the electron and positron that will produce a measurable effect. We begin by describing the effect qualitatively first, and we will compute it in full in the subsequent subsections.

Qualitatively, the origin of vacuum polarization lies in the fact that vacuum fluctuations of the Dirac field amount to the creation of virtual pairs of an electron and a positron. These particles are virtual in the sense that there is not enough energy available to make them materialize as real physical electron and positron. By the energy-time uncertainty relation, these particles can exist only for a very short time, after which they must annihilate one another. But during their short life-time, the pair forms a small electric dipole. And this (virtual) dipole has a screening effect on the electric charge which is completely analogous to the effect produced by a real electric dipole like water. As a result, if a charge $q$ is introduced at a point $P$ in the Dirac vacuum, then the effective charge felt must decrease with distance away from $P$.

Is it possible to have the opposite effect ? Namely, could the effective charge increase as the distance increases ? Not in electro-dynamics. In non-Abelian gauge theories (Yang-Mills theories) however, this is possible, and in fact generic within certain ranges of parameters, and this effect is equivalent to the property of asymptotic freedom.