Quantum Mechanics I

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Bibliography

[1] Modern Quantum Mechanics, Sakurai

[2] The Feynman Lectures in Physics, Feynman

[3] Lectures on Quantum Mechanics, Weinberg

Preface

This script is based on Refs. [1–3]. These books are great and students are encouraged to study them as a first priority. The purpose of the present notes, which contain some personalized material, is to facilitate the author for his lecture presentations. Students are of course welcome to read the script if they find it useful. However, the script should not replace the study of the recommended and other literature.

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Chapter 1

Quantum behavior

1.1 Atomic mechanics

For a long time, light was thought to behave like waves and electrons were thought to behave like particles. There are phenomena which violate these main "rules". So they behave neither like particles nor like waves. However, it is true that light, electrons, protons and all subatomic particles behave the same. This common subatomic behavior is very different from our intuition of large objects. We will demonstrate the difference of the quantum and classic behavior by a thought "two-slit" experiment first with macroscopic bullets, second with waves and third with subatomic particles such as electrons.

1.2 Basic two slit experiments

1.2.1 An experiment with bullets

We have a gun firing very hard indestructible bullets towards a wall. The wall has two slits which are at a close distance and are big enough so that they can pass through.

Behind the wall there is a "detector", a material which can stop the bullets. We can take a look at it afterwards and see how the bullets are distributed in space after they have gone through the holes. We perform the experiment in three stages:

- First, we leave open "Hole 1" and cover up the second hole. We find that the bullets are distributed according to P_1, a Gaussian centered around the Hole 1.
- Then, we leave open "Hole 2" while we cover up "Hole 1". We find a similar Gaussian P_2 centered around Hole 2.
- Finally, we leave open both holes. We find a distribution which

$$P_{12} = P_1 + P_2 \,. \tag{1.1}$$

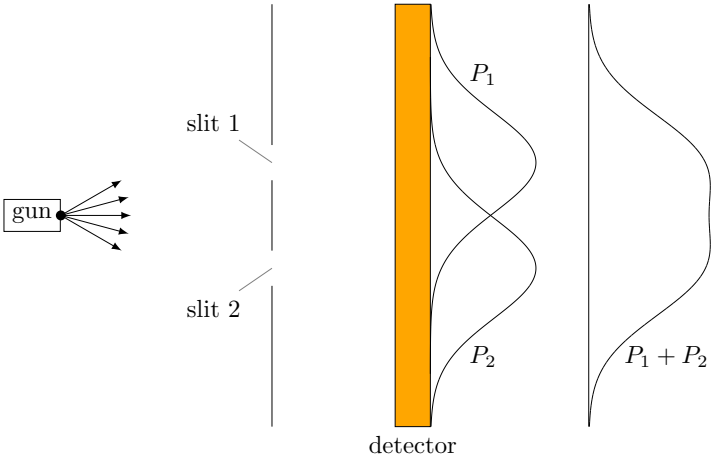


Figure 1.1: A two slit experiment with bullets.

The probability that a bullet goes through the holes is the sum of the probabilities that it passes either through hole 1 or through hole 2.

1.2.2 An experiment with waves

We now perform a different experiment where we create a spherical wave at some distance in front of the wall with the two holes. The detector measures the intensity of the wave arriving at it, which is proportional to the square of the amplitude:

$$I \sim |A|^2 .$$

We perform the experiment in three stages:

- First, we leave open "Hole 1" and cover up the second the second hole. We find that the intensity I_1 is a function centered around the Hole 1.
- Then, we leave open "Hole 2" while we cover up "Hole 1". We find a similar function intensity I_2 centered around Hole 2.
- Finally, we leave open both holes. We find a distribution $I_{12} \neq I_1 + I_2$.

There is a simple explanation why the intensity I_{12} is not equal to the sum of the intensities when either one of the two holes is covered. The amplitude

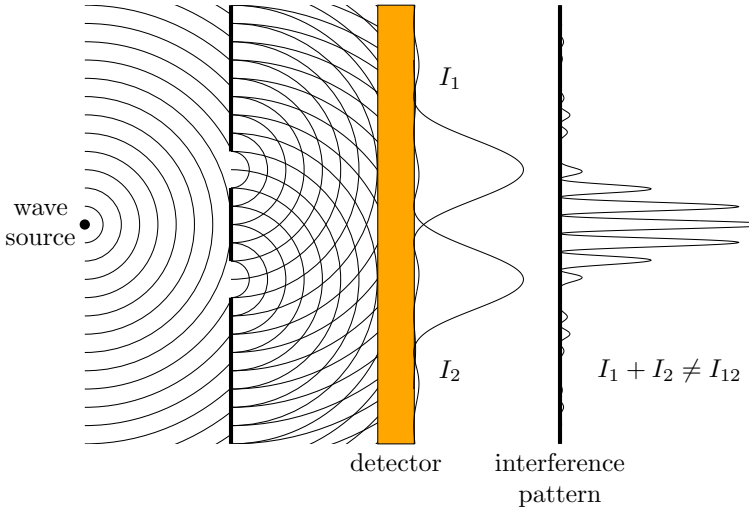


Figure 1.2: A two slit experiment with waves.

of the wave is given by the sum of the amplitudes,

$$A_{12} = A_1 + A_2$$

where A_1 and A_2 can be both positive or negative. The total intensity,

$$\begin{aligned} I_{12} &\sim |A_{12}|^2 \\ &= I_1 + I_2 + 2\sqrt{|I_1|\,|I_2|}\cos\delta \end{aligned} \tag{1.2}$$

includes an interference term, giving the characteristic interference pattern of Fig 1.2.

1.2.3 An experiment with electrons

We now shoot electrons at the wall. What happens is pictured in Fig 1.3.

This is a surprising result. If an electron went through either hole 1 or hole 2, we would not have found $P_{12} \neq P_1 + P_2$. Are electrons waves? Well, no. We always detect one "full" electron at the time at the detector. For example, we can reconstruct the full energy of an electron as it dissipates it in the detector, or if the detector is inside a magnetic field, the electron track has the curvature of charge one, etc.

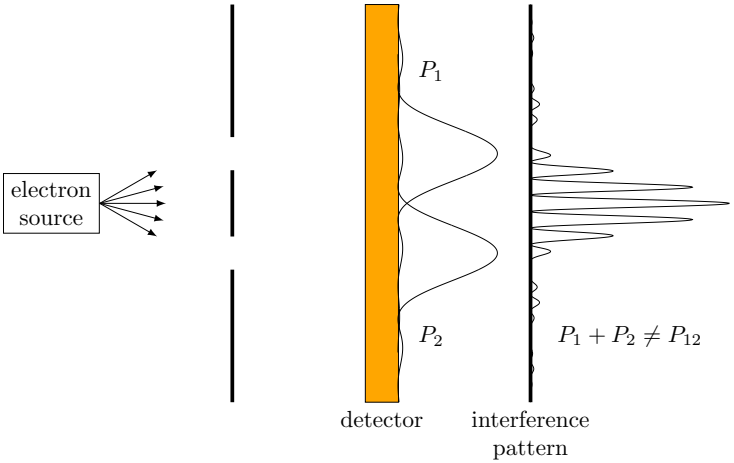


Figure 1.3: A two slit experiment with electrons with wave behavior.

So, the electron arrives at the detector as a particle and the probability of arrival is distributed like the intensity of a wave.

1.3 Watching electrons

Let's put a light source behind the two holes. Deflected light from the vicinity of hole 1 or hole 2 can tell us where the electron passed through. What happens? Indeed, we can see a flash coming from the hole every time that an electron passes through. However, we find the following probability pattern. The interference pattern is destroyed when we can verify experimentally that the electrons go through either hole 1 or hole 2. If we switch off the light, the interference leading to $P_{12} \neq P_1 + P_2$ is restored.

Let's now try to understand how the light affects our measurement. Before going ahead with modifying the light characteristics, we equip our detector with a sound system. Each time an electron hits on the detector we also hear a click.

What happens with a dimmer light? We observe two types of events.

i) Events where a flash comes from hole 1 or hole 2 and we hear a click immediately after coming from the detector.

ii) Events where we only hear a click from the detector without seeing any flash.

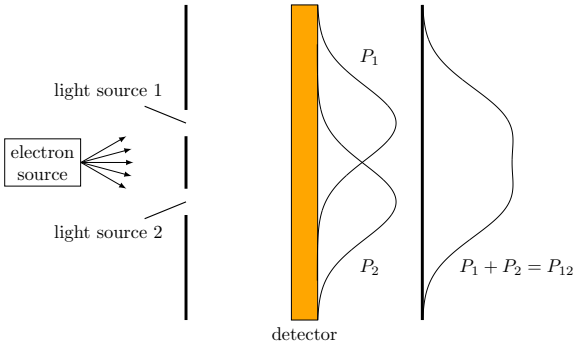


Figure 1.4: A two slit experiment with electrons. In this experiment, we observe which hole the electrons pass through.

We plot the probability distribution for the above categories of the events. For the events where we have seen a light, we find a distribution as in Fig. 1.4 with no interference. For the events where we have not seen the light but we have heard the sound we get a probability distribution as in Fig. 1.3 with an interference pattern. The interference pattern gets destroyed if we are able to observe the hole from where the electrons passed.

The intensity of the light is not its only physical characteristic. When we dim it, we reduce the amplitude of the electromagnetic wave. This means that there is a smaller density of "light particles" (photons) and therefore some electrons can pass through the holes without crashing onto one of them. It is then when we only hear a sound at the moment the electron arrives at the detector without having seen a flash from a hole before. But we can also tune the wavelength of the light. There is a simple relation between the momentum of the photons and the wavelength,

$$p = \frac{h}{\lambda},$$

where h is a (the Planck) constant. Photons are less energetic and the light is "gentler" if we increase the wavelength using infrared light or even radio waves.

So, let's start increasing gradually the wavelength without changing the intensity. We find that at the beginning there is no change in the type of probability distribution for the electrons arriving at the detector. As long as the wavelength is shorter than the distance of the two holes, we can tell whether a flash light came from one or the other hole and we find no inter-

ference pattern

$$P_{12}(\lambda) = P_1(\lambda) + P_2(\lambda), \qquad \lambda \sim \text{small}.$$

If we increase the wavelength to a size comparable to the distance of the two holes, we find something dramatic. The flash becomes fuzzy and it is not possible to tell anymore whether it comes from the first or the second hole. Then, we find that an interference is restored.

$$P_{12}(\lambda) \neq P_1(\lambda) + P_2(\lambda), \qquad \lambda \sim \text{hole distance or larger}.$$

In conclusion, there is no configuration of our apparatus for which we can determine which hole the electrons went through without destroying the interference pattern.

1.4 Back to the bullet experiment

If the laws of quantum mechanics are universal, for light particles, electrons, protons and macroscopic objects, why then did we not observe an interference pattern for the experiment with the bullets? The reason is that the wavelength

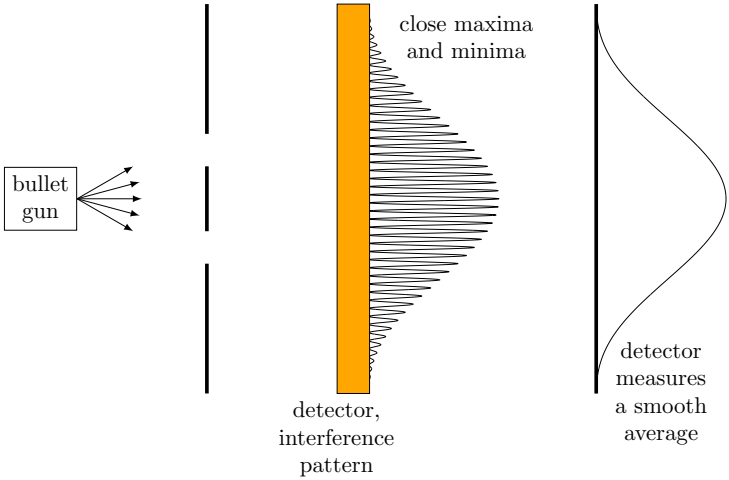


Figure 1.5: A two slit experiment with bullets.

of a large object is very short. The minima and maxima of the interference pattern are very dense and they cannot be discerned by the resolution of our

detectors. Instead, we measure a smooth average over the distance of several wavelengths as in Fig.1.5.

1.5 First principles of quantum mechanics

Let's define an "ideal" experiment as one in which all initial and final conditions are completely specified. An event is a set of such initial and final conditions. (For example, a bullet leaves the gun, arrives at the detector and nothing else happens.)

i) The probability of an event in an ideal experiment is given by the square of the absolute value of a complex number, which is called the probability amplitude

$$P = |\phi|^2 , \quad \begin{cases} \phi \equiv \text{probability amplitude} \\ P \equiv \text{probability} \end{cases} \tag{1.3}$$

ii) If an event can occur in several ways, there is interference

$$\begin{aligned} \phi &= \phi_1 + \phi_2 \\ P &= |\phi_1 + \phi_2|^2 . \end{aligned} \tag{1.4}$$

iii) If an experiment can determine whether one or another alternative happened the interference is destroyed

$$P = P_1 + P_2. \tag{1.5}$$

Note that we compute probabilities. We cannot know what an electron does at any given instance.

1.6 The laws for combining amplitudes

This is a good point to formalize and develop further the principles of section 1.5. We will denote the probability amplitude of an event using the "bra-ket" notation of Dirac:

$$\langle \text{final condition} | \text{initial condition} \rangle$$

For example, we can write the amplitude for an electron leaving the source s and arriving at the point x of the detector as

$$\langle \text{arrives at } x | \text{leaves from } s \rangle$$

or, shortly,

$$\langle x|s\rangle\,,$$

and the corresponding probability is

$$P = |\langle x|s\rangle|^2\,.$$

According to our second principle, if an event can occur in more than one way, then we must add the amplitudes for all alternatives and we have interference. For example, in our two slit experiment where the electron could pass through either of the slits, we write

$$\langle x|s\rangle = \langle x|s\rangle_{\substack{\text{through}\\ \text{slit 1}}} + \langle x|s\rangle_{\substack{\text{through}\\ \text{slit 2}}}\,. \tag{1.6}$$

We now introduce a new rule for amplitudes (which leads to the third principle of the previous section). If an event can be expressed as a sequence of other events then the amplitude factorizes. For example, we can write

$$\left\langle \begin{matrix}\text{arrives}\\ \text{at } x\end{matrix} \middle| \begin{matrix}\text{leaves}\\ \text{source } s\end{matrix} \right\rangle_{\substack{\text{through}\\ \text{slit 1}}} = \left\langle \begin{matrix}\text{arrives}\\ \text{at } x\end{matrix} \middle| \begin{matrix}\text{leaves}\\ \text{slit 1}\end{matrix} \right\rangle \left\langle \begin{matrix}\text{arrives}\\ \text{at slit 1}\end{matrix} \middle| \begin{matrix}\text{leaves}\\ \text{source } s\end{matrix} \right\rangle$$

or, shortly,

$$\langle x|s\rangle_{\substack{\text{through}\\ \text{slit 1}}} = \langle x|1\rangle\,\langle 1|s\rangle\,.$$

Then

$$\langle x|s\rangle = \langle x|1\rangle\,\langle 1|s\rangle + \langle x|2\rangle\,\langle 2|s\rangle\,.$$

1.6.1 Revisiting the two-slit experiment

Let us now revisit the two-slit experiment where we throw electrons at them and use a light source behind the slits in an attempt to see which slit is chosen by an electron before it arrives at the detector. For the purpose of "seeing" the flashes we place two photon-detectors one to the left of the left hole and one to the right of the right hole. Let's focus at the events which will be seen by the detector D_1. The amplitude is

$$\begin{aligned}\mathcal{M}_1 &= \left\langle \begin{matrix}\text{electron arrives at } x\\ \text{photon strikes } D_1\end{matrix} \middle| \begin{matrix}\text{electron leaves}\\ \text{source } s\end{matrix} \right\rangle \\ &= \langle x|1\rangle\,A_{1\to 1}(\lambda)\,\langle 1|s\rangle + \langle x|2\rangle\,A_{2\to 1}(\lambda)\,\langle 2|s\rangle\,.\end{aligned} \tag{1.7}$$

$A_{1\to 1}(\lambda)$ is the amplitude that a photon strikes an electron in hole 1 and it is deflected into the detector D_1. Similarly, $A_{2\to 1}(\lambda)$ is the amplitude that

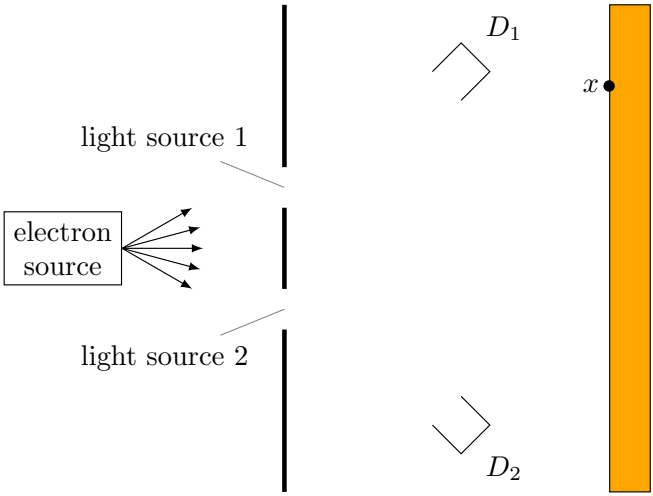


Figure 1.6: A two slit experiment with electrons. Trying to see which slit they are going through.

a photon strikes an electron in hole 2 and it is deflected into the detector D_1. The detector D_1 is placed closer to hole 1 and for small wavelengths $A_{2\to1}$ is much smaller than $A_{1\to1}$. The interference term in the probability $P_1 = |\mathcal{M}_1|^2$ vanishes for $A_{2\to1} = 0$. Instead, for large wavelength λ the photon cannot be localized precisely enough and $A_{2\to1} \sim A_{1\to1}$; then, there is interference.

Similarly, we can write an expression for the amplitude where the photon scattered from the electron strikes detector D_2:

$$\begin{aligned}\mathcal{M}_2 &= \left\langle \begin{matrix}\text{electron arrives at } x\\ \text{photon strikes } D_2\end{matrix} \middle| \begin{matrix}\text{electron leaves}\\ \text{source } s\end{matrix} \right\rangle \\ &= \langle x|1\rangle\, A_{1\to2}(\lambda)\, \langle 1|s\rangle + \langle x|2\rangle\, A_{2\to2}(\lambda)\, \langle 2|s\rangle\,.\end{aligned} \tag{1.8}$$

What is then the probability for the photon to strike either D_1 or D_2? Notice that we now ask for the combined probability of two different events with different final conditions. We should not combine the two amplitudes into a common amplitude ($\mathcal{M} \neq \mathcal{M}_1 + \mathcal{M}_2$). Our rule of combining amplitudes applies to alternative ways of a single event (where the initial and final conditions are the same for all alternatives). If the events differ, for their combined probability we add up the probabilities of each separate event. In our specific

case,

$$\begin{aligned} P\left(\text{light in } D_1 \text{ or } D_2\right) &= P\left(\text{light in } D_1\right) + P\left(\text{light in } D_2\right) \\ &= \left|\mathcal{M}_1\right|^2 + \left|\mathcal{M}_2\right|^2 . \end{aligned}$$

1.6.2 A subatomic travel from Zurich to China?

Our product rule for amplitudes can puzzle our physics intuition from macroscopic physics. Think of a particle at a position $\mathbf{x}_1$ which transitions to a position $\mathbf{x}_2$. The corresponding amplitude is

$$\langle \mathbf{x}_2 | \mathbf{x}_1 \rangle .$$

Let $\mathbf{y}$ be an intermediate position in the journey of the particle. According to our rules for combining amplitudes we must have:

$$\langle \mathbf{x}_2 | \mathbf{x}_1 \rangle = \langle \mathbf{x}_2 | \mathbf{y} \rangle \langle \mathbf{y} | \mathbf{x}_1 \rangle .$$

However, if we have no knowledge of which point exactly the particle passed through (e.g. by putting up a wall with only a hole open) we must sum up all positions.

$$\langle \mathbf{x}_2 | \mathbf{x}_1 \rangle = \sum_{\mathbf{y}} \langle \mathbf{x}_2 | \mathbf{y} \rangle \langle \mathbf{y} | \mathbf{x}_1 \rangle .$$

In the sum, we are supposed to include all positions $\mathbf{y}$ no matter how far they reside from $\mathbf{x}_1, \mathbf{x}_2$ or how improbable they appear to us from our knowledge of classical physics.

It turns out that amplitudes for classically improbable transitions are suppressed. Up to some normalization, the transition amplitude of a free particle (no forces are exerted on it) of momentum $\mathbf{p}$ from a position $\mathbf{x}$ to a position $\mathbf{y}$ is

$$\mathcal{M}_{\mathbf{x}\to\mathbf{y}} \sim \frac{e^{-\frac{i}{\hbar}\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}}{|\mathbf{x}-\mathbf{y}|}, \tag{1.9}$$

where $\mathbf{p}$ is the classical momentum of the particle and $\hbar = \frac{h}{2\pi}$ (Planck's) constant. We note that the amplitude is suppressed for large distances and that the motion along the direction of the momentum produces a maximum phase in the exponential.

Probability amplitudes depend in general both in space and time. The time evolution of the amplitudes is determined by the equation of Schrödinger, which we shall see in the future.

Chapter 2

Quantum measurement and quantum states

In this chapter we shall explore further the basic rules of probability amplitudes and introduce quantum states.

2.1 Stern-Gerlach experiment

Let's think of a magnetic dipole/loop current localized in a small volume, with a magnetic moment $\boldsymbol{\mu}$. The potential energy when the current is inside a magnetic field is

$$U = -\boldsymbol{\mu} \cdot \mathbf{B} \,. \tag{2.1}$$

Inside a inhomogeneous magnetic field a force will be exerted in the magnetic dipole so that it minimizes its energy. The force will be

$$\mathbf{F} = -\boldsymbol{\nabla} U = \boldsymbol{\nabla} \left(\boldsymbol{\mu} \cdot \mathbf{B} \right) . \tag{2.2}$$

For a magnetic field which varies, for example, in the $z-$direction there is a force exerted on the magnetic dipole in the same direction,

$$F_z = \mu_z \frac{\partial B_z}{\partial z}. \tag{2.3}$$

In classical physics, we can attempt to describe atoms as dipoles, i.e. currents which are localized in a tiny space. We now perform a conceptually very simple experiment, the Stern-Gerlach experiment. We produce a beam of atoms and we direct the beam towards a magnet with a inhomogeneous magnetic field. In classical physics we expect that the value of μ_z is a continuous variable. The effect of the gradient magnetic field should then be to spread out the beam along the $z-$direction as in Fig. **??**. This is not what really happens. Instead, we find that the beam of atoms is split as in Fig. 2.2 in a number of beams which the original beam is split into depends on the

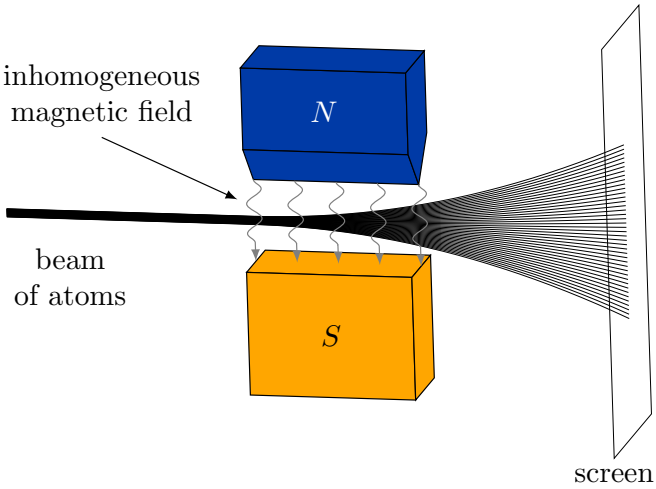


Figure 2.1: Stern-Gerlach experiment: Expectation from classical electrodynamics in a description of atoms as magnetic dipoles. (*This is not what happens in reality!)*

kind of the atoms and a property of them called "spin" [1]. Atoms with spin-$\frac{1}{2}$ split into two beams, atoms with spin-1 split into three beams and so on; in general atoms with spin-j split into $2j + 1$ beams.

2.2 The Stern-Gerlach filter

2.2.1 Experimental setup

In the following, we shall take a beam of atoms with spin-1 and examine further experimentally the three separated beams which originate from a Stern-Gerlach apparatus. We construct a Stern-Gerlach filter. This filter takes a beam of atoms and passes it first through a magnetic field with a gradient in a certain direction, as in the Stern-Gerlach experiment, splitting the beam into three. The split beams are channeled through gates which we can decide at wish to keep them open or have them closed. Afterwards, magnets re-unite the beams which pass through the gates and let them come out from an exit point as a single beam.

[1] It is not yet time to describe spin. We will only say for now that it is a intrinsic angular momentum of subatomic particles which can be detected even when these particles are motionless.

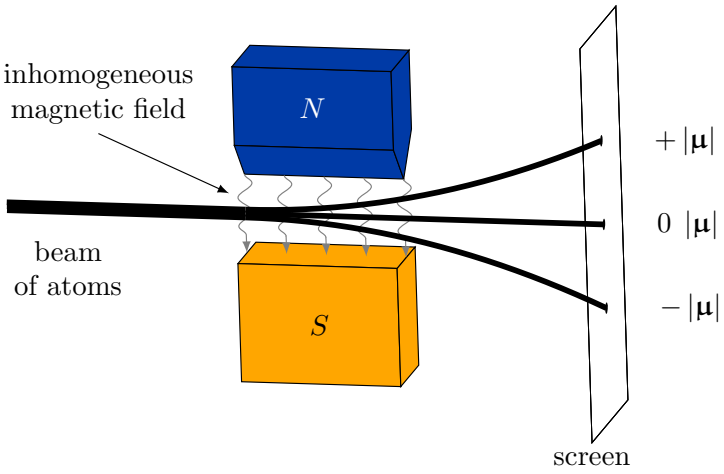


Figure 2.2: Stern-Gerlach experiment: The beam splits into a number of separated beams. The magnetic moments of the atoms assume discrete values.

The filter serves the purpose of selecting atoms of a certain state out of the Stern-Gerlach experiment. We can produce three types of "pure" beams with our Stern-Gerlach filter.

i) Atom beams in the state $|\hat{z}, +\rangle$, where we close the lower two gates and allow only the "upper" beam to go through.

ii) Atom beams in the state $|\hat{z}, 0\rangle$, where we block the upper and lower beams and let the non-deflected central beam to go through.

iii) Atom beams in the state $|\hat{z}, -\rangle$, where we close the upper two gates and allow only the "lower" beam to go through.

The unit vector $\hat{z}$ denotes the orientation of the magnetic field gradient in the Stern-Gerlach apparatus.

2.2.2 Successive aligned Stern-Gerlach filters

We shall now perform experiments passing atom beams through two successive Stern-Gerlach filters (Filter 1 and Filter 2), both having the same gradient for the magnetic field.

In a first experiment, we block the middle and lower gates of both filters. Filter 1 gives a beam of atoms at the state $|\hat{z}, +\rangle$. We observe that the *full*

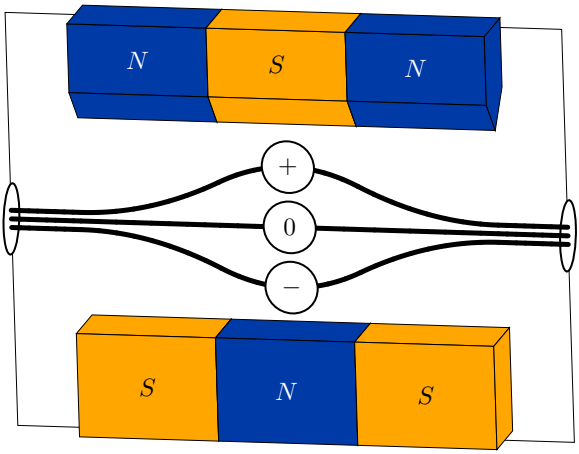


Figure 2.3: Stern-Gerlach filter for spin-1 atoms with a gate +,0 and −.

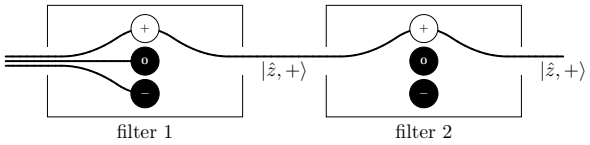


Figure 2.4: Two aligned Stern-Gerlach filters for spin-1 atoms.

beam passes through the second filter, which is also designed to select the same $|\hat{z},+\rangle$ state. We then conclude that the probability amplitude for the transition from a state $|\hat{z},+\rangle$ to the same state $|\hat{z},+\rangle$ is unity [2]

$$\langle \hat{z},+|\hat{z},+\rangle = 1. \tag{2.4}$$

In a second experiment, we close the middle and lower gates of Filter 1 and the upper and lower gates of Filter 2. Filter 1 selects atoms in the state $|\hat{z},+\rangle$ and Filter 2 selects atoms in the state $|\hat{z},0\rangle$. We observe that no beam passes through the second filter. Therefore the probability amplitude for the transition from the state $|\hat{z},+\rangle$ to the state $|\hat{z},0\rangle$ vanishes,

$$\langle \hat{z},0|\hat{z},+\rangle = 0. \tag{2.5}$$

[2] up to a phase $\exp(i\alpha)$ which drops out when computing the modulus square of the amplitude.

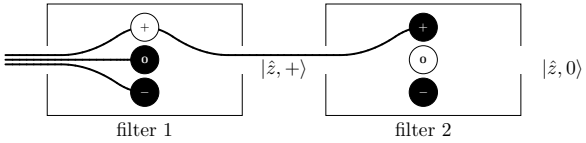


Figure 2.5: Two aligned Stern-Gerlach filters for spin-1 atoms.

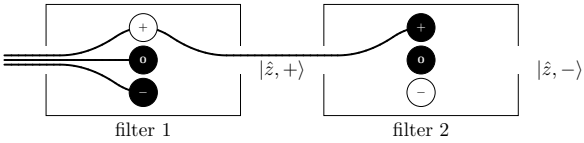


Figure 2.6: Two aligned Stern-Gerlach filters for spin-1 atoms.

The same result holds for transitions from $|\hat{z},+\rangle$ to $|\hat{z},-\rangle$,

$$\langle \hat{z},-|\hat{z},+\rangle = 0. \tag{2.6}$$

The following equations summarize our results for the transitions among the "pure" states $|\hat{z},+\rangle, |\hat{z},-\rangle, |\hat{z},0\rangle$:

$$\langle \hat{z},+|\hat{z},+\rangle = \langle \hat{z},0|\hat{z},0\rangle = \langle \hat{z},-|\hat{z},-\rangle \ = 1 \tag{2.7a}$$

and

$$\langle \hat{z},+|\hat{z},0\rangle = \langle \hat{z},0|\hat{z},+\rangle = \langle \hat{z},+|\hat{z},-\rangle \ = 0\,, \tag{2.7b}$$

$$\langle \hat{z},-|\hat{z},+\rangle = \langle \hat{z},0|\hat{z},-\rangle = \langle \hat{z},-|\hat{z},0\rangle \ = 0\,. \tag{2.7c}$$

2.2.3 Successive rotated Stern-Gerlach filters

We now perform a more interesting experiment with two Stern-Gerlach filters in a row, where the second filter is rotated by an angle θ. Specifically, in Filter 1 the magnetic field $\mathbf{B}$ varies along the $\hat{z}$ direction and in Filter 2 $\mathbf{B}$ varies along the $\hat{n}$ direction, with $\hat{n}\cdot\hat{z} = \cos\theta$. The first filter splits a beam of spin-1 atoms along the $\hat{z}-$axis and it can select atoms in the "pure" states

$$|\hat{z},+\rangle, |\hat{z},-\rangle, |\hat{z},0\rangle\,.$$

The second filter splits a beam of spin-1 atoms along the $\hat{n}-$axis and it can select atoms in the "pure" states

$$|\hat{n},+\rangle, |\hat{n},-\rangle, |\hat{n},0\rangle\,.$$

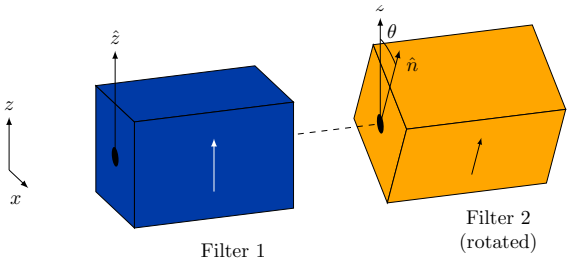


Figure 2.7: Two Stern-Gerlach filters with their directions of $\mathbf{B}-$field variation roated at an angle θ.

In our sequential experiments, we can find the probability that an atom transitions from a definite $|\hat{z}, \{+, 0, -\}\rangle$ state to a definite $|\hat{n}, \{+, 0, -\}\rangle$ state. We find that all such transitions are indeed possible and therefore the probability amplitudes

$$\langle \hat{n}, a|\hat{z}, b\rangle\,, \quad a, b \in \{+, 0, -\}$$

are different from zero.

We also observe that a transition from a $|\hat{z}, a\rangle$ state to any state $|\hat{n}, b\rangle$ takes always place with a 100% certainty. This gives that

$$\left|\langle \hat{n}, +|\hat{z}, +\rangle\right|^2 + \left|\langle \hat{n}, 0|\hat{z}, +\rangle\right|^2 + \left|\langle \hat{n}, -|\hat{z}, +\rangle\right|^2 = 1\,, \tag{2.8a}$$

$$\left|\langle \hat{n}, +|\hat{z}, -\rangle\right|^2 + \left|\langle \hat{n}, 0|\hat{z}, -\rangle\right|^2 + \left|\langle \hat{n}, -|\hat{z}, -\rangle\right|^2 = 1\,, \tag{2.8b}$$

$$\left|\langle \hat{n}, +|\hat{z}, 0\rangle\right|^2 + \left|\langle \hat{n}, 0|\hat{z}, 0\rangle\right|^2 + \left|\langle \hat{n}, -|\hat{z}, 0\rangle\right|^2 = 1\,. \tag{2.8c}$$

2.2.4 Three filters

We now consider an experiment with three Stern-Gerlach filters. The first and the third apparatus have a direction of $\mathbf{B}-$field variation along the positive $\hat{z}$ axis. The second apparatus is rotated at an angle θ with a $\mathbf{B}-$field variation pointing along $\hat{n}$. We arrange that the first filter sets the atoms in the state $|\hat{z}, +\rangle$ and that the second filter puts them at a state $|\hat{n}, 0\rangle$. What happens when the atoms pass through the third filter? Do the atoms have a memory that they have been before in a $|\hat{z}, +\rangle$ state? No! The atoms can transition to any of the three states $|\hat{z}, \{+, 0, -\}\rangle$ despite the fact that they have once been made to be in a pure $|\hat{z}, +\rangle$ state.

Indeed, we can easily show that the fraction of atoms that ends up in any of the $|\hat{z}, \{+, 0\}\rangle$ states through the last filter is independent of the transition

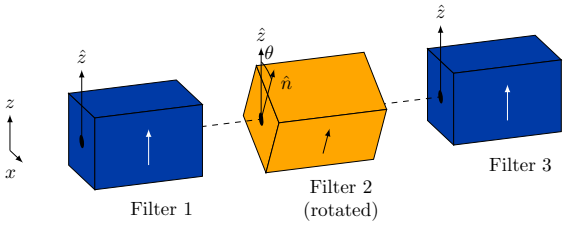


Figure 2.8: Three Stern-Gerlach filters in a row. The first and the third apparatus have a direction of $\mathbf{B}-$field variation along the positive $\hat{z}$ axis. The second apparatus is rotated at an angle θ with a $\mathbf{B}-$field variation pointing along $\hat{n}$.

through the first filter. The amplitudes for the transition through the second and third filter from the $|\hat{z},+\rangle$ to, say, either a $|\hat{z},+\rangle$ or a $|\hat{z},-\rangle$ state are

$$\langle \hat{z},+|\hat{n},0\rangle \langle \hat{n},0|\hat{z},+\rangle$$

and

$$\langle \hat{z},-|\hat{n},0\rangle \langle \hat{n},0|\hat{z},+\rangle$$

respectively. The ratio of probabilities for the two transitions is

$$\frac{\left|\langle \hat{z},+|\hat{n},0\rangle \langle \hat{n},0|\hat{z},+\rangle\right|^2}{\left|\langle \hat{z},-|\hat{n},0\rangle \langle \hat{n},0|\hat{z},+\rangle\right|^2} = \frac{\left|\langle \hat{z},+|\hat{n},0\rangle\right|^2}{\left|\langle \hat{z},-|\hat{n},0\rangle\right|^2}$$

and it does not depend on the state of the beam prior to the second filter.

2.3 Base states

The previous results illustrate one of the basic principles of quantum mechanics: Atomic systems can be decomposed through a filtering process into *base states*. The evolution of the system in any of these states is independent of the past and depends solely on the nature of the base state. The base states depend on the filtering process. For example, the states $|\hat{z},\{+,0,-\}\rangle$ are one set of base states and the states $|\hat{n},\{+,0,-\}\rangle$ are another.

Let's now go back to our three-filter experiment and do the following:

i) open only the $\hat{z}-$"+" gate in the first filter

ii) open only the $\hat{n}-$"0" gate in the second filter

iii) open only the $\hat{z}-$"−" gate in the third filter

If the beam exiting the first filter has N atoms, there will be $N \times |\langle \hat{z}, -|\hat{n}, 0\rangle|^2$ atoms exiting the last filter.

Now, let's open all the gates in the second filter. How many atoms will go through this time? The result of this experiment is very intriguing. No atom exits our apparatus! It is so, that our filter has no effect if none of the base-states are selected. We can then write

$$\sum_{\text{all } i} \langle \hat{z}, -|i\rangle \langle i|\hat{z}, +\rangle = 0, \quad i \in \big|\hat{n}, \{+, 0, -\}\big\rangle. \tag{2.9}$$

To verify that this is a generic property of a "wide open" filter we check with a third Stern-Gerlach filter which filter in a completely different direction $\hat{r}$ than the other two filters. If the first filter is set to prepare the atoms in a state $|\phi\rangle$ and the third filter is set to prepare the atoms in a state $|\chi\rangle$, we find that the open second filter does not affect at all the transition from $|\phi\rangle$ to $|\chi\rangle$:

$$\langle \chi|\phi\rangle = \sum_{\text{all } i} \langle \chi|i\rangle \langle i|\phi\rangle \,. \tag{2.10}$$

Let us list here the properties of base states:

i) If a system is in a base state then the future evolution is independent of the past.

ii) Base states satisfy equation 2.10

iii) Base states are completely different from each other

$$\langle i|j\rangle = \delta_{ij}. \tag{2.11}$$

Base states are not unique and they depend on the filtering method. For example, a Stern-Gerlach filter in the $\hat{n}$ direction and a Stern-Gerlach experiment in a different $\hat{r}$ direction yield a different set of base states.

Let us now compare equation 2.10 and equation 2.8a. In order for both of them to be valid, we require one more rule for the conjugation of probability amplitudes. Namely,

$$\langle \phi|\chi\rangle^* = \langle \chi|\phi\rangle \,. \tag{2.12}$$

2.4 States and vector spaces

We will now take a bold step. We will postulate that atomic states live in a vector space. We will also assume that the pure states filtered with the aid of

a physical measurement, such as angular momentum in the $\hat{z}$ direction, form an orthogonal basis in that vector space. In our example, we can write

$$|\hat{z},+\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\hat{z},0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |\hat{z},-\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{2.13}$$

A generic state will be expressed as a superposition of basis states,

$$|\phi\rangle = \phi_1 |\hat{z},+\rangle + \phi_2 |\hat{z},0\rangle + \phi_3 |\hat{z},-\rangle = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{pmatrix}. \tag{2.14}$$

We will also equip the vector space of with an inner product, which we will physically identify with a transition amplitude. For

$$|\phi\rangle = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{pmatrix}, \quad |\chi\rangle = \begin{pmatrix} \chi_1 \\ \chi_2 \\ \chi_3 \end{pmatrix}, \tag{2.15}$$

we define

$$\langle\phi|\chi\rangle = \phi_1^* \chi_1 + \phi_2^* \chi_2 + \phi_3^* \chi_3. \tag{2.16}$$

Equivalently, we can define dual vectors, "bra" in Dirac's notation, as

$$\langle\phi| = (\phi_1^*, \phi_2^*, \phi_3^*), \tag{2.17}$$

and we can think of the inner product of as a multiplication of a dual "bra" vector and a customary "ket" vector. It will be more practical to us to think of the inner product in this equivalent way.

The above assumptions of a vector space and an inner product are consistent with the physical properties that we inferred with our experimentations using the Stern-Gerlach apparatus. For example, the property

$$\langle\phi|\chi\rangle = \phi_1^* \chi_1 + \phi_2^* \chi_2 + \phi_3^* \chi_3 = (\chi_1^* \phi_1 + \chi_2^* \phi_2 + \chi_3^* \phi_3)^* = \langle\chi|\phi\rangle^* \tag{2.18}$$

emerges naturally. Let us now focus on the "completeness"identity,

$$\langle\phi|\chi\rangle = \sum_i \langle\phi|i\rangle \langle i|\chi\rangle = \langle\phi| \left(\sum_i |i\rangle \langle i| \right) |\chi\rangle. \tag{2.19}$$

with $|i\rangle \in \{|\hat{z},+\rangle, |\hat{z},0\rangle, |\hat{z},-\rangle\}$. From the vector representation of the base states,

$$\sum_i |i\rangle \langle i| = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} (1,0,0) + \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} (0,1,0) + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} (0,0,1) = 1_{3\times 3} \tag{2.20}$$

we naturally derive this result too.

Recall the values of L_z angular momentum that we observed experimentally for each element in our basis of states. We have

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \to \hbar, \quad \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \to 0, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \to -\hbar. \tag{2.21}$$

We can define a matrix

$$\hat{L}_z \equiv \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{2.22}$$

with the property that the basis vector states are its eigenvectors and the corresponding eigenvalues are the values of angular momentum L_z measured in each state. Namely

$$\hat{L}_z \left|\hat{z},+\right\rangle = \hbar \left|\hat{z},+\right\rangle \tag{2.23}$$
$$\hat{L}_z \left|\hat{z},0\right\rangle = 0 \left|\hat{z},0\right\rangle \tag{2.24}$$
$$\hat{L}_z \left|\hat{z},+\right\rangle = -\hbar \left|\hat{z},+\right\rangle \tag{2.25}$$
$$\tag{2.26}$$

We pass a beam of atoms, all prepared identically to be at the same state $|\psi\rangle$, through a Stern-Gerlach apparatus. We will measure the following average value of the angular momentum L_z

$$\langle L_z \rangle = \left|\langle \hat{z},+|\psi\rangle\right|^2 \hbar + \left|\langle \hat{z},0|\psi\rangle\right|^2 0 + \left|\langle \hat{z},+|\psi\rangle\right|^2 (-\hbar). \tag{2.27}$$

Using that $\langle\phi|\chi\rangle = \langle\chi|\phi\rangle^*$ and that the matrix $\hat{L}_z$ has the set $|\hat{z},\{+,0,-\}\rangle$ as eigenvectors, we cast the above equation as

$$\begin{aligned} \langle L_z \rangle &= \langle\psi|\hat{z},+\rangle \langle\hat{z},+|\psi\rangle \hbar + \langle\psi|\hat{z},0\rangle \langle\hat{z},0|\psi\rangle 0 + \langle\psi|\hat{z},-\rangle \langle\hat{z},-|\psi\rangle (-\hbar) \\ &= \langle\psi| \hat{L}_z \left|\hat{z},+\right\rangle \langle\hat{z},+|\psi\rangle + \langle\psi| \hat{L}_z \left|\hat{z},0\right\rangle \langle\hat{z},0|\psi\rangle + \langle\psi| \hat{L}_z \left|\hat{z},-\right\rangle \langle\hat{z},-|\psi\rangle \\ &= \langle\psi| \left[\hat{L}_z \left(\sum_{i\in\{+.0.-1\}} |\hat{z},i\rangle \langle\hat{z},i| \right) \right] |\psi\rangle \end{aligned} \tag{2.28}$$

Now, we can use that

$$\sum_{i\in\{+.0.-1\}} |\hat{z},i\rangle \langle\hat{z},i| = 1. \tag{2.29}$$

And we obtain that the average value of the physical measuuremt for our observable, the angular momentum component L_z, is given by

$$\langle L_z \rangle = \langle \psi | \, \hat{L}_z \, | \psi \rangle \, . \tag{2.30}$$

Similarly, if we start from the experimental statement that the sum of all probabilities for any of the transitions

$$|\psi\rangle \longrightarrow |\hat{z}, i\rangle \, , \quad i \in \{+.0. - 1\}$$

is a unity, we can conclude that

$$\langle \psi | \psi \rangle = 1. \tag{2.31}$$

The matrix operator $\hat{L}_z$ is a "generator" of a symmetry transformation. The connection to symmetry will be explored at more depth in subsequent lectures. In here, we will just give a first glimpse of it. After a standard linear algebra computation, we can compute a weighted exponential of $\hat{L}_z$ as

$$U(\theta) \equiv \exp\left(-i \frac{L_z}{\hbar} \theta\right) = \begin{pmatrix} e^{-i\theta} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\theta} \end{pmatrix} \tag{2.32}$$

θ is an arbitrary parameter for now, but we will be able to relate it to a rotation angle. Let us now define a new transformed state

$$|\psi'\rangle = U(\theta) \, |\psi\rangle \, . \tag{2.33}$$

The average value of L_z in the transformed state is

$$\langle L_z \rangle' = \langle \psi' | \, \hat{L}_z \, | \psi' \rangle = \langle \psi | \, U^\dagger(\theta) \, \hat{L}_z \, U(\theta) \, | \psi \rangle \, . \tag{2.34}$$

We can easily show that

$$U^\dagger(\theta) \, \hat{L}_z \, U(\theta) = \hat{L}_z \tag{2.35}$$

from which we conclude that

$$\langle L_z \rangle' = \langle L_z \rangle \, . \tag{2.36}$$

Classically, we expect that a vector remains unchanged if we perform a rotation by an angle θ around its axis. The matrix $U(\theta)$ is, as we will learn in detail later, encoding the action of this rotational symmetry on the space of quantum states. The classical result also holds in quantum mechanics, but for average values in measurements of physical observables.

Chapter 3

Quantum Mechanics and Linear Algebra

In quantum mechanics we are interested in computing the probability amplitudes $\langle b|a\rangle$ for transitions from an initial state $|a\rangle$ to a final state $|b\rangle$. In this chapter, we will postulate that such amplitudes are the inner products of vectors in a space of physical states.

$$\langle b|a\rangle \leftrightarrow \mathbf{b}\cdot\mathbf{a}.$$

Mathematically, the space of quantum states belongs to a category of a vector space known as a Hilbert space. All physical information for a physical system, e.g. a particle, an atom, a system of many particles, etc is encoded in these vectors in a Hilbert space. In what follows, we will describe the properties of the Hilbert space of quantum states.

3.1 Ket-space

Physical states are represented by vectors in a complex vector space. We call such a vector state a *ket*. Kets possess complete information about the physical system. The dimensionality of the ket space is equal to the number of base states which we can obtain with a filtering experiment, such as our Stern-Gerlach experiment.

i) Two kets can be added yielding a new ket for another physical state

$$|\alpha\rangle + |\beta\rangle = |\gamma\rangle\,. \tag{3.1}$$

ii) The multiplication of a ket with a complex number yields a new ket which corresponds however to the same physical state as the original

$$c\,|\chi\rangle \;\text{ and }\; |\chi\rangle \rightarrow \text{same physical state.} \tag{3.2}$$

3.2 Operators

The state of a physical system can change during an experiment or by letting the system evolve with time. We represent mathematically changes in physical states by the action of operators on kets:

$$A\,|\psi\rangle = |\phi\rangle \qquad (\text{Operator}\,|\text{state}\rangle = |\text{new state}\rangle). \tag{3.3}$$

For a given operator A, there are some special states, $|i\rangle$, which are not changed, up to a multiplicative factor λ_i, by the action of the operator,

$$A\,|i\rangle = \lambda_i\,|i\rangle\,. \tag{3.4}$$

The values λ_i are called the eigenvalues of the operator. The eigenstates of a physical operator are postulated to correspond to base states: Any other physical state $|\phi\rangle$ can be written as a superposition of the base states.

$$\forall\,|\phi\rangle\ \ \exists\,\{c_i\}:\quad |\phi\rangle = \sum_i c_i\,|i\rangle\,.$$

3.3 Dual space

We define a dual space of "bra" states $\langle\phi|$,

$$|\phi\rangle \leftrightarrow \langle\phi|\ . \tag{3.5}$$

By dual we mean that all information about the bra $\langle\phi|$ is already encoded in the ket $|\phi\rangle$ and we only need to use it for a different purpose. We can think of kets as states of an "initial condition" and bras as states of a "final condition". The duality means that all states are eligible as starting or ending states of an experiment. For a general superposition of ket states, the bra dual reads

$$c_1\,|a_1\rangle + \ldots + c_n\,|c_n\rangle \leftrightarrow c_1^*\,\langle a_1| + \ldots + c_n^*\,\langle c_n|\,, \tag{3.6}$$

where we conjugate the multiplicative factors in front of every bra component.

3.4 Inner product

The dual bra-space serves to define probability amplitudes as inner products:

$$\langle a|b\rangle \quad (\text{inner product}). \tag{3.7}$$

We postulate that

$$\langle a|b\rangle = \langle b|a\rangle^*\,, \tag{3.8}$$

and that the "square" of a state is positive definite:

$$\langle\phi|\phi\rangle \geq 0, \quad \forall\ |\phi\rangle\,. \tag{3.9}$$

We call $\sqrt{\langle\phi|\phi\rangle}$ the norm of the state $|\phi\rangle$. We can normalize all states to have a unit norm without altering the physics,

$$|\phi\rangle \to \left|\tilde{\phi}\right\rangle = \frac{|\phi\rangle}{\sqrt{\langle\phi|\phi\rangle}}, \tag{3.10}$$

where $\left\langle\tilde{\phi}\middle|\tilde{\phi}\right\rangle = 1$.

3.5 Properties of operators and their duals

i) Two operators are said to be equal, $X = Y$, if

$$X\,|\phi\rangle = Y\,|\phi\rangle\,, \quad \forall\ |\phi\rangle\,. \tag{3.11}$$

ii) An operator is zero, $X = 0$, if

$$X\,|\phi\rangle = 0, \quad \forall\ |\phi\rangle\,. \tag{3.12}$$

iii) Operators can be added together, with properties

$$X + Y = Y + X\,, \tag{3.13}$$

$$X + (Y + Z) = X + (Y + Z) = X + Y + Z\,. \tag{3.14}$$

iv) Operators can be multiplied together with the property

$$\begin{aligned} X(YZ) &= (XY)Z \\ &= XYZ\,. \end{aligned} \tag{3.15}$$

v) However, the multiplication order is important and, in general,

$$XY \neq YX.$$

The dual of an operator acting on a ket $X\,|\phi\rangle$ is in general a different operator

$$X\,|\phi\rangle \leftrightarrow \langle\phi|\,X^\dagger, \tag{3.16}$$

with

$$X^\dagger \neq X.$$

$X^\dagger$ is called the "Hermitian adjoint" of X. Operators with the special property that $X^\dagger = X$ are called hermitian operators.

The dual of a product of operators is

$$(XY)^\dagger = Y^\dagger X^\dagger. \tag{3.17}$$

Proof. Let's write

$$Y\left|a\right\rangle = \left|b\right\rangle,$$

where the dual is

$$\left\langle b\right| = \left\langle a\right| Y^\dagger.$$

Then

$$XY\left|a\right\rangle = X(Y\left|a\right\rangle) = X\left|b\right\rangle \leftrightarrow \left\langle b\right| X^\dagger = \left\langle a\right| Y^\dagger X^\dagger,$$

which proves our assertion. □

We can define an outer product $\left|b\right\rangle\left\langle a\right|$, which is an operator turning a generic state $\left|\phi\right\rangle$ to a state $\left|b\right\rangle$

$$\left(\left|b\right\rangle\left\langle a\right|\right)\left|\phi\right\rangle = \left|b\right\rangle\left(\left\langle a|\phi\right\rangle\right) = \left(\left\langle a|\phi\right\rangle\right)\left|b\right\rangle, \tag{3.18a}$$

$$(\text{operator})\left|\text{state}\right\rangle = \ldots = (\text{number})\left|\text{new state}\right\rangle. \tag{3.18b}$$

The dual of an outer product is also an outer product

$$\left(\left|\phi\right\rangle\left\langle\psi\right|\right)^\dagger = \left|\psi\right\rangle\left\langle\phi\right|. \tag{3.19}$$

Indeed,

$$\left(\left|\phi\right\rangle\left\langle\psi\right|\right)\left|a\right\rangle = \left|\phi\right\rangle\left(\left\langle\psi|a\right\rangle\right) \leftrightarrow \left\langle\phi\right|\left(\left\langle\psi|a\right\rangle\right)^* = \left(\left\langle a|\psi\right\rangle\right)\left\langle\phi\right| = \left\langle a\right|\left(\left|\psi\right\rangle\left\langle\phi\right|\right).$$

3.6 Hermitian operators

For a general operator, X, we can prove that

$$\left\langle a\right| X\left|b\right\rangle = \left\langle b\right| X^\dagger\left|a\right\rangle^* \tag{3.20}$$

Proof.

$$\left\langle a\right| X\left|b\right\rangle = \left\langle a\right|\left(X\left|b\right\rangle\right) = \left(\left(\left\langle b\right| X^\dagger\right)\left|a\right\rangle\right)^* = \left\langle b\right| X^\dagger\left|a\right\rangle^*.$$

□

Hermitian operators $H^\dagger = H$ have the special property that

$$\langle a| H |b\rangle = \langle b| H |a\rangle^* .$$

We can prove the following:

i) The eigenvalues of a Hermitian operator are real.

Proof. For a Hermitian operator H with eigenstates $|i\rangle$,

$$H |i\rangle = \lambda_i |i\rangle .$$

The dual of the above equation is

$$\langle i| H = \lambda_i^* \langle i| ,$$

where we have exploited the hermiticity of H ($H^\dagger = H$). Multiplying the first equation with $\langle i|$ from the left and the second equation with $|i\rangle$ from the right, we obtain that

$$\langle i| H |i\rangle = \lambda_i = \lambda_i^*,$$

which proves that the eigenvalue λ_i is real. □

ii) The eigenstates of a Hermitian operator with non-degenerate eigenvalues are orthogonal.

Proof. Following the same reasoning as above, we can easily show that for two eigenstates $|i\rangle , |j\rangle$ of a Hermitian operator H we can write the quantity $\langle i| A |j\rangle$ in two alternative ways:

$$\langle i| A |j\rangle = \lambda_i \langle i|j\rangle = \lambda_j \langle i|j\rangle$$

which leads to

$$(\lambda_i - \lambda_j) \langle i|j\rangle = 0.$$

For non-degenerate eigenvalues, i.e.

$$\lambda_i \neq \lambda_j, \quad \forall |i\rangle \neq |j\rangle$$

we conclude that

$$\langle i|j\rangle = 0, \quad \forall |i\rangle \neq |j\rangle$$

and the eigenstates are orthogonal. □

We typically normalize eigenstates of Hermitian operators to be orthonormal:

$$\langle i|j\rangle = \delta_{ij}. \tag{3.21}$$

We postulate that a Hermitian operator A which corresponds to a physical observable has a "complete" set of eigenstates $\{|i\rangle\}$. Every other physical state can be written as a superposition:

$$\forall\, |\phi\rangle \;\; \exists\{c_i\} \;:\; |\phi\rangle = \sum_i c_i\, |i\rangle\,. \tag{3.22}$$

The coefficients c_i can be determined to be the transition amplitude from the state $|\phi\rangle$ to the eigenstate $|i\rangle$:

$$c_i = \langle i|\phi\rangle\,. \tag{3.23}$$

Indeed,

$$\sum_j c_j\, |j\rangle = |\phi\rangle$$

$$\rightsquigarrow \sum_j c_j\, \langle i|j\rangle = \langle i|\phi\rangle$$

$$\rightsquigarrow \sum_j c_j \delta_{ij} = \langle i|\phi\rangle$$

$$\rightsquigarrow c_i = \langle i|\phi\rangle\,.$$

From Eq. 3.22 and Eq. 3.23 we obtain that for every state $|\phi\rangle$,

$$|\phi\rangle = \sum_i \left(\langle i|\phi\rangle\right) |i\rangle\,, \tag{3.24}$$

which we can re-arrange into.

$$|\phi\rangle = \left(\sum_i |i\rangle\, \langle i|\right) |\phi\rangle\,, \tag{3.25}$$

Thus, for base-states $|i\rangle$ which are eigenstates of a non-degenerate Hermitian operator, we have that:

$$1 = \sum_{\text{all } i} |i\rangle\, \langle i|\,. \tag{3.26}$$

For a normalized state $|\phi\rangle$ we have that

$$1 = \langle\phi|\phi\rangle = \sum_i \langle\phi|i\rangle \langle i|\phi\rangle \tag{3.27}$$

$$\rightsquigarrow 1 = \sum_i |\langle i|\phi\rangle|^2 . \tag{3.28}$$

This is consistent with the probabilistic interpretation of the inner product, associating the probability $P(|\phi\rangle \to |i\rangle)$ for a transition from a state $|\phi\rangle$ to an eigenstate with the square of the inner product

$$P(|\phi\rangle \to |i\rangle) = |\langle i|\phi\rangle|^2 . \tag{3.29}$$

In a filtering experiment (corresponding to the operator A with eigenstates $|i\rangle$) of a quantum mechanical system (such as an atom in a state $|\phi\rangle$) the probability that the system passes through one of the filters (the state ϕ collapses to one of the eigenstates $|i\rangle$) is one

$$\sum_{\text{all } i} P(|\phi\rangle \to |i\rangle) = 1 . \tag{3.30}$$

The operator $\Lambda_i \equiv |i\rangle \langle i|$ projects a general state onto the eigenstate $|i\rangle$ of the Hermitian operator A. Indeed,

$$\begin{aligned} \Lambda_i |\phi\rangle &= \big(|i\rangle \langle i|\big) |\phi\rangle = \big(\langle i|\phi\rangle\big) |i\rangle \\ &= \big[\text{amplitude}(|\phi\rangle \to |i\rangle)\big] \times |i\rangle . \end{aligned} \tag{3.31}$$

This operator has the defining property of a projector,

$$\begin{aligned} \Lambda_i \Lambda_j &= \big(|i\rangle \langle i|\big) \big(|j\rangle \langle j|\big) = |i\rangle \langle i|j\rangle \langle j| \\ &= |i\rangle \delta_{ij} \langle j| = |i\rangle \langle i| \delta_{ij} \\ &= \Lambda_i \delta_{ij} . \end{aligned}$$

For $i = j$, we find that $\Lambda_i^2 = \Lambda_i$, which tells us that filtering a quantum system onto a pure state $|i\rangle$ successively does induce any further change to the system after the filtering of the first time. For $i \neq j$, we find that $\Lambda_i \Lambda_j = 0$. A system which is already filtered onto a pure state $|i\rangle$ cannot transition directly into a different pure state of the same observable.

3.7 Matrix representation of states and operators

Consider a Hermitian operator A with a set of eigenstates $\{|i\rangle\}, i = 1 \ldots N$. These satisfy the orthonormality condition $\langle j|i\rangle = \delta_{ij}$. We can represent these eigenstates as vectors,

$$|1\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad |2\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \quad \cdots \quad , \quad |N\rangle \doteq \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}. \tag{3.32a}$$

We represent the dual bra-eigenstates as

$$\begin{aligned} &\langle 1| \doteq (1, 0, \ldots, 0)\,, \\ &\langle 2| \doteq (0, 1, \ldots, 0)\,, \quad \cdots \quad , \quad \langle N| \doteq (0, 0, \ldots, 1)\,. \end{aligned} \tag{3.32b}$$

The above representations of the bra and ket eigenstates are consistent with their orthonormality condition. For example,

$$\langle 1|2\rangle \doteq (1, 0, \ldots, 0) \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix} = 0$$

and

$$\langle 2|2\rangle \doteq (0, 1, \ldots, 0) \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix} = 1$$

etc.

A general state $|\phi\rangle$ must satisfy

$$|\phi\rangle = \sum_i \langle i|\phi\rangle\, |i\rangle \tag{3.33}$$

This can be represented as

$$|\phi\rangle \doteq \langle 1|\phi\rangle \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \langle 2|\phi\rangle \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix} + \ldots + \langle N|\phi\rangle \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix} \tag{3.34}$$

yielding,

$$|\phi\rangle \doteq \begin{pmatrix} \langle 1|\phi\rangle \\ \langle 2|\phi\rangle \\ \vdots \\ \langle N|\phi\rangle \end{pmatrix}.$$

For a bra state $\langle\phi|$ we write

$$\langle\phi| = \langle\phi| \sum_i |i\rangle\langle i| = \sum_i \langle\phi|i\rangle \langle i| = \sum_i \langle i|\phi\rangle^* \langle i| \,. \tag{3.35}$$

This is represented as

$$\langle\phi| \doteq \left(\langle 1|\phi\rangle^*, \langle 2|\phi\rangle^*, \ldots, \langle N|\phi\rangle^*\right). \tag{3.36}$$

The inner product of two general states is

$$\langle a|b\rangle = \langle a| \left(\sum_i |i\rangle\langle i|\right) |b\rangle = \sum_j \langle a|i\rangle \langle i|b\rangle = \sum_i \langle i|a\rangle^* \langle i|b\rangle \,. \tag{3.37}$$

This is consistent with the result that we obtain by using our representation,

$$\langle a|b\rangle \doteq \left(\langle 1|a\rangle^*, \langle 2|a\rangle^*, \ldots, \langle N|a\rangle^*\right) \begin{pmatrix} \langle 1|b\rangle \\ \langle 2|b\rangle \\ \vdots \\ \langle N|b\rangle \end{pmatrix} \tag{3.38}$$

A general operator X can be written as

$$X = \left(\sum_i |i\rangle \langle i|\right) X \left(\sum_j |j\rangle \langle j|\right) = \sum_{ij} |i\rangle \langle i| X |j\rangle \langle j| \,. \tag{3.39}$$

The operator is represented as an $N \times N$ matrix,

$$X \doteq \begin{pmatrix} \langle 1| X |1\rangle & \langle 1| X |2\rangle & \ldots & \langle 1| X |N\rangle \\ \langle 2| X |1\rangle & \langle 2| X |2\rangle & \ldots & \langle 2| X |N\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle N| X |1\rangle & \langle N| X |2\rangle & \ldots & \langle N| X |N\rangle \end{pmatrix}. \tag{3.40}$$

For the case of the outer product operator, we obtain the following representation

$$|a\rangle\langle b| \doteq \begin{pmatrix} \langle 1|a\rangle \langle 1|b\rangle^* & \langle 1|a\rangle \langle 2|b\rangle^* & \ldots & \langle 1|a\rangle \langle N|b\rangle^* \\ \langle 2|a\rangle \langle 1|b\rangle^* & \langle 2|a\rangle \langle 2|b\rangle^* & \ldots & \langle 2|a\rangle \langle N|b\rangle^* \\ \vdots & \vdots & \ddots & \vdots \\ \langle N|a\rangle \langle 1|b\rangle^* & \langle N|a\rangle \langle 2|b\rangle^* & \ldots & \langle N|a\rangle \langle N|b\rangle^* \end{pmatrix}. \tag{3.41}$$

3.8 Compatible and incompatible observables

Two Hermitian operators which commute with each other,

$$[A, B] \equiv AB - BA = 0, \tag{3.42}$$

are called compatible. If they do not commute, $[A, B] \neq 0$, they are incompatible. We shall prove a couple of theorems which elucidate the meaning of this terminology.

Theorem 3.1. *For two hermitian operators $A, B : [A, B] = 0$, where A has a spectrum of eigenstates $|i\rangle$ with non-degenerate eigenvalues,*

$$A\,|i\rangle = \lambda_i\,|i\rangle\,,$$

i) B is a diagonal matrix in the representation of the $|i\rangle$ basis,

ii) The set of $|i\rangle$ states is also a set of eigenstates of the B operator.

Proof. For any two eigenstates $|i\rangle\,, |j\rangle$ of A we have that

$$\begin{aligned} 0 &= [A, B] \\ \rightsquigarrow 0 &= \langle i|\, AB - BA\,|j\rangle = \langle i|\, AB\,|j\rangle - \langle i|\, BA\,|j\rangle \\ &= (\lambda_i - \lambda_j)\,\langle i|\, B\,|j\rangle\,.^{1} \end{aligned}$$

For $|i\rangle \neq |j\rangle$, given that the eigenvalues are not degenerate, we have that $\lambda_i \neq \lambda_j$. Thus, it must be that $\langle i|\, B\,|j\rangle = 0$. Only the diagonal elements, $i = j$, are allowed to be different than zero. We write:

$$\langle i|\, B\,|j\rangle = \delta_{ij}\,\langle i|\, B\,|i\rangle\,, \tag{3.43}$$

which is the first statement of our theorem.
The B operator can be written as

$$\begin{aligned} B &= \left(\sum_i |i\rangle\langle i|\right) B \left(\sum_j |j\rangle\langle j|\right) \\ &= \sum_{ij} |i\rangle\,\langle i|\, B\,|j\rangle\,\langle j| \\ &= \sum_{ij} |i\rangle\,\delta_{ij}\,\langle j|\,\big(\langle i|\, B\,|i\rangle\big) \\ &= \sum_i \big(\langle i|\, B\,|i\rangle\big)\,|i\rangle\langle i|. \end{aligned}$$

[1] $\langle i|\, AB - BA\,|j\rangle$ can be seen as $\langle i|\,(AB - BA)\,|j\rangle$.

Acting on an eigenstate $|m\rangle$ of the A operator, we have

$$\begin{aligned} B|m\rangle &= \sum_i \left(\langle i| B |i\rangle\right) |i\rangle\langle i| |m\rangle \\ &= \sum_i \left(\langle i| B |i\rangle\right) |i\rangle \delta_{im} \\ &= \left(\langle m| B |m\rangle\right) |m\rangle \end{aligned}$$

which proves that the eigenstates $|m\rangle$ of A are also eigenstates of the commuting operator B. □

Theorem 3.2. *If two operators do not commute, $[A, B] \neq 0$, their common eigenstates do not form a complete set.*

Proof. We can prove the above by assuming the opposite, i.e. the common eigenstates of A, B, denoted by $|a, b\rangle$ and satisfying

$$\begin{aligned} A|a, b\rangle &= a|a, b\rangle , \\ B|a, b\rangle &= b|a, b\rangle , \end{aligned}$$

form a complete set. Then a general state can be written as

$$|\phi\rangle = \sum_{a,b} c_{ab} |a, b\rangle . \tag{3.44}$$

Acting with the commutator on an arbitrary state $|\phi\rangle$, we obtain that

$$[A, B]|\phi\rangle = \sum_{a,b} c_{ab} (AB - BA)|a, b\rangle = \sum_{a,b} c_{ab} (ab - ba)|a, b\rangle = 0. \tag{3.45}$$

From the above we conclude that the commutator vanishes, $[A, B] = 0$, which is in contradiction to our hypothesis. □

3.9 Expectation value and uncertainty of Hermitian operators (measurements)

Consider a Hermitian operator A which corresponds to a physical observable, such as energy, momentum, position, spin magnetic moment, etc. We associate the average value measured in an experiment (which is repeated infinitely many times) for the quantity corresponding to A with the expectation value of the operator with respect to the system's state $|\phi\rangle$:

$$\langle A\rangle = \langle\phi| A |\phi\rangle . \tag{3.46}$$

Let's use the eigenstates $|i\rangle$ of the operator A as a basis of physical states. These have eigenvalues λ_i, where

$$A\,|i\rangle = \lambda_i\,|i\rangle\,. \tag{3.47}$$

The expectation value of A can be written as

$$\langle A\rangle = \langle\phi|\left(\sum_i |i\rangle\langle i|\right) A \left(\sum_j |j\rangle\langle j|\right)|\phi\rangle\,, \tag{3.48}$$

which yields

$$\langle A\rangle = \sum_i \lambda_i\,|\langle i|\phi\rangle|^2\,. \tag{3.49}$$

We can re-write this expression as

$$\langle A\rangle = \sum_i \lambda_i \mathrm{Prob}(|\phi\rangle \to |i\rangle) \tag{3.50}$$

The expectation value is a sum over all possible eigenvalues weighted by the probability that the state of the system collapses to the corresponding eigenstate. If $|\phi\rangle$ is itself an eigenstate of A, e.g. $|\phi\rangle = |j\rangle$ the expectation value of the measurement is simply the eigenvalue λ_j:

$$\langle A\rangle = \langle j|\,A\,|j\rangle = \sum_i \lambda_i\,|\langle i|j\rangle|^2 = \sum_i \lambda_i\delta_{ij} = \lambda_j. \tag{3.51}$$

In addition to the average of mesurements for an observable in a quantum mechanical system, we can compute the uncertainty in these measurements. This is defined as

$$\left\langle(\Delta A)^2\right\rangle \equiv \left\langle\left(A - \langle A\rangle\,\mathbf{1}\right)^2\right\rangle. \tag{3.52}$$

[2] Indeed,

$$\left\langle(\Delta A)^2\right\rangle = \left\langle A^2\right\rangle - \langle A\rangle^2\,, \tag{3.53}$$

which we can easily prove,

$$\begin{aligned}\left\langle\left(A - \langle A\rangle\right)^2\right\rangle &= \left\langle A^2\right\rangle - 2\left\langle A\,\langle A\rangle\right\rangle + \langle A\rangle^2 = \left\langle A^2\right\rangle - 2\,\langle A\rangle^2 + \langle A\rangle^2 \\ &= \left\langle A^2\right\rangle - \langle A\rangle^2\,,\end{aligned} \tag{3.54}$$

[2] From now on we will drop the **1**.

where

$$\begin{aligned}\left\langle A\left\langle A\right\rangle\right\rangle &= \left\langle\phi\right| A \underbrace{\left\langle\phi\right| A \left|\phi\right\rangle}_{\text{number}} \left|\phi\right\rangle = \left\langle\phi\right| A \left|\phi\right\rangle \left\langle\phi\right| A \left|\phi\right\rangle = \left(\left\langle\phi\right| A \left|i\right\rangle\right)^2 \\ &= \left\langle A\right\rangle^2 .\end{aligned} \tag{3.55}$$

Notice that the uncertainty for a system in an eigenstate of A is zero,

$$\left\langle(\Delta A)^2\right\rangle = \left\langle i\right| A^2 \left|i\right\rangle - \left\langle i\right| A \left|i\right\rangle^2 = \lambda_i^2 - \lambda_i^2 = 0. \tag{3.56}$$

3.10 The uncertainty principle

In this section, we shall derive Heisenberg's uncertainty principle for any pair of incompatible (non-commuting) Hermitian (physical) operators A, B.
We start with

$$\begin{aligned}\left\langle(A-\left\langle A\right\rangle)(B-\left\langle B\right\rangle)\right\rangle &= \left\langle AB - A\left\langle B\right\rangle - \left\langle A\right\rangle B + \left\langle A\right\rangle\left\langle B\right\rangle\right\rangle \\ &= \left\langle AB\right\rangle - \left\langle A\right\rangle\left\langle B\right\rangle \\ &= \frac{1}{2}\left\langle[A,B]\right\rangle + \frac{1}{2}\left\langle AB+BA\right\rangle - \left\langle A\right\rangle\left\langle B\right\rangle \\ &= \frac{1}{2}\left\langle[A,B]\right\rangle \\ &\quad + \frac{1}{2}\left\langle \left(A-\left\langle A\right\rangle\right)\left(B-\left\langle B\right\rangle\right) + \left(B-\left\langle B\right\rangle\right)\left(A-\left\langle A\right\rangle\right)\right\rangle \\ &= \frac{1}{2}\left\langle[A,B]\right\rangle + \frac{1}{2}\left\langle\{A-\left\langle A\right\rangle, B-\left\langle B\right\rangle\}\right\rangle\end{aligned} \tag{3.57}$$

where the anti-commutator is defined as

$$\{X,Y\} \equiv XY + YX. \tag{3.58}$$

The anti-commutator of Hermitian operators is also a Hermitian operator. Indeed,

$$\begin{aligned}\{X,Y\}^\dagger &= (XY)^\dagger + (YX)^\dagger = Y^\dagger X^\dagger + X^\dagger Y^\dagger \\ &= YX + XY = XY + YX = \{X,Y\}\end{aligned}$$

On the other hand, the commutator of two Hermitian operators is anti-Hermitian [3]. Indeed,

$$[A,B]^\dagger = [B^\dagger, A^\dagger] = [B,A] = -[A,B].$$

Now we can prove an important theorem:

[3] (an operator Z is anti-Hermitian if its adjoint is $Z^\dagger = -Z$)

Theorem 3.3. *The expectation value of a Hermitian operator is real, while the expectation value of an anti-Hermitian operator is imaginary.*

Proof. Indeed, the real and imaginary parts of the expectation value for an operator A are

$$\Re\left(\langle A\rangle\right) = \frac{\langle A\rangle + \langle A\rangle^*}{2} = \frac{1}{2}\left\langle\phi\right| A + A^\dagger \left|\phi\right\rangle \tag{3.59}$$

$$\Im\left(\langle A\rangle\right) = \frac{\langle A\rangle - \langle A\rangle^*}{2i} = \frac{1}{2i}\left\langle\phi\right| A - A^\dagger \left|\phi\right\rangle \tag{3.60}$$

The real part vanishes if A is anti-Hermitian, $A^\dagger = -A$, while the imaginary part vanishes if A is Hermitian, $A^\dagger = A$. □

In the rhs of Eq. 3.57, the first term is then purely imaginary while the second term is real. Both give an independent positive definitive contribution in the absolute value square of the lhs, and we can write

$$\left|\left\langle (A - \langle A\rangle)(B - \langle B\rangle)\right\rangle\right|^2 = \left|\frac{1}{2}\left\langle [A,B]\right\rangle\right|^2 + \left|\frac{1}{2}\left\langle \{A - \langle A\rangle\,, B - \langle B\rangle\}\right\rangle\right|^2 . \tag{3.61}$$

This leads to the inequality,

$$\left|\langle (A - \langle A\rangle)\,(B - \langle B\rangle)\rangle\right|^2 \geq \left|\frac{1}{2}\left\langle [A,B]\right\rangle\right|^2 . \tag{3.62}$$

Now we shall use a Schwarz inequality,

$$\left|\langle a|b\rangle\right|^2 \leq \langle a|a\rangle\,\langle b|b\rangle\,, \tag{3.63}$$

which we can prove easily by the postulate $\langle\phi|\phi\rangle \geq 0$ for

$$|\phi\rangle = |a\rangle - \frac{\langle b|a\rangle}{\langle b|b\rangle}\,|b\rangle\,.$$

Applying Schwarz's inequality to

$$|a\rangle = (A - \langle A\rangle)\,|\phi\rangle$$

and

$$|b\rangle = (B - \langle B\rangle)\,|\phi\rangle$$

we obtain,

$$\left|\langle (A - \langle A\rangle)(B - \langle B\rangle)\rangle\right|^2 \leq \left\langle (A - \langle \mathbf{A}\rangle)^2\right\rangle \left\langle (B - \langle \mathbf{B}\rangle)^2\right\rangle \tag{3.64}$$

Combining the inequalities 3.57 - 3.62 we obtain the "uncertainty principle":

$$\left\langle (\Delta A)^2\right\rangle \left\langle (\Delta B)^2\right\rangle \geq \frac{1}{4}\left|\langle [A,B]\rangle\right|^2 \tag{3.65}$$

3.11 Change of basis

Incompatible operators offer different sets of base-kets to describe the states of a quantum mechanical system (furnishing a different "representation" for each one of such operators).

Given two sets of base-kets there is a unitary operator which can transform general states and operators from one basis to the other. Consider two Hermitian operators A, B and their corresponding sets of eigenstates $\{|a_i\rangle\}, \{|b_i\rangle\}$ where,

$$A\,|a_i\rangle = a_i\,|a_i\rangle\,, \tag{3.66}$$
$$B\,|b_i\rangle = b_i\,|b_i\rangle\,, \tag{3.67}$$

and

$$\langle a_i|a_j\rangle = \langle b_i|b_j\rangle = \delta_{ij}. \tag{3.68}$$

There is a unitary operator U which transforms a state $|a_i\rangle$ into a state $|b_i\rangle$:

$$|b_i\rangle = U\,|a_i\rangle\,, \tag{3.69}$$

with

$$UU^\dagger = U^\dagger U = 1. \tag{3.70}$$

Explicitly, we can easily verify that

$$U = \sum_k |b_k\rangle\,\langle a_k|\,. \tag{3.71}$$

Indeed,

$$\begin{aligned} U\,|a_i\rangle &= \sum_k |b_k\rangle\,\langle a_k|a_i\rangle = \sum_k |b_k\rangle\,\delta_{ki} \\ &= |b_i\rangle\,. \end{aligned} \tag{3.72}$$

Similarly,

$$\begin{aligned} U^\dagger\,|b_i\rangle &= \sum_k \left(|b_k\rangle\,\langle a_k|\right)^\dagger\,|b_i\rangle = \sum_k \left(|a_k\rangle\,\langle b_k|\right)|b_i\rangle = \sum_k |a_k\rangle\,\delta_{ki} \\ &= |a_i\rangle\,. \end{aligned} \tag{3.73}$$

Finally,

$$\begin{aligned} U^\dagger U &= \left(\sum_j |a_j\rangle\,\langle b_j|\right)\left(\sum_k |b_k\rangle\,\langle a_k|\right) = \sum_{jk} |a_j\rangle\,\langle b_j|b_k\rangle\,\langle a_k| \\ &= \sum_{jk} |a_j\rangle\,\delta_{jk}\,\langle a_k| = \sum_j |a_j\rangle\,\langle a_j| = 1\,, \end{aligned} \tag{3.74}$$

and

$$\begin{aligned} UU^\dagger &= \left(\sum_j |b_j\rangle \langle a_j|\right)\left(\sum_k |a_k\rangle \langle b_k|\right) = \sum_{jk} |b_j\rangle \langle a_j|a_k\rangle \langle b_k| \\ &= \sum_{jk} |b_j\rangle \delta_{jk} \langle b_k| = \sum_j |b_j\rangle \langle b_j| = 1\,. \end{aligned} \tag{3.75}$$

3.11.1 Transformation matrix

The transformation matrix

$$U = \sum_k |b_k\rangle\langle a_k| \tag{3.76}$$

is represented in the basis of $\{|a_i\rangle\}$ as

$$\langle a_j| U |a_i\rangle = \sum_k \langle a_j|b_k\rangle \langle a_k|a_i\rangle = \sum_k \langle a_j|b_k\rangle \delta_{ki} = \langle a_j|b_i\rangle\,. \tag{3.77}$$

An arbitrary state $|\phi\rangle$ is written as

$$|\phi\rangle = \sum_k c_k |a_k\rangle = \sum_k \langle a_k|\phi\rangle |a_k\rangle \doteq \begin{pmatrix} \langle a_1|\phi\rangle \\ \langle a_2|\phi\rangle \\ \vdots \\ \langle a_N|\phi\rangle \end{pmatrix} \tag{3.78}$$

and in the $\{|a_i\rangle\}$ basis it is represented as a column vector with elements $\langle a_i|\phi\rangle$. Similarly, in the $\{|b_i\rangle\}$ basis it is represented as a column vector with elements $\langle b_i|\phi\rangle$.

$$|\phi\rangle = \sum_k d_k |b_k\rangle = \sum_k \langle b_k|\phi\rangle |b_k\rangle \doteq \begin{pmatrix} \langle b_1|\phi\rangle \\ \langle b_2|\phi\rangle \\ \vdots \\ \langle b_N|\phi\rangle \end{pmatrix} \tag{3.79}$$

The two column vectors are related as follows:

$$\begin{aligned} \langle b_i|\phi\rangle &= \sum_k \langle b_i|a_k\rangle \langle a_k|\phi\rangle \\ &= \sum_k \langle a_i| U^\dagger |a_k\rangle \langle a_k|\phi\rangle\,. \end{aligned} \tag{3.80}$$

In matrix form

$$\underbrace{\begin{pmatrix} \vdots \\ \langle b_i|\phi\rangle \\ \vdots \end{pmatrix}}_{\text{new basis}} = \underbrace{\begin{pmatrix} \ddots & \vdots & \iddots \\ \dots & \langle a_i|\, U^\dagger\, |a_k\rangle & \dots \\ \iddots & \vdots & \ddots \end{pmatrix}}_{\substack{\langle a_i|U^\dagger|a_k\rangle \text{ at } i\text{th row} \\ \text{and } k\text{th column}}} \underbrace{\begin{pmatrix} \vdots \\ \langle a_k|\phi\rangle \\ \vdots \end{pmatrix}}_{\text{old basis}} \tag{3.81}$$

Let's now look at changing representations for operators. In the two bases, $\{|a_i\rangle\}$ and $\{|b_i\rangle\}$, an operator X is represented by the matrices

$$\langle a_j|\, X\, |a_i\rangle \quad \text{and} \quad \langle b_j|\, X\, |b_i\rangle\,,$$

respectively. We write:

$$\begin{aligned} \langle b_j|\, X\, |b_i\rangle &= \sum_{k\ell} \langle b_j|a_k\rangle\, \langle a_k|\, X\, |a_\ell\rangle\, \langle a_\ell|b_i\rangle \\ &= \sum_{k\ell} \langle a_j|\, U^\dagger\, |a_k\rangle\, \langle a_k|\, X\, |a_\ell\rangle\, \langle a_\ell|\, U\, |a_i\rangle \end{aligned} \tag{3.82}$$

Which, in matrix notation is written as [4]

$$\begin{aligned} &\underbrace{\begin{pmatrix} \langle b_j|\, X\, |b_i\rangle \end{pmatrix}}_{\text{new basis}} \\ &= \begin{pmatrix} \langle a_j|\, U^\dagger\, |a_k\rangle \end{pmatrix} \underbrace{\begin{pmatrix} \langle a_k|\, X\, |a_\ell\rangle \end{pmatrix}}_{\text{old basis}} \begin{pmatrix} \langle a_\ell|\, U\, |a_i\rangle \end{pmatrix}. \end{aligned} \tag{3.83}$$

3.11.2 Trace of operators

The trace of an operator is defined as

$$\mathrm{tr}(X) = \sum_i \langle a_i|\, X\, |a_i\rangle\,, \tag{3.84}$$

[4] In the same manner as Eq. 3.81

and it is independent of the representation. Indeed, for two representation $\{|a_i\rangle\}$, $\{|b_i\rangle\}$, we have:

$$\begin{aligned}
\sum_i \langle a_i| X |a_i\rangle &= \sum_{ijk} \langle a_i|b_j\rangle \langle b_j| X |b_k\rangle \langle b_k|a_i\rangle \\
&= \sum_{jk} \langle b_k| \underbrace{\left(\sum_i |a_i\rangle\langle a_i| \right)}_{1} |b_j\rangle \langle b_j| X |b_k\rangle \\
&= \sum_{jk} \langle b_k|b_j\rangle \langle b_j| X |b_k\rangle \\
&= \sum_{jk} \delta_{jk} \langle b_j| X |b_k\rangle \\
&= \sum_i \langle b_i| X |b_i\rangle .
\end{aligned}$$

It is easy to prove the typical properties for traces, such as

$$\mathrm{tr}(XY) = \mathrm{tr}(YX). \tag{3.85}$$

We also note that the trace of an outer product is an inner product,

$$\mathrm{tr}\left(|c\rangle\langle b|\right) = \sum_i \langle a_i|c\rangle \langle b|a_i\rangle = \langle b| \left(\sum_i |a_i\rangle\langle a_i| \right) |c\rangle = \langle b|c\rangle . \tag{3.86}$$

3.12 Eigenstates and eigenvalues

Suppose that we know the representation $\langle a_i| X |a_j\rangle$ of an operator X in a basis $\{|a_i\rangle\}$. We would like to compute the eigenstates of X in the same representation. We have

$$\begin{aligned}
X |b_i\rangle &= b_i |b_i\rangle \\
\rightsquigarrow X \sum_l |a_l\rangle\langle a_l| |b_i\rangle &= b_i |b_i\rangle \\
\rightsquigarrow \langle a_\lambda| X \sum_l |a_l\rangle\langle a_l| |b_i\rangle &= b_i \langle a_\lambda|b_i\rangle \\
\rightsquigarrow \sum_l \langle a_\lambda| X |a_l\rangle \langle a_l|b_i\rangle &= b_i \langle a_\lambda|b_i\rangle
\end{aligned}$$

which, in matrix notation, is cast as

$$\begin{pmatrix} \langle a_1| X |a_1\rangle & \dots & \langle a_1| X |a_N\rangle \\ \vdots & \ddots & \vdots \\ \langle a_N| X |a_1\rangle & \dots & \langle a_N| X |a_N\rangle \end{pmatrix} \begin{pmatrix} \langle a_1|b_i\rangle \\ \vdots \\ \langle a_N|b_i\rangle \end{pmatrix} = b_i \begin{pmatrix} \langle a_1|b_i\rangle \\ \vdots \\ \langle a_N|b_i\rangle \end{pmatrix} . \tag{3.87}$$

We can find the eigenvalues b_i and eigenstates

$$\begin{pmatrix} \langle a_1|b_i\rangle \\ \vdots \\ \langle a_N|b_i\rangle \end{pmatrix} \tag{3.88}$$

as eigenvalues and eigenstates of the matrix in the lhs of Eq. 3.87. The eigenvalues satisfy,

$$\det(X - b_i\mathbf{1}) = 0. \tag{3.89}$$

Knowing the eigenvalues the eigenstates can be constructed as usual in linear algebra by substituting b_i explicitly in Eq. 3.87 and solving for the $\langle a_i|b_i\rangle$'s.

3.13 Unitary equivalent observables

Two operators A, B are equivalent if they can be related by a unitary transformation.

$$B = UAU^\dagger, \qquad U^\dagger = U^{-1}. \tag{3.90}$$

These operators have the same eigenvalues and their eigenstates are related by the same unitary transformation.

$$\begin{aligned} A\,|a\rangle &= a\,|a\rangle \\ \rightsquigarrow A\underbrace{U^\dagger U}_{1}\,|a\rangle &= a\underbrace{U^\dagger U}_{1}|a\rangle \\ \rightsquigarrow \left(UAU^\dagger\right)(U\,|a\rangle) &= aUU^\dagger U\,|a\rangle \\ \rightsquigarrow B\,(U\,|a\rangle) &= a\,(U\,|a\rangle)\,. \end{aligned} \tag{3.91}$$

The operator B satisfies an eigenvalues equation

$$B\,|b\rangle = b\,|b\rangle\,.$$

Comparing with the above, we conclude that the eigenstates of the operator B are

$$|b\rangle = U\,|a\rangle\,,$$

and the eigenvalues are

$$b = a\,.$$

Chapter 4

Time evolution

Before we introduce Quantum Mechanics, it will be useful to recall how we described the dynamics of simple mechanical systems in classical physics. In Quantun Mechanics, we will postulate principles that extend a picture of Classical Mechanics.

4.1 Time evolution in classical mechanics

Consider, for simplicity, a one-dimensional mechanical system whose dynamical behavior is encoded in a Lagrangian

$$L\left(x(t), \dot{x}(t)\right).$$

The Lagrangian depends on the position and the velocity, which are functions of time. We will focus on energy conserving systems, in which the Lagrangian acquires all of its time dependence through these functions and has no other explicit time dependence,

$$\frac{\partial L}{\partial t} = 0. \tag{4.1}$$

The time evolution of the position and the velocity obeys the principle of least action. This states that the action is stable,

$$\delta S = 0\,, \tag{4.2}$$

under small variations of the physical trajectory

$$x(t) \to x(t) + \delta x(t). \tag{4.3}$$

Eq. 4.2, leads to the Euler-Lagrange differential equation

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0. \tag{4.4}$$

For example, a particle moving in one-dimension under the influence of a force potential $V(x)$ has a Lagrangian

$$L = \frac{1}{2}m\dot{x}^2 - V(x), \tag{4.5}$$

and the corresponding Euler-Lagrange equation yields Newtons law

$$m\ddot{x} + \frac{\partial V}{\partial x} = 0. \tag{4.6}$$

An alternative description of the same dynamics can be obtained through the Hamiltonian formalism. We define first the canonical momentum,

$$p = \frac{\partial L}{\partial \dot{x}}, \tag{4.7}$$

which, in general, is a function of both the position and velocity,

$$p = p\left(x(t), \dot{x}(t)\right). \tag{4.8}$$

We now define the Hamiltonian

$$H(x, p) = p\dot{x} - L, \tag{4.9}$$

and pick the pair of (x, p) as our independent variables, "inverting" Eq. (4.8), and considering the velocity as a function of position and momentum,

$$\dot{x} = \dot{x}\left(x, p\right). \tag{4.10}$$

Differentiating the Hamiltonian with the position, we have

$$\frac{\partial H}{\partial x} = \ldots = -\dot{p}, \tag{4.11}$$

while differentiating with respect to the momentum we arrive at

$$\frac{\partial H}{\partial p} = \ldots = \dot{x}. \tag{4.12}$$

Therefore, alternatively to the second-order Euler-Lagrangian differential equation, we can describe the dynamical system with the pair of first-order differential equations of Hamilton

$$\dot{p} = -\frac{\partial H}{\partial x}\,, \quad \dot{x} = \frac{\partial H}{\partial p}\,. \tag{4.13}$$

Let us now consider a generic physical quantity,

$$A = A(x, p, t). \tag{4.14}$$

Differentiating with respect to time, we have

$$\frac{dA}{dt} = \frac{\partial A}{\partial p}\,\dot{p} + \frac{\partial A}{\partial x}\,\dot{x} + \frac{\partial A}{\partial t}\,. \tag{4.15}$$

Substituting above the Hamilton equations (4.13), we obtain

$$\frac{dA}{dt} = \{A, H\} + \frac{\partial A}{\partial t}. \tag{4.16}$$

where the Poisson bracket for two functions $f(x, p)$ and $g(x, p)$ is given by

$$\{f, g\} \equiv \frac{\partial f}{\partial x}\frac{\partial g}{\partial p} - \frac{\partial f}{\partial p}\frac{\partial g}{\partial x}. \tag{4.17}$$

For example, the canonical momentum for a particle in a potential, corresponding to the Lagrangian of Eq. (4.5), is

$$p = \frac{\partial L}{\partial \dot{x}} = m\dot{x}, \tag{4.18}$$

which we invert to read

$$\dot{x} = \frac{p}{m}. \tag{4.19}$$

The Hamiltonian is then computed to be

$$H = p\dot{x} - L = \frac{p^2}{2m} + V(x), \tag{4.20}$$

and Hamilton's equations are

$$\dot{x} = \frac{p}{m}\,, \dot{p} = -\frac{\partial V}{\partial x}. \tag{4.21}$$

and the general evolution equation reads

$$\frac{dA}{dt} = \left\{A, \frac{p^2}{2m} + V(x)\right\} + \frac{\partial A}{\partial t} \tag{4.22}$$

We will study the theoretical implications of the time-evolution equation for generic physical quantities A above and the Poisson brackets, soon.

4.1.1 Properties of Poisson brackets

We can derive the following properties of Poisson brackets from their definition in Eq. (4.17).

- Anti-commutation,

$$\{A, B\} = -\{B, A\} \tag{4.23}$$

- Linearity

$$\{A, B + C\} = \{A, B\} + \{A, C\}\,, \tag{4.24}$$

- Product rule,

$$\{A, B\,C\} = B\,\{A, C\} + \{A, B\}\,C \tag{4.25}$$

- Action on position and momentum

$$\{x, p\} = 1\,, \quad \{x, x\} = 0\,, \quad \{p, p\} = 0\,. \tag{4.26}$$

In addition, Poisson brackets satisfy the Jacobi identity

$$\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0. \tag{4.27}$$

We can now also show the inverse. For the class of functions of position and momentum which have a series representation as in

$$f(x, p) = \sum_{n,m=0}^{\infty} c_{nm} x^n p^m, \tag{4.28}$$

the properties of Eqs. (4.23) - (4.26), lead back to the definition of Eq. (4.17). The proof can be somewhat lengthy but relies on simple induction.
We first prove inductively that

$$\{x, x^m\} = 0, \quad \{p, p^m\} = 0, \tag{4.29}$$

and

$$\{x, p^m\} = m p^{m-1} = \frac{\partial}{\partial p}\, p^m, \quad \{x^m, p\} = m x^{m-1} = \frac{\partial}{\partial x}\, x^m. \tag{4.30}$$

Then, it follows that for a generic function $f(x, p)$, as of Eq. 4.17, the Poisson bracket with respect to position (momentum) is equivalent to the derivative with respect to momentum (position),

$$\{x, f\} = \frac{\partial f}{\partial p}\,, \quad \{f, p\} = \frac{\partial f}{\partial x}\,. \tag{4.31}$$

Now, we can show inductively that

$$\{x^n, f(x,p)\} = nx^{n-1}\frac{\partial f}{\partial p} = \frac{\partial\, x^n}{\partial x}\,\frac{\partial f}{\partial p}, \quad \{f(x,p), p^n\} = np^{n-1}\frac{\partial f}{\partial x} = \frac{\partial\, p^n}{\partial p}\frac{\partial f}{\partial x} \tag{4.32}$$

Now, in Eq. (4.32) and in the anticommutation, Eq. (4.23), linearity, Eq. (4.24), and product rule, Eq. (4.25), of the Poisson brackets we have all the ingredients needed to return back to Eq. (4.17).

$$\begin{aligned}\{f(x,p), g(x,p)\} &= \left\{\sum_{nm} c_{nm} x^n p^m, g(x,p)\right\} = \sum_{nm} c_{nm}\,\{x^n p^m, g\} \\ &= \sum_{nm} c_{nm}\, x^n\,\{p^m, g\} + \sum_{nm} c_{nm}\,\{x^n, g\}\, p^m = \sum_{nm} c_{nm}\,[-x^n\,\{g, p^m\} + \{x^n, g\}\, p^m] \\ &= \sum_{nm} c_{nm}\left[-x^n\,\frac{\partial p^m}{\partial p}\,\frac{\partial g}{\partial x} + \frac{\partial x^n}{\partial x}\,p^m\,\frac{\partial g}{\partial p}\right] = \frac{\partial f}{\partial x}\,\frac{\partial g}{\partial p} - \frac{\partial f}{\partial p}\,\frac{\partial g}{\partial x}. \end{aligned} \tag{4.33}$$

4.1.2 A way to think of classical time evolution

We have just then shown, that the definition of Poisson brackets in Eq. (4.17) is equivalent to the properties of Eqs (4.23)-Eqs (4.26). We can then choose to formulate time evolution as follows.

The dynamics of a physical system is encoded in its Hamiltonian,

$$H(x_i, p_i)$$

which depends on space coordinates x_i and canonical momenta p_i. A physical quantity $A(x_i, p_i, t)$ evolves in time according to

$$\frac{dA}{dt} = \{A, H\} + \frac{\partial A}{\partial t}, \tag{4.34}$$

and the Poisson brackets are defined to satisfy

$$\{x_i, x_j\} = \{p_i, p_j\} = 0, \quad \{x_i, p_j\} = \delta_{ij}, \tag{4.35}$$

as well as, anticommutation, linearity, and the product rule of Eqs. (4.23)-(4.25). The above statements are all what one needs to describe the dynamic evolution of a classical system.

4.2 Time evolution in quantum mechanics

Physical systems are in quantum states $|\psi\rangle$ of a Hilbert space. Physical quantities, such as the position and momentum, are hermitian operators acting on this space,

$$\hat{x}_i\,, \hat{p}_i\,, \ldots$$

The mean value of experimental measurements of an observable quantity $\mathcal{O}(x_i, p_i)$, which is represented by an operator $\hat{\mathcal{O}}$ in Hilbert space, is given by

$$\langle \mathcal{O} \rangle = \langle \psi | \, \hat{\mathcal{O}}(\hat{x}_i, \hat{p}_i) \, | \psi \rangle \, . \tag{4.36}$$

Quantum time evolution has a very similar form as classical evolution, in the form presented in the subsection 4.1.2. A central object in classical evolution has been the Poisson brackets of position and momentum. What is the analogous object for the corresponding quantum mechanical operators? Dirac observed that the commutator of two operators,

$$[A, B] \equiv AB - BA$$

possesses algebraic properties analogous to the classical Poisson brackets, i.e.

$$\begin{aligned} [A, B] &= -\,[B, A] \, , & (4.37)\\ [A, B + C] &= [A, B] + [A, C] \, , & (4.38)\\ [A, BC] &= B\,[A, C] + [A, B]\,C \, , & (4.39)\\ [A, [B, C]] + [B, [C, A]] + [C, [A, B]] &= 0 \, . & (4.40) \end{aligned}$$

In classical mechanics, the Poisson bracket of a coordinate and its canonical momentum is a constant (unit). We will postulate the same for the commutator of their quantum mechanical operators,

$$[\hat{x}, \hat{p}] = \text{constant}$$

The constant must then be imaginary, given that the positions and momenta are hermitian,

$$\text{constant}^* = [\hat{x}, \hat{p}]^\dagger = \left[\hat{p}^\dagger, \hat{x}^\dagger\right] = -\,[\hat{x}, \hat{p}] = -\text{constant}. \tag{4.41}$$

In analogy to classical mechanics, it comes natural to postulate the following commutation relations for positions and momenta

$$[\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0 \, , \quad [\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij} \, . \tag{4.42}$$

Comparing Eqs. (4.42) and the Poisson bracket "postulates" for classical mechanics in Eq. (4.35) it is motivated to identify the quantum mechanical analogue of the Poisson bracket as the commutator,

$$\{A, B\} \to \frac{1}{i\hbar} \left[\hat{A}, \hat{B}\right] . \tag{4.43}$$

Inspired by this analogy and Eq. (4.34), it seems natural to postulate the following time evolution for operators of physical operators $\hat{\mathcal{O}}\left(\hat{x}_i, \hat{p}_i\right)$ in quantum mechanics,

$$\frac{d\hat{\mathcal{O}}}{dt} = \frac{1}{i\hbar}\left[\hat{\mathcal{O}}, \hat{H}\right], \tag{4.44}$$

where $\hat{H}$ is the Hamiltonian operator. Eq. (4.44) has the solution,

$$\hat{\mathcal{O}}(t) = e^{\frac{i}{\hbar}Ht}\hat{\mathcal{O}}_0 e^{-\frac{i}{\hbar}Ht}. \tag{4.45}$$

4.2.1 Ehrenfest theorem

In the above, in complete analogy to their classical mechanics counterparts, we have endowed quantum mechanical operators with a time dependence. However, quantum operators are not physically determined experimentally. What is measured is their expectation values for quantum states in Hilbert space. For such a state, $|\psi_0\rangle$, the average value is

$$\left\langle \hat{O}(t) \right\rangle = \langle\psi_0| \hat{O}(t) |\psi_0\rangle . \tag{4.46}$$

The time evolution of the measured average value of the observable satisfies the differential equation

$$\begin{aligned} \frac{d}{dt}\left\langle \hat{O}(t) \right\rangle &= \langle\psi_0| \frac{d}{dt}\hat{O}(t) |\psi_0\rangle \\ &= \frac{1}{i\hbar}\langle\psi_0| \left[\hat{O}, \hat{H}\right] |\psi_0\rangle . \end{aligned} \tag{4.47}$$

Let us concretely consider the Hamiltonian of a particle in a potential,

$$H = \frac{\hat{p}^2}{2M} + V\left(\hat{x}\right) , \tag{4.48}$$

and specialize to $\hat{O} = \hat{x}$ and $\hat{O} = \hat{p}$. Then, from Eq. (4.47) and the commutation relations

$$[\hat{x}(t), \hat{x}(t)] = [\hat{p}(t), \hat{p}(t)] = 0, \quad [\hat{x}(t), \hat{p}(t)] = 0 , \tag{4.49}$$

we obtain (**Exercise**),

$$\frac{d}{dt}\langle\hat{x}(t)\rangle = \frac{\langle\hat{p}(t)\rangle}{M} , \tag{4.50}$$

$$\frac{d}{dt}\langle\hat{p}(t)\rangle = -\left\langle V\left(\hat{x}(t)\right)\right\rangle . \tag{4.51}$$

These equations are analogous to Hamilton's equations of classical mechanics. As in classical mechanics, we can combine them into a second order differential equation, yielding

$$M\frac{d^2}{dt^2}\langle\hat{x}(t)\rangle = -\langle V(\hat{x}(t))\rangle\,. \tag{4.52}$$

The result of Eq. (4.52) is Ehrenfest's theorem and generalizes Newton's law to quantum mechanics.

While Eq. 4.52 is in form similar to the classical law of Newton, its solution for the quantum average value of the trajectory, $\langle\hat{x}(t)\rangle$, can be qualitatively and quantitatively very different than the classical trajectory. This is because, in general,

$$\langle V(\hat{x})\rangle \neq V(\langle\hat{x}\rangle)\,. \tag{4.53}$$

4.2.2 Heisnberg and Schrödinger picture

In so far, we have endowed the physical quantum operators with time evolution while we took the quantum states $|\psi_0\rangle$ to be time independent. This description of time evolution is known as the *Heisenberg picture* but it is not unique. Eq. (4.46) allows further possibilities. Heisenberg's picture will be more convenient for studying time evolution in Quantum Field Theory. An equally useful description is commonly used and it is known Schrödinger's picture.

In Schrödinger's picture, operators are teken to be constant in time and time evolution is carried by the states. Indeed, we can rearrenge the right-hand side of Eq. (4.46) shifting time evolution from the operator to the quantum states

$$\langle\psi_0|\,\hat{O}(t)\,|\psi_0\rangle = \langle\psi(t)|\,\hat{O}_0\,|\psi(t)\rangle\,, \tag{4.54}$$

where

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}Ht}\,|\psi_0\rangle\,. \tag{4.55}$$

This shift of picture does not affect the prediction for the physically measured value of the observable and, of course, both Heisenberg and Schödinger pictures, are physically equivalent. It is easy to see by differentiating the above equation with respect to time, that the time-dependent states (Schrödinger picture) satisfy Schrödinger's equation

$$i\hbar\frac{\partial}{\partial t}\,|\psi(t)\rangle = \hat{H}\,|\psi(t)\rangle\,. \tag{4.56}$$

4.3 Time evolution in the Schrödinger picture

In the previous sections, we followed Dirac's reasoning and guessed the time evolution of a class of observable operators by extending the classical mechanics formalism of Poisson brackets. In here, we will revisit time evolution in the Schrödinger picture, in which the time evolution is carried out by the states and not operators. We will realize that we can infer fundamental properties of time evolution from the fact that quantum states are vectors of a Hilbert space. Our description of time evolution needs to be consistent with the mathematical language of kets, bras and operators upon which we have formulated the principle of quantum mechanics. This language is very restrictive and leads to an elegant and austere formalism for time evolution. Consider a state which evolves as:

$$|\phi, t_0\rangle \to |\phi, t\rangle\,, \qquad t \geq t_0. \tag{4.57}$$

We introduce a time evolution operator and write a relation of the two states at times t_0 and t as

$$|\phi, t\rangle = U(t - t_0)\,|\phi, t_0\rangle\,. \tag{4.58}$$

The operator $U(t-t_0)$ is a time evolution operator which as for now we have only defined its purpose and name. We can guess some of the properties of the time evolution operation easily.

1. Let us consider a normalized state $|\phi, t_0\rangle$, satisfying

   $$\langle\phi, t_0|\phi, t_0\rangle = 1 \tag{4.59}$$

   We would like that the time evolution operator does not destroy the normalization of the states:

   $$\langle\phi, t|\phi, t\rangle = 1 \tag{4.60}$$

   . This is satisfied if the time evolution operator is unitary

   $$U^\dagger(t - t_0)U(t - t_0) = 1, \quad t > t_0\,. \tag{4.61}$$

   We will take Eq. (4.61) to hold as one of our starting assumptions.

2. We also expect that a time evolution $t_0 \to t_1 > t_0$ followed by a time evolution $t_1 \to t_2 > t_1$ is equivalent to a time evolution $t_0 \to t_2$

   $$U(t_2 - t_1)U(t_1 - t_0) = U(t_2 - t_0). \tag{4.62}$$

3. Finally, we anticipate that

$$\lim_{t \to t_0} U(t - t_0) = 1. \tag{4.63}$$

For small times, all of the above are satisfied if

$$U(\Delta t) = 1 - i\Omega\Delta t + \mathcal{O}((\Delta t)^2), \tag{4.64}$$

$$\Omega^\dagger = \Omega \tag{4.65}$$

.

with

We postulate that

$$\Omega = \frac{H}{\hbar}, \tag{4.66}$$

where H is the Hamiltonian operator. This is inspired by classical mechanics as in our earlier discussion.

4.4 Schrödinger equation

We start by the product property for a time translation in the interval

$$(t_0 = 0, t + \Delta t) \tag{4.67}$$

with Δt being infinitesimal.

$$\begin{aligned} U(t + \Delta t) &= U(\Delta t)U(t) \\ \rightsquigarrow U(t + \Delta t) &= \left(1 - i\frac{H}{\hbar}\Delta t\right) U(t) \\ \rightsquigarrow U(t) + \Delta t\frac{\partial}{\partial t}U(t) &= \left(1 - i\frac{H}{\hbar}\Delta t\right) U(t) \\ \overset{\cdot i\hbar/\Delta t}{\rightsquigarrow} i\hbar\frac{\partial}{\partial t}U(t) &= HU(t). \end{aligned} \tag{4.68}$$

The operators of the left and right sides of the last equation acting on a state at the starting time $t_0 = 0$ give

$$i\hbar \frac{\partial}{\partial t} U(t) \left|\phi, t_0 = 0\right\rangle = H U(t) \left|\phi, t_0 = 0\right\rangle \tag{4.69}$$

Recalling that

$$U(t) \left|\phi, t_0 = 0\right\rangle = \left|\phi, t\right\rangle , \tag{4.70}$$

we obtain the equation of Schrödinger

$$i\hbar \frac{\partial}{\partial t} \left|\phi, t\right\rangle = H \left|\phi, t\right\rangle . \tag{4.71}$$

We see that the only axiom in Schrödinger's equation is to identify the operator H with the Hamiltonian. The form of the equation and the Hemiticity of H are derived from demanding states to be vectors in Hilbert space and that time evolution is a unitary operator (4.61). Notice, also, that as our derivation is based on examining time evolution in infinitessimally small intervals. The Hamiltonian can always be assumed to be a constant within their infinitessimal duration [1]. Thus, we can take Schrödinger's equation to be valid for time dependent Hamiltonians $H(t)$.

In the familiar case of a constant Hamiltonian, $H(t) = H$, the solution of Schrödinger's equation is

$$\left|\phi, t\right\rangle = e^{-\frac{i}{\hbar}(t - t_0)\cdot H} \left|\phi, t_0\right\rangle . \tag{4.72}$$

which we also found For a time-dependent Hamiltonian with

$$[H(t_1), H(t_2)] = 0, \quad \forall\, t_1, t_2 \in \underbrace{[t_0, t]}_{\text{interval}} \tag{4.73}$$

we can prove that

$$\left|\phi, t\right\rangle = e^{-\frac{i}{\hbar}\int_{t_0}^{t} \mathrm{d}t' H(t')} \left|\phi, t_0\right\rangle . \tag{4.74}$$

The exponential of an operator X, as of the Hamiltonian above, is defined through its series expansion

$$e^X = 1 + X + \frac{X^2}{2!} + \ldots \tag{4.75}$$

The generic solution of Schrödingers equation can be formally written as a "time ordered exponential" that we will present in QM2 and QFT1.

[1] If not, then make Δt smaller

4.5 Eigenstates of the Hamiltonian operator and time evolution

Consider a constant Hamiltonian operator H with eigenstates $|n\rangle$ and eigenvalues E_n

$$H\,|n\rangle = E_n\,|n\rangle\,. \tag{4.76}$$

A general state at an initial time t_0 is written as

$$|\psi, t_0\rangle = \left(\sum_n |n\rangle\langle n|\right)|\psi, t_0\rangle\,. \tag{4.77}$$

Acting with the time evolution operator we obtain

$$\begin{aligned} U(t-t_0)\,|\psi, t_0\rangle &= U(t-t_0)\left(\sum_n |n\rangle\langle n|\right)|\psi, t_0\rangle \\ \rightsquigarrow |\psi, t\rangle &= e^{-\frac{i}{\hbar}(t-t_0)\cdot H}\left(\sum_n |n\rangle\langle n|\right)|\psi, t_0\rangle \\ \rightsquigarrow |\psi, t\rangle &= \sum_n |n\rangle\, e^{-\frac{i}{\hbar}(t-t_0)\cdot E_n}\,\langle n|\psi, t_0\rangle\ . \end{aligned} \tag{4.78}$$

For the special situation where the initial state is also an eigenstate,

$$|\psi, t_0\rangle = |m\rangle\,,$$

we obtain

$$\begin{aligned} |\psi, t\rangle &= \sum_n |n\rangle\, e^{-\frac{i}{\hbar}(t-t_0)\cdot E_n}\,\langle n|m\rangle \\ \rightsquigarrow |\psi, t\rangle &= \sum_n |n\rangle\, e^{-\frac{i}{\hbar}(t-t_0)\cdot E_n}\delta_{nm} \\ \\ \rightsquigarrow |\psi, t\rangle &= |m\rangle\, e^{-\frac{i}{\hbar}(t-t_0)\cdot E_m} \end{aligned} \tag{4.79}$$

The time evolved state is the original eigenstate up to a phase factor unimportant for physics. **Once a physical system is in an eigenstate of the Hamiltonian, it will always remain in this eigenstate.**

Assuming again that the system is in an eigenstate of the Hamiltonian, the expectation value of a physical observable A at a later time t will be

$$\begin{aligned} \langle A\rangle_t &= \langle\phi, t|\,A\,|\phi, t\rangle = \langle m|\, e^{+\frac{i}{\hbar}(t-t_0)\cdot H} A e^{-\frac{i}{\hbar}(t-t_0)\cdot H}\,|m\rangle \\ &= \langle m|\, e^{+\frac{i}{\hbar}(t-t_0)\cdot E_m} A e^{-\frac{i}{\hbar}(t-t_0)\cdot E_m}\,|m\rangle = \langle m|\,A\,|m\rangle \end{aligned} \tag{4.80}$$

Therefore, **expectation values of physical observables remain unchanged if the system is in an eigenstate of the Hamiltonian.**

Otherwise, we anticipate that expectation values "oscillate" among various values with time. For an initial state (at $t_0 = 0$)

$$|\phi\rangle = \sum_m |m\rangle \langle m|\phi\rangle ,$$

we have that at a later time the expectation value becomes

$$\begin{aligned}
\langle A\rangle_t &= \langle \phi, t| A |\phi, t\rangle \\
&= \langle \phi| e^{+\frac{i}{\hbar}(t-t_0)\cdot H} A e^{-\frac{i}{\hbar}(t-t_0)\cdot H} |\phi\rangle \\
&= \sum_{n,m} \langle \phi|m\rangle \langle m| e^{+\frac{i}{\hbar}(t-t_0)\cdot H} A e^{-\frac{i}{\hbar}(t-t_0)\cdot H} |n\rangle \langle n|\phi\rangle \\
&= \sum_{n,m} \langle \phi|m\rangle \langle m| e^{+\frac{i}{\hbar}(t-t_0)\cdot E_m} A e^{-\frac{i}{\hbar}(t-t_0)\cdot E_n} |n\rangle \langle n|\phi\rangle \\
&= \sum_{n,m} e^{-i(t-t_0)\cdot\omega_{nm}} \langle m|\phi\rangle^* \langle n|\phi\rangle \langle n| A |m\rangle , \qquad (4.81)
\end{aligned}$$

where the "oscillation" frequencies are

$$\omega_{nm} = \frac{E_n - E_m}{\hbar}. \qquad (4.82)$$

Chapter 5

Two-state systems

In this Chapter, we will study the evolution with time of simple quantum mechanical systems. The simplest situation occures when the Hilbert space has a basis with only two states. For example, a particle with spin-$\frac{1}{2}$ can be found in two states, a spin "up" and a spin "down" state. We will see, that all two-state systems can be described with the same formalism.

5.1 Spin precession

Consider an electron, which is a spin-$\frac{1}{2}$ particle, inside a magnetic field. The potential energy of a classical magnetic dipole is given by

$$U = -\boldsymbol{\mu} \cdot \mathbf{B},$$

where μ is the dipole magnetic moment, proportional to the angular momentum of the rotating electric charge. Inspired by this, we define a quantum mechanical Hamiltonian operator

$$H = -\left(\frac{e}{m_e c}\right) \mathbf{S} \cdot \mathbf{B}, \tag{5.1}$$

where $\mathbf{S}$ is the spin operator and $\mathbf{B}$ is the magnetic field. Let us take the magnetic field to be along the $\hat{z}$ direction,

$$\mathbf{B} = B\hat{z}.$$

Thus

$$H = -\left(\frac{eB}{m_e c}\right) S_z \equiv \omega S_z, \tag{5.2}$$

with

$$\omega \equiv \frac{|e|B}{m_e c}. \tag{5.3}$$

The Hamiltonian and the operator of spin in the z-direction, S_z, commute. Therefore, they must have a common set of eigenvalues. The spin operator

has two eigenstates

$$S_z \left|\pm\right\rangle = \pm\frac{\hbar}{2}\left|\pm\right\rangle, \tag{5.4}$$

which are also energy eigenstates with eigenvalues

$$H\left|\pm\right\rangle = E_\pm\left|\pm\right\rangle, \quad E_\pm = \pm\frac{\hbar\omega}{2}. \tag{5.5}$$

The time evolution operator is

$$U(t) = e^{-\frac{iHt}{\hbar}} = e^{-\frac{i\omega t S_z}{\hbar}}. \tag{5.6}$$

Acting on an initial state

$$\left|\phi\right\rangle = c_+\left|+\right\rangle + c_-\left|-\right\rangle \tag{5.7}$$

we obtain

$$\left|\phi, t\right\rangle = c_+ e^{-i\omega t/2}\left|+\right\rangle + c_- e^{+i\omega t/2}\left|-\right\rangle \tag{5.8}$$

. The coefficients $c_\pm$ are such that

$$\left\langle\phi|\phi\right\rangle = 1 \tag{5.9}$$

,

$$\rightsquigarrow \left|c_+\right|^2 + \left|c_-\right|^2 = 1. \tag{5.10}$$

Note that there is an orthogonal state $\left|\psi\right\rangle$ to $\left|\phi\right\rangle$,

$$\left|\psi\right\rangle = c_-^*\left|+\right\rangle - c_+^*\left|-\right\rangle, \tag{5.11}$$

such that

$$\left\langle\phi|\psi\right\rangle = c_- c_+ - c_+ c_- = 0.$$

The probability that the electron is found again at the same state $\left|\phi\right\rangle$ after some time t is given by

$$P_1(t) = \left|\left\langle\phi|\phi, t\right\rangle\right|^2 = \ldots = 1 - 4|c_+|^2|c_-|^2\sin^2\left(\frac{\omega t}{2}\right) \tag{5.12}$$

If we set $|c_+| = \sin\theta$ and, thus, $|c_-| = \cos\theta$, the probability can be written as

$$P_1(t) = \left|\left\langle\phi|\phi, t\right\rangle\right|^2 = \ldots = 1 - \sin^2\left(\frac{\omega t}{2}\right)\sin^2(2\theta). \tag{5.13}$$

Notice that for $\theta = 0, \frac{\pi}{2}$, which corresponds to $\left|\phi\right\rangle$ being an eigenstate $\left|\pm\right\rangle$ of the Hamiltonian, the probability that the electron remains in the same state

is 100% at all times. For all other states, $\theta \neq 0, \frac{\pi}{2}$, the probability oscillates with time. There exist, however, periodic times,

$$t = n\frac{2\pi}{\omega}, \quad n = 0, 1, 2, \ldots$$

for which the probability to measure the system in the original, arbitrarily chosen, state is always one,

$$P_1\left(t = \frac{2\pi}{\omega}\right) = 1.$$

The probability to transition to the orthogonal state ψ after some time t is

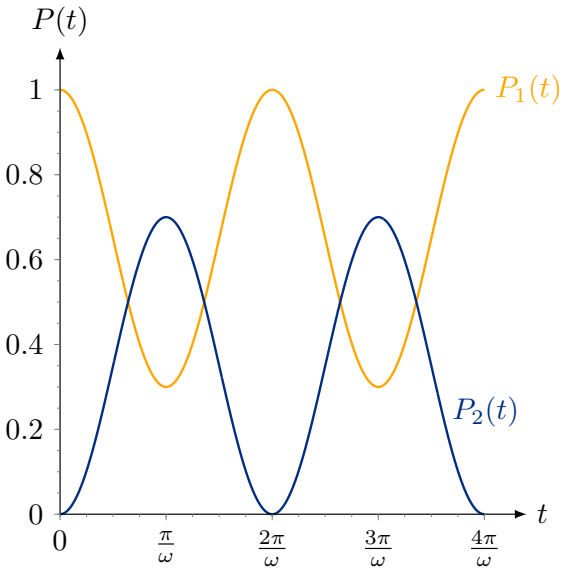


Figure 5.1: The probability P_1 for a transition to the initial state and the probabiltity for a transition to its orthogonal state after some time t as a function of t.

$$P_2(t) = |\langle\psi|\phi, t\rangle|^2 = \ldots = \sin^2\left(\frac{\omega t}{2}t\right)\sin^2(2\theta)\,. \tag{5.14}$$

As you can observe, the total probability is conserved

$$P_1 + P_2 = 1.$$

5.2 A generic two-state system

Consider a system with only two base states

$$|1\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |2\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

A generic state can be written, in this basis, as

$$\begin{aligned} |\psi\rangle &= |1\rangle \langle 1|\psi\rangle + |2\rangle \langle 2|\psi\rangle \\ &\doteq \begin{pmatrix} \langle 1|\psi\rangle \\ \langle 2|\psi\rangle \end{pmatrix} \end{aligned} \tag{5.15}$$

The action of the Hamiltonian on a ganeric state is

$$H|\psi\rangle = \sum_{i,j} |i\rangle \langle i| H |j\rangle \langle j|\psi\rangle \tag{5.16}$$

and it is represented as

$$H|\psi\rangle \doteq \begin{pmatrix} \langle 1| H |1\rangle & \langle 1| H |2\rangle \\ \langle 2| H |1\rangle & \langle 2| H |2\rangle \end{pmatrix} \begin{pmatrix} \langle 1|\psi\rangle \\ \langle 2|\psi\rangle \end{pmatrix} \tag{5.17}$$

The Hamiltonian matrix of the system, as represented in this basis is of the general form

$$H \doteq \begin{pmatrix} H_{11} & H_{12} \\ H_{12}^* & H_{22} \end{pmatrix}, \tag{5.18}$$

where

$$H_{ij} = H_{ji}^* = \langle i| H |j\rangle,$$

so that

$$H^\dagger = H.$$

Notice that the diagonal elements must be real $H_{11*} = H_{11}, H_{22*} = H_{22}$ while the non-diagonal elements can be complex.

We shall assume for now that the Hamiltonian is independent of time,

$$H(t) = H, \quad \forall\, t\,. \tag{5.19}$$

The Hamiltonian has two energy eigenstates with eigenvalues E satisfying

$$\det \begin{pmatrix} H_{11} - E & H_{12} \\ H_{12}^* & H_{22} - E \end{pmatrix} = 0\,. \tag{5.20}$$

This yields the solutions

$$E_\pm = \frac{H_{11} + H_{22} \pm \sqrt{\Delta}}{2}, \quad \Delta = (H_{11} - H_{22})^2 + 4|H_{12}|^2. \tag{5.21}$$

The energy eigenstates, $|E_\pm\rangle$, satisfy

$$(H - E_\pm \mathbf{1})\,|E_\pm\rangle = 0\,. \tag{5.22}$$

We find (exercise) that

$$|E_\pm\rangle = \frac{1}{\sqrt{|H_{12}|^2 + (E_\pm - H_{11})^2}} \begin{pmatrix} H_{12} \\ E_\pm - H_{11} \end{pmatrix}, \tag{5.23}$$

where we have normalized so that $\langle E_\pm | E_\pm \rangle = 1$. They also satisfy (exercise)

$$\langle E_\pm | E_\mp \rangle = 0.$$

Having found the eigenvalues and eigestates of the Hamiltonian, we can simplify the study of time evolution by changing to a new basis of our Hilbert space, with elements the Hamiltonina eigenstates,

$$|E_+\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |E_-\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

In the new basis, the Hamiltonian is represented as

$$H \doteq \begin{pmatrix} \langle E_+|\,H\,|E_+\rangle & \langle E_+|\,H\,|E_-\rangle \\ \langle E_-|\,H\,|E_+\rangle & \langle E_-|\,H\,|E_-\rangle \end{pmatrix} \doteq \begin{pmatrix} E_+ & 0 \\ 0 & E_- \end{pmatrix} \tag{5.24}$$

TheHamiltonian takes the form of a diagonal matrix. The time evolution operator is now computed by exponentiated this diagonal matrix. With standard linear algebra, we find that

$$U(t) = \exp\left(-\frac{iHt}{\hbar}\right) \doteq \begin{pmatrix} \exp\left(-\frac{iE_+t}{\hbar}\right) & 0 \\ 0 & \exp\left(-\frac{iE_-t}{\hbar}\right) \end{pmatrix} \tag{5.25}$$

It is easy to verify that the evolution operator does not change (except up to a phase) the energy eigenstates:

$$U(t)\,|E_\pm\rangle = \exp\left(-\frac{iE_\pm}{\hbar}\right)|E_\pm\rangle\,. \tag{5.26}$$

To obtain the representation of $U(t)$ in the $\{|1\rangle, |2\rangle\}$ basis, we use that

$$\langle i_1| U(t) |i_2\rangle = \sum_{kl} \langle i_1|e_k\rangle \langle e_k| U(t) |e_l\rangle \langle e_l|i_2\rangle, \quad i_{1,2} \in \{1,2\}, e_{1,2} \in \{E_+, E_-\}. \tag{5.27}$$

In matrix notation we have

$$\overbrace{\begin{pmatrix} \langle 1| U(t) |1\rangle & \langle 1| U(t) |2\rangle \\ \langle 2| U(t) |1\rangle & \langle 2| U(t) |2\rangle \end{pmatrix}}^{\substack{\text{time evolution operator} \\ \text{in } \{|1\rangle, |2\rangle\} \text{ basis}}}$$
$$= \underbrace{\begin{pmatrix} \langle 1|E_+\rangle & \langle 1|E_-\rangle \\ \langle 2|E_+\rangle & \langle 2|E_-\rangle \end{pmatrix}}_{\substack{\text{basis transformation} \\ \{|E_+\rangle, |E_-\rangle\} \to \{|1\rangle, |2\rangle\}}} \underbrace{\begin{pmatrix} \langle E_+| U(t) |E_+\rangle & \langle E_+| U(t) |E_-\rangle \\ \langle E_-| U(t) |E_+\rangle & \langle E_-| U(t) |E_-\rangle \end{pmatrix}}_{\substack{\text{time evolution operator} \\ \text{in } \{|E_+\rangle, |E_-\rangle\} \text{ basis}}} \underbrace{\begin{pmatrix} \langle E_+|1\rangle & \langle E_+|2\rangle \\ \langle E_-|1\rangle & \langle E_-|2\rangle \end{pmatrix}}_{\substack{\text{basis transformation} \\ \{|1\rangle, |2\rangle\} \to \{|E_+\rangle, |E_-\rangle\}}}, \tag{5.28}$$

5.3 The ammonia molecule

In this section we will describe a simplified model of the ammonia molecule NH_3. The molecule consists of three hydrogen and one nitrogen atoms and can be depicted as in Fig 5.2. Let us make the simplifying assumption that the collective motion of the molecule is not important and focus only on the spinning motion of the molecule around its axis. The molecule can spin in two different ways; the nitrogen atom is "above" the plane of the hydrogen atoms or "below" that plane. We denote the two states corresponding to the two types of rotations as $|1\rangle, |2\rangle$. Ignoring all other motions, we can consider these kets as base kets:

$$|1\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |2\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{5.29}$$

We assume that the system is completely symmetric under exchanging the states $|1\rangle, |2\rangle$. Specifically, the expectation value for the energy in the two states is the same:

$$\langle 1| H |1\rangle = \langle 2| H |2\rangle = E_0. \tag{5.30}$$

We also allow for a probability that with time the nitrogen atom can push the hydrogen plane and flip its state:

$$\langle 1| H |2\rangle = \langle 2| H |1\rangle = -A. \tag{5.31}$$

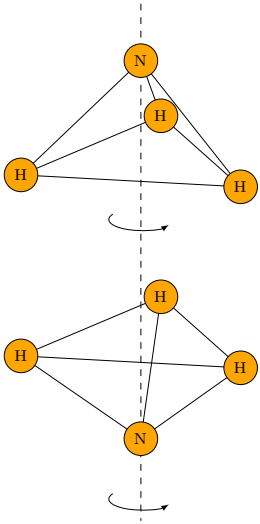


Figure 5.2: The rotation of the molecule of ammonia around its axis can be described as a two-state system.

The Hamiltonian of the system can be written as

$$H \doteq \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}. \tag{5.32}$$

The energy eigenvalues are

$$E_\pm = E_0 \pm A \tag{5.33}$$

and the corresponding eigenstates are

$$|+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad |-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \tag{5.34}$$

The time evolution operator is a function of the Hamiltonian:

$$U(t) = e^{-\frac{iHt}{\hbar}}. \tag{5.35}$$

Exercise 5.1. *Show that the matrix $U(t)$ is a polynomial with no quadratic or higher order terms in H.*

In the $\{|+\rangle, |-\rangle\}$ basis

$$U(t) \doteq \begin{pmatrix} \langle +| U(t) |+\rangle & \langle +| U(t) |-\rangle \\ \langle -| U(t) |+\rangle & \langle -| U(t) |-\rangle \end{pmatrix} \tag{5.36}$$

$$= \begin{pmatrix} \exp\left(-\frac{i(E+A)t}{\hbar}\right) & 0 \\ 0 & \exp\left(-\frac{i(E-A)t}{\hbar}\right) \end{pmatrix}. \tag{5.37}$$

We now compute the transformation matrix,

$$|b\rangle \langle a|, \quad |a\rangle \in \{|+\rangle, |-\rangle\}, \quad |b\rangle \in \{|1\rangle, |2\rangle\}.$$

The time evolution operator in the $\{|1\rangle, |2\rangle\}$ basis is

$$U(t) \doteq \exp\left(-\frac{iE_0 t}{\hbar}\right) \begin{pmatrix} \cos\left(\frac{At}{\hbar}\right) & i\sin\left(\frac{At}{\hbar}\right) \\ i\sin\left(\frac{At}{\hbar}\right) & \cos\left(\frac{At}{\hbar}\right) \end{pmatrix}. \tag{5.38}$$

Unsurprisingly, we also find that if we start from any other state at $t = 0$ the system changes. For a general state, $|\psi, t_0 = 0\rangle$ with norm $\langle \psi, t_0 | \psi, t_0 \rangle$

$$|\psi, t_0 = 0\rangle \doteq e^{i\phi} \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}, \tag{5.39}$$

we find that it evolves as

$$|\psi, t\rangle \doteq e^{i(\phi - E_0 t/\hbar)} \begin{pmatrix} \cos\theta\cos\left(\frac{At}{\hbar}\right) + i\sin\theta\sin\left(\frac{At}{\hbar}\right) \\ \sin\theta\cos\left(\frac{At}{\hbar}\right) + i\cos\theta\sin\left(\frac{At}{\hbar}\right) \end{pmatrix}. \tag{5.40}$$

The probability P_1 that the ammonia molecule is found to be at the same state $|\psi, t_0 = 0\rangle$ after some time t has elapsed is

$$P_1 = \left|\langle \psi, t_0 = 0 | \psi, t\rangle\right|^2 = 1 - \sin^2\left(\frac{At}{\hbar}\right)\cos^2(2\theta). \tag{5.41}$$

We notice that for times

$$t = \frac{n\pi\hbar}{A}, \quad n = 0, 1, 2, \ldots \tag{5.42}$$

the molecule is certainly $P_1 = 1$ back to the original state. For values of θ corresponding to the energy eigenstates, $\theta = \pm\frac{\pi}{4}$, the molecule remains in the original state at all times.

At $t_0 = 0$ we can find a state $|\xi, t_0 = 0\rangle$ which is orthogonal to $|\psi, t_0 = 0\rangle$, satisfying

$$\langle \psi, t_0 = 0 | \xi, t_0 = 0 \rangle = 0.$$

Namely,

$$|\xi, t_0 = 0\rangle \doteq e^{i\phi} \begin{pmatrix} \sin\theta \\ -\cos\theta \end{pmatrix}. \tag{5.43}$$

The probability P_2 that the ammonia molecule transitions after some time t from the state $|\psi, t_0 = 0\rangle$ to its orthogonal $|\xi, t_0 = 0\rangle$ is

$$P_2 = \left| \langle \xi, t_0 = 0 | \psi, t \rangle \right|^2 = \sin^2 \left(\frac{At}{\hbar} \right) \cos^2(2\theta), \tag{5.44}$$

and we find that

$$P_1 + P_2 = 1.$$

The time evolution is completely analogous to the evolution of a spin-1/2 particle inside a magnetic field which we have studied earlier.

5.4 The ammonia molecule inside an electric field

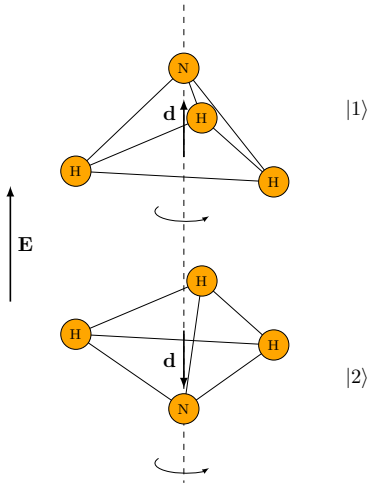


Figure 5.3: The molecule inside an electric field develops an electric dipole moment with a vertical direction from the nitrogen atom to the plane of the hydrogen atoms.

The distribution of the electric charges in the ammonia molecule is not spatially symmetric; it has a non-zero electric dipole moment with a vertical direction from the hydrogen plane to the nitrogen atom. When the molecule is placed inside an electric field $\boldsymbol{\mathcal{E}}$, the energy of the molecule in the states $|1\rangle, |2\rangle$ is not the same anymore since in one state the dipole moment d is in the direction of the electric field and in the other against it. We then have the Hamiltonian

$$H \doteq \begin{pmatrix} E_0 + d\mathcal{E} & -A \\ -A & E_0 - d\mathcal{E} \end{pmatrix} \tag{5.45}$$

The energy eigenvalues are

$$E_\pm = E_0 \pm \sqrt{A^2 + d^2\mathcal{E}^2}. \tag{5.46}$$

For weak electric fields, $d\mathcal{E} \ll E_0$, we can approximate [1]

$$E_\pm \approx E_0 \pm A \pm \frac{d^2\mathcal{E}^2}{2A}. \tag{5.47}$$

In an inhomogeneous electric field, the molecules will move to the regions of the field where they can minimize their energy. The force acting on a molecule in a $|\pm\rangle$ state is,

$$\mathbf{F}_\pm = -\boldsymbol{\nabla} E_\pm = \mp \frac{d^2}{2A} \boldsymbol{\nabla}\mathcal{E}^2 \,. \tag{5.48}$$

The electric force acts opposite to the molecules in the two energy eigenstates and separates them.

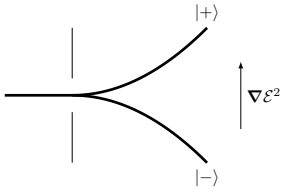


Figure 5.4: The force on ammonia molecules inside an inhomogeneous electric field is opposite for the two energy eigenstates.

5.5 Ammonia in an oscillating electric field

Let us put the ammonia molecule in a time varying electric field

$$\mathcal{E}\cos(\omega t).$$

[1] second order Taylor approximation

The Hamiltonian in the basis of rotation states $\{|1\rangle, |2\rangle\}$ is

$$H(t) \doteq \begin{pmatrix} E_0 + d\mathcal{E}\cos(\omega t) & -A \\ -A & E_0 - d\mathcal{E}\cos(\omega t) \end{pmatrix}. \tag{5.49}$$

Notice (exercise) that the Hamiltonian at one time t_1 does not commute with the Hamiltonian at a later time t_2:

$$[H(t_1), H(t_2)] \neq 0\,.$$

We now need to solve Schrödinger's equation

$$i\hbar\frac{\partial}{\partial t}|\psi, t\rangle = H(t)\,|\psi, t\rangle \tag{5.50}$$

in a more complicated situaiton where the Hamiltonian varies with time. We can exploit the fact that we already know how to solve Schrödinger's equation for a vanishing electric field. For small electric fields, the "bulk" of the evolution should be determined by this static solution. For

$$H_0 = H(t)|_{\mathcal{E}=0} = \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}, \tag{5.51}$$

we found two energy eigenstates, $\{|+\rangle, |-\rangle\}$ with eigenvalues $E_+ = E_0 + |A|, E_- = E_0 - |A|$. It will be most convenient to bring the H_0 Hamiltonian (what we envisage to be the dominant part of the Hamiltonian) in a diagonal form, by working with the energy eigenstates of H_0 as a basis of our Hilbert space.

To change basis, we need the transformation matrix

$$V = \begin{pmatrix} \langle +|1\rangle & \langle -|1\rangle \\ \langle +|2\rangle & \langle -|2\rangle \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}. \tag{5.52}$$

We have that

$$\begin{pmatrix} |+\rangle \\ |-\rangle \end{pmatrix} = V \begin{pmatrix} |1\rangle \\ |2\rangle \end{pmatrix} = \begin{pmatrix} \frac{|1\rangle+|2\rangle}{\sqrt{2}} \\ \frac{|1\rangle-|2\rangle}{\sqrt{2}} \end{pmatrix}, \tag{5.53}$$

and, because it happens that $V^2 = 1$, we also have that

$$\begin{pmatrix} |1\rangle \\ |2\rangle \end{pmatrix} = V \begin{pmatrix} |+\rangle \\ |-\rangle \end{pmatrix} = \begin{pmatrix} \frac{|+\rangle+|-\rangle}{\sqrt{2}} \\ \frac{|+\rangle-|-\rangle}{\sqrt{2}} \end{pmatrix}. \tag{5.54}$$

In the $\{|+\rangle, |-\rangle\}$ basis we have

$$H_0 = \begin{pmatrix} E_0 + |A| & 0 \\ 0 & E_0 - |A| \end{pmatrix}. \tag{5.55}$$

The full Hamiltonian $H(t)$ is not diagonal in the new basis, as $|+\rangle, |-\rangle$ are only eigenstates of H_0. Indeed, we find that in the $\{|+\rangle, |-\rangle\}$ basis,

$$H_0 = \begin{pmatrix} E_0 + |A| & d\mathcal{E}\cos(\omega t) \\ d\mathcal{E}\cos(\omega t) & E_0 - |A| \end{pmatrix}. \tag{5.56}$$

Notice that the non-diagonal elements of the Hamiltonian are indeed small for a small electrical field.

Without loss of generality, without making an approximation yet, we write

$$|\psi, t\rangle = \exp\left(-\frac{iH_0 t}{\hbar}\right)|\phi, t\rangle, \tag{5.57}$$

where, in the convenient $\{|+\rangle, |-\rangle\}$ basis, the evolution operator for a free ammonia molecule is also diagonal,

$$\exp\left(-\frac{iH_0 t}{\hbar}\right) = \exp\left(-\frac{iE_0 t}{\hbar}\right)\begin{pmatrix} e^{-\frac{i\omega_0 t}{2}} & 0 \\ 0 & e^{+\frac{i\omega_0 t}{2}} \end{pmatrix}, \tag{5.58}$$

with

$$\omega_0 = \frac{2|A|}{\hbar}. \tag{5.59}$$

With our substitution of Eq. 5.57, Schrödinger's equation becomes

$$i\hbar\frac{\partial}{\partial t}|\phi, t\rangle = H_I(t)|\phi, t\rangle, \tag{5.60}$$

with

$$\begin{aligned} H_I(t) &= \exp\left(+\frac{iH_0 t}{\hbar}\right)[H(t) - H_0]\exp\left(-\frac{iH_0 t}{\hbar}\right) \\ &= d\mathcal{E}\cos(\omega t)\begin{pmatrix} 0 & e^{+i\omega_0 t} \\ e^{-i\omega_0 t} & 0 \end{pmatrix} \end{aligned} \tag{5.61}$$

In components, Schrödinger's equation becomes

$$\begin{aligned} &i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\phi_+(t)\\ \phi_-(t)\end{pmatrix} \\ &= \frac{d\mathcal{E}}{2}\begin{pmatrix} 0 & e^{+i(\omega_0-\omega)t} + e^{+i(\omega_0+\omega)t} \\ e^{-i(\omega_0-\omega)t} + e^{-i(\omega_0+\omega)t} & 0 \end{pmatrix}\begin{pmatrix}\phi_+(t)\\ \phi_-(t)\end{pmatrix}. \end{aligned} \tag{5.62}$$

where

$$\phi_\pm(t) \equiv \langle \pm|\phi\rangle. \tag{5.63}$$

Now, we will assume that the electric field is small ($d\mathcal{E} \ll E_0$). The $|\phi, t\rangle$ ket should not change very fast in comparison to the rapidly oscillating exponential terms with frequency $\omega + \omega_0$. These oscillations average to a zero value and do not contribute much to the change of the ρ_i coefficients. We make an approximation and ignore them. The exponentials with frequency $\omega - \omega_0$ are also rapidly oscillating unless the two frequencies are very close to each other, which is what we will arrange by tuning our electrical field. We write

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \phi_+(t) \\ \phi_-(t) \end{pmatrix} \approx \frac{d\mathcal{E}}{2} \begin{pmatrix} 0 & e^{+i(\omega_0-\omega)t} \\ e^{-i(\omega_0-\omega)t} & 0 \end{pmatrix} \begin{pmatrix} \phi_+(t) \\ \phi_-(t) \end{pmatrix}. \tag{5.64}$$

5.5.1 Transitions at resonance

Let's consider the situation where the frequency of the electric field is tuned to be $\omega = \omega_0$.

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \phi_+(t) \\ \phi_-(t) \end{pmatrix} \approx \frac{d\mathcal{E}}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \phi_+(t) \\ \phi_-(t) \end{pmatrix} = \hbar\Omega_{\mathcal{E}} \begin{pmatrix} \phi_-(t) \\ \phi_+(t) \end{pmatrix} \tag{5.65}$$

with

$$\Omega_{\mathcal{E}} = \frac{d\mathcal{E}}{2\hbar} \tag{5.66}$$

which are of the same form as our familiar equations for the canonical position and canonical momentum of a simple (classical) harmonic oscillator. The solution of our system of differential equations is

$$\begin{pmatrix} \phi_+(t) \\ \phi_-(t) \end{pmatrix} = \begin{pmatrix} \cos(\Omega_{\mathcal{E}}t) & -i\sin(\Omega_{\mathcal{E}}t) \\ -i\sin(\Omega_{\mathcal{E}}t) & \cos(\Omega_{\mathcal{E}}t) \end{pmatrix} \begin{pmatrix} \phi_+(0) \\ \phi_-(0) \end{pmatrix} \tag{5.67}$$

We can now calculate the time dependence of the $|\psi, t\rangle$ state from,

$$\begin{aligned} \begin{pmatrix} \psi_+(t) \\ \psi_-(t) \end{pmatrix} &= \exp\left(-\frac{iH_0t}{\hbar}\right) \begin{pmatrix} \phi_+(t) \\ \phi_-(t) \end{pmatrix} \\ = \exp\left(-\frac{iE_0t}{\hbar}\right) &\begin{pmatrix} e^{-\frac{i\omega_0 t}{2}} & 0 \\ 0 & e^{+\frac{i\omega_0 t}{2}} \end{pmatrix} \begin{pmatrix} \cos(\Omega_{\mathcal{E}}t) & -i\sin(\Omega_{\mathcal{E}}t) \\ -i\sin(\Omega_{\mathcal{E}}t) & \cos(\Omega_{\mathcal{E}}t) \end{pmatrix} \begin{pmatrix} \phi_+(0) \\ \phi_-(0) \end{pmatrix} \\ = \exp\left(-\frac{iE_0t}{\hbar}\right) &\begin{pmatrix} \cos(\Omega_{\mathcal{E}}t)e^{-\frac{i\omega_0 t}{2}} & -i\sin(\Omega_{\mathcal{E}}t)e^{-\frac{i\omega_0 t}{2}} \\ -i\sin(\Omega_{\mathcal{E}}t)e^{+\frac{i\omega_0 t}{2}} & \cos(\Omega_{\mathcal{E}}t)e^{+\frac{i\omega_0 t}{2}} \end{pmatrix} \begin{pmatrix} \psi_+(0) \\ \psi_-(0) \end{pmatrix} \end{aligned} \tag{5.68}$$

In the last step, we have used that $|\psi, t = 0\rangle = |\phi, t = 0\rangle$.
Let us assume that at $t = 0$, we start with a molecule at the state of highest energy,

$$|\psi, t = 0\rangle = |+\rangle\,. \tag{5.69}$$

Then, after time t the state will be

$$\begin{pmatrix}\psi_+(t)\\ \psi_-(t)\end{pmatrix} = = \exp\left(-\frac{iE_0t}{\hbar}\right)\begin{pmatrix}\cos(\Omega_{\mathcal{E}}t)e^{-\frac{i\omega_0 t}{2}} & -i\sin(\Omega_{\mathcal{E}}t)e^{-\frac{i\omega_0 t}{2}}\\ -i\sin(\Omega_{\mathcal{E}}t)e^{+\frac{i\omega_0 t}{2}} & \cos(\Omega_{\mathcal{E}}t)e^{+\frac{i\omega_0 t}{2}}\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}$$
$$= \begin{pmatrix}\cos(\Omega_{\mathcal{E}}t)e^{-\frac{i\omega_0 t}{2}}\\ -i\sin(\Omega_{\mathcal{E}}t)e^{+\frac{i\omega_0 t}{2}}\end{pmatrix} \tag{5.70}$$

The probability that the molecule transitions to the lower energy state

$$P\left(|+\rangle \to |-\rangle\right) = |\psi_-(t)|^2 = \sin^2(\Omega_{\mathcal{E}}t) \tag{5.71}$$

This is periodic. After certain times controlled by the frequency $\omega_{\mathcal{E}}$ the molecule will certainly transition to the lowest energy state. Similarly, the probability for the molecule to be found again in the state $|+\rangle$ is

$$P\left(|+\rangle \to |+\rangle\right) = |\psi_+(t)|^2 = \cos^2(\Omega_{\mathcal{E}}t). \tag{5.72}$$

5.5.2 Microwave amplification with stimulated emission of radiation

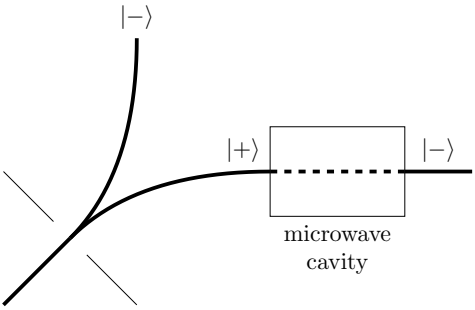


Figure 5.5: The ammonia maser

We now discuss the ammonia maser which is based on the quantum behavior of the two-state molecule. By means of a static inhomogeneous electric field in a "Stern-Gerlach" type of apparatus with an electric field, we can separate molecules in the two energy eigenstates. Molecules in the upper state are directed into a cavity with an oscillating electric field having the resonance frequency $\omega = \omega_0 = 2A/\hbar$. After time $T = \frac{2\pi}{\Omega_{\mathcal{E}}}$ the molecules will transition to the lower energy eigenstate, losing energy equal to the difference of the

two energy eigenvalues. This energy feeds back to the oscillating electric field. To avoid that the molecules transition back to the original state, thus recapturing the released energy, we arrange the length of the cavity such that the molecules exit the cavity in time T.

Exercise: Prove that

$$\int_{-\infty}^{+\infty} \mathrm{d}x \, \frac{\sin^2 x}{x^2} = \pi. \tag{5.73}$$

5.5.3 Transition off resonance

We now solve the differential equation for very small times t and $\omega \sim \omega_0$.

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \phi_+(t) \\ \phi_-(t) \end{pmatrix} \approx \frac{d\mathcal{E}}{2} \begin{pmatrix} 0 & e^{+i(\omega_0-\omega)t} \\ e^{-i(\omega_0-\omega)t} & 0 \end{pmatrix} \begin{pmatrix} \phi_+(t) \\ \phi_-(t) \end{pmatrix}. \tag{5.74}$$

Assuming that we start from a $|+\rangle$ state corresponding to $\phi_+(0) = 1, \phi_-(0) = 0$, for very small times the coefficient $\phi_+(t)$ will remain very close to 1. Then, we have

$$i\hbar \frac{\partial}{\partial t} \phi_-(t) = \frac{d\mathcal{E}}{2} e^{-i(\omega_0-\omega)t} \tag{5.75}$$

which yields

$$\phi_-(t) = \frac{d\mathcal{E}}{2\hbar} \frac{1 - e^{-i(\omega-\omega_0)t}}{\omega - \omega_0} \tag{5.76}$$

The probability for a transition is

$$P\left(|+\rangle \to |-\rangle\right) = \left[\frac{d\mathcal{E}}{\hbar}\right]^2 \frac{\sin^2\left[(\omega-\omega_0)t/2\right]}{\left[\omega-\omega_0\right]^2} \tag{5.77}$$

This is a function peaked very much around $\omega = \omega_0$.

Exercise: Plot it! Unless we are spot-on on the frequency of the MASER, a transition does not occur.

Chapter 6

Position and momentum

6.1 Continuous spectra

So far, we have restricted our discussions to quantum mechanical systems which can be described by a discrete basis of states. We will now discuss operators for physical quantities with a continuous spectrum of eigenvalues. For these operators and their eigenstates, we need some generalisations. Primary examples are the quantum operators for the position and momenta of particles which have as real valued continuous spectrum of eigenvalues.

As we have already developed a formalism of quantum mechanics for operators with discrete eigenvalues, we can generalise the same formalism to continuous spectra with a limiting procedure. For simplicity, we will describe the method assuming an one-dimensional, rather than three-dimensional, space of postions described by a single continuous variable x. The values of x are eigenvalues of an operator $\hat{x}$,

$$\hat{x}\ |x\rangle = x\ |x\rangle\ . \tag{6.1}$$

We will approximate the space by a set of equally distanced discrete points x_i and we will assume that these points are separated with a spacing a from next neighbours. We can obtain the physical continuous space by increasing the density of discrete points taking the limit of zero spacing, $a \to 0$. Before we take this limit, the eigenvalues of the position operator are discrete,

$$\hat{x}\ |x_i\rangle = x_i\ |x_i\rangle \quad i = 1, 2 \ldots \tag{6.2}$$

In accordance to the quantum mechanics principles that we have introduced in the discrete case, we will take that the position eigenstates are orthogonal. We write the following orthogonality condition,

$$\langle x_i | x_j \rangle = \frac{1}{a}\,\delta_{ij}\,. \tag{6.3}$$

Anticipating the continuous limit, $a \to 0$, and that the a state $|x_i\rangle$ stands for an infinite number of continuous states in its vicinity, in the above we

have normalised the states $|x_i\rangle$ to the density $1/a$ of states, rather than to one. A general state $|\psi\rangle$ can be written as a superposition of discrete position eigenstates,

$$|\psi\rangle = \sum_i c_i \, |x_i\rangle \, . \tag{6.4}$$

Multiplying with a position bra $\langle x_j|$, we obtain

$$\begin{aligned} \langle x_j|\psi\rangle &= \sum_i c_i \, \langle x_j|x_i\rangle = \sum_i c_i \, \frac{1}{a}\delta_{ij} = \frac{c_j}{a} \\ &\rightsquigarrow c_j = a \, \langle x_j|\psi\rangle \, . \end{aligned} \tag{6.5}$$

Thus,

$$|\psi\rangle = \sum_i a \, |x_i\rangle \, \langle x_i|\psi\rangle \, . \tag{6.6}$$

We can now take the continuous limit of a zero spacing, $a \to 0$, in Eq. (6.6). The sum over an infinite number of points, is an integral [1]

$$\lim_{a\to 0} \sum_i a = \int dx \, . \tag{6.7}$$

We then have,

$$|\psi\rangle = \int dx \, |x\rangle \, \langle x|\psi\rangle \, . \tag{6.8}$$

As $|\psi\rangle$ can be any state, we then have the completeness relation for continuum spectra,

$$\int dx \, |x\rangle\langle x| = \mathbf{1} \, . \tag{6.9}$$

The probability that a particle is measured at the position corresponding to the state $|x_i\rangle$, in the discretised space, is given by [2]

$$P\left(|\psi\rangle \to |x_i\rangle\right) = \left| \frac{\langle x_i|\psi\rangle}{\sqrt{\langle x_i|x_i\rangle}\sqrt{\langle\psi|\psi\rangle}} \right|^2 = \frac{\left|\langle x_i|\psi\rangle\right|^2}{\langle x_i|x_i\rangle} = a \left|\langle x_i|\psi\rangle\right|^2 . \tag{6.10}$$

[1] Recall how the Riemann integral was defined in your Analysis lectures.

[2] Note, that it is wrong to write $P\left(|\psi\rangle \to |x_i\rangle\right) = \left|\langle x_i|\psi\rangle\right|^2$ as the ket $|x_i\rangle$ is not normalised to unity, $\langle x_i|x_i\rangle = 1/a \neq 1$.

You can check that the sum of all such probabilities is one,

$$\begin{aligned}\sum_i P\left(|\psi\rangle \to |x_i\rangle\right) &= \sum_i a\,|\langle x_i|\psi\rangle|^2 = \ldots = \langle\psi|\left(\sum_i a\,|x_i\rangle\,\langle x_i|\psi\rangle\right)\\ &= \langle\psi|\psi\rangle = 1\,,\end{aligned} \tag{6.11}$$

as it should. We can now take the continuous limit of the above result,

$$\begin{aligned}1 &= \langle\psi|\psi\rangle = \lim_{a\to 0}\sum_i a\,|\langle x_i|\psi\rangle|^2\\ &= \int dx\,|\langle x|\psi\rangle|^2\,.\end{aligned} \tag{6.12}$$

We found that the sum of all probabilities is an integral over a probability density,

$$\rho(x) \equiv |\langle x|\psi\rangle|^2\,. \tag{6.13}$$

The probability of a particle to be located in a region of length dx around a point x is

$$dP(x) = \rho(x)dx\,. \tag{6.14}$$

The amplitude $\langle x|\psi\rangle$ is the *wavefunction* of the particle.

Let us now return to the orthogonality condition of position states of Eq. (6.3). Rearranging and summing over i we have that

$$\sum_i a\,\langle x_i|x_j\rangle = \sum_i \delta_{ij} = 1. \tag{6.15}$$

In the continuum limit, the above turns into

$$\int dx\,\langle x|x'\rangle = 1\,. \tag{6.16}$$

From the above, we conclude that

$$\langle x|x'\rangle = \delta\left(x - x'\right)\,. \tag{6.17}$$

The analysis we made above is generic and it applies to general operators with a continuum spectrum of eigenvalues. We summarize below our conclusions, highlighting the correspondence to the discrete case. For a Hermitian operator Ξ with eigenstates $|\xi\rangle$ and eigenvalues ξ

$$\Xi\,|\xi\rangle = \xi\,|\xi\rangle\,, \tag{6.18}$$

where ξ is a continuous variable, we have

Discrete	Continuous
Kronecker δ_{ij}	Dirac $\delta(\xi - \xi')$
$\langle i\|j\rangle = \delta_{ij}$	$\langle \xi\|\xi'\rangle = \delta(\xi - \xi')$
$\|\psi\rangle = \sum_i \|i\rangle \langle i\|\psi\rangle$	$\|\psi\rangle = \int \mathrm{d}\xi \ \|\xi\rangle \langle \xi\|\psi\rangle$
$\sum_i P(\|\psi\rangle \to \|\xi_i\rangle) = 1$	$\int d\xi \, dP(\xi) = \int d\xi \ \|\langle \xi\|\psi\rangle\|^2 = 1$

6.2 Position operator and eigenstates

Let us now discuss position states in a three-dimensional space. We define hermitian position operators $\hat{x}, \hat{y}, \hat{z}$ which commute with each other:

$$[\hat{x}, \hat{y}] = [\hat{y}, \hat{z}] = [\hat{z}, \hat{x}] = 0. \tag{6.19}$$

The vanishing commutators correspond to the physical requirement that all position coordinates of a particle can, in principle, be measured simultaneously without an uncertainty (in the sense of a quantum uncertainty principle). These operators have a common set of eigenstates, $|x, y, z\rangle$, with

$$\begin{aligned} \hat{x}\,|x, y, z\rangle &= x\,|x, y, z\rangle \\ \hat{y}\,|x, y, z\rangle &= y\,|x, y, z\rangle \\ \hat{z}\,|x, y, z\rangle &= z\,|x, y, z\rangle \end{aligned} \tag{6.20}$$

We identify the eigenvalues x, y, z with the positions in the $x-, y-, z-$directions accordingly. Employing a compact notation, we can write

$$|\mathbf{r}\rangle \equiv |x, y, z\rangle \,. \tag{6.21}$$

Also, when there is no risk of confusion of the position operators and their eigenstates, we may drop the $\hat{}$ notation for the operators.

The eigenstates of the position operator

$$\hat{\mathbf{r}}\,|\mathbf{r}\rangle = \mathbf{r}\,|\mathbf{r}\rangle$$

are orthonormal

$$\langle \mathbf{r}_1|\mathbf{r}_2\rangle = \delta^{(3)}(\mathbf{r}_1 - \mathbf{r}_2)$$

and form a complete basis such that every other one-particle state can be written as a superposition

$$|\phi\rangle = \int \mathrm{d}^3\mathbf{r} \ |\mathbf{r}\rangle \langle \mathbf{r}|\phi\rangle \ . \tag{6.22}$$

A quantum state $|\phi\rangle$ can be expressed as a superposition of position eigenstates.

$$|\phi\rangle = \int \mathrm{d}^3\mathbf{r}\ |\mathbf{r}\rangle\,\langle\mathbf{r}|\phi\rangle\,. \tag{6.23}$$

An experimental measurement of the position will collapse a general state $|\phi\rangle$ to a state $|\mathbf{r}\rangle$:

$$|\phi\rangle \longrightarrow |\mathbf{r}\rangle$$

with a probability density amplitude $\langle\mathbf{r}|\phi\rangle$. This amplitude is the wavefunction. The probability for a transition to a infinitesimal volume $\mathrm{d}^3\mathbf{r}$ around the position $\mathbf{r}$ is

$$P\left(|\phi\rangle \to (\ \mathrm{d}^3\mathbf{r} \text{ around } \mathbf{r})\right) = \mathrm{d}^3\mathbf{r}\ \left|\langle\mathbf{r}|\phi\rangle\right|^2\,. \tag{6.24}$$

A description of quantum states in terms of wave-functions corresponds to a representation of quantum states in the basis of eigenstates of the position operator. Although important, the position operator and the wavefunction representation are not more special than other operators and the representations of Hilberts space states that they furnish. However, traditionally, many of the results of quantum mechanics have been worked out in the position representation first. For example, scalar products of quantum states are

$$\begin{aligned} \langle a|b\rangle &= \int \mathrm{d}^3\mathbf{r}\ \langle a|\mathbf{r}\rangle\,\langle\mathbf{r}|b\rangle \\ \rightsquigarrow \langle a|b\rangle &= \int \mathrm{d}^3\mathbf{r}\ \psi_a^*(\mathbf{r})\psi_b(\mathbf{r}). \end{aligned} \tag{6.25}$$

6.3 Momentum operator and eigenstates

As for the position operators, we have hermitian operators for the components of the momentum which commute among each other,

$$[\hat{p}_x, \hat{p}_y] = [\hat{p}_y, \hat{p}_z] = [\hat{p}_z, \hat{p}_x] = 0. \tag{6.26}$$

The vanishing commutators originate from the physical requirement that all momenta components of a particle can, in principle, be measured simultaneously without an uncertainty (in the sense of a quantum uncertainty principle). These operators have a common set of eigenstates, $|x, y, z\rangle$, with

$$\begin{aligned} \hat{p}_x\,|p_x, p_y, p_z\rangle &= p_x\,|p_x, p_y, p_z\rangle \\ \hat{p}_y\,|p_x, p_y, p_z\rangle &= p_y\,|p_x, p_y, p_z\rangle \\ \hat{p}_z\,|p_x, p_y, p_z\rangle &= p_z\,|p_x, p_y, p_z\rangle \end{aligned} \tag{6.27}$$

We identify the eigenvalues p_x, p_y, p_z with the momenta in the $x-, y-, z-$directions accordingly. Employing a compact notation, we can write

$$|\mathbf{p}\rangle \equiv |p_x, p_y, p_z\rangle \,. \tag{6.28}$$

The three eigenvalue equations of Eq. (6.27) take the compact form,

$$\hat{\mathbf{p}}\,|\mathbf{p}\rangle = \mathbf{p}\,|\mathbf{p}\rangle \ . \tag{6.29}$$

As we have seen in Section 4.2, the link of quantum and classical mechanics requires that the position and momentum components in a certain direction do not commute. We repeat here the complete set of position and momentum commutators,

$$[\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0\,, \quad [\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}\,. \tag{6.30}$$

The above commutation relations imply, from the uncertainty principle of Eq. (3.65), that the position and the momentum components in a certain direction for a quantum system in a state $|\psi\rangle$ cannot be measured with infinite precision,

$$(\Delta x)\,(\Delta p_x) \geq \frac{|\langle\psi|\,[x, p_x]\,|\psi\rangle|}{2} = \frac{|\langle\psi|\psi\rangle\ i\hbar|}{2} = \frac{\hbar}{2}\,. \tag{6.31}$$

6.4 Translation operator

The position-momentum commutation relations of Eqs. (6.30) gift the quantum mechanical operator of momentum with the property of generating space translations on the Hilbert space of quantum systems. To see that, let us define an operator

$$\hat{P}(\Delta\mathbf{x}) = 1 - \frac{i}{\hbar}\hat{\mathbf{p}}\cdot\Delta\mathbf{x} \tag{6.32}$$

where $\boldsymbol{\Delta x}$ is a vector corresponding to a space interval. The commutator of the operator $\hat{P}$ and a position operator is,

$$\begin{aligned}\left[\hat{x}, \hat{P}(\Delta\mathbf{x})\right] &= -\frac{i}{\hbar}\,[\hat{x}, \hat{\mathbf{p}}\cdot\Delta\mathbf{x}] \\ &= -\frac{i}{\hbar}\,([\hat{x}, \hat{p}_x]\,\Delta x + [\hat{x}, \hat{p}_y]\,\Delta y + [\hat{x}, \hat{p}_z]\,\Delta z) \\ &= \Delta x. \end{aligned} \tag{6.33}$$

Collectively, for the commutators with all three position operators, we obtain,

$$\left[\hat{\mathbf{r}}, \hat{P}(\Delta\mathbf{x})\right] = \Delta\mathbf{x}. \tag{6.34}$$

Let us now consider the state

$$|\mathbf{x}'\rangle \equiv \hat{P}(\Delta\mathbf{x})\,|\mathbf{x}\rangle\,. \tag{6.35}$$

Probing it with a position operator, we have

$$\begin{aligned}
\hat{\mathbf{r}}\,|\mathbf{x}'\rangle &= \hat{\mathbf{r}}\hat{P}(\Delta\mathbf{x})\,|\mathbf{x}\rangle \\
&= \left[\hat{\mathbf{r}}, \hat{P}(\Delta\mathbf{x})\right]|\mathbf{x}\rangle + \hat{P}(\Delta\mathbf{x})\hat{\mathbf{r}}\,|\mathbf{x}\rangle \\
&= \Delta\mathbf{x}\,|\mathbf{x}\rangle + \hat{P}(\Delta\mathbf{x})\,\mathbf{x}\,|\mathbf{x}\rangle \\
&= (\mathbf{x}+\Delta\mathbf{x})\;\hat{P}(\Delta\mathbf{x})\;|\mathbf{x}\rangle + \Delta\mathbf{x}\frac{i}{\hbar}\hat{\mathbf{p}}\cdot\Delta\mathbf{x}
\end{aligned} \tag{6.36}$$

Let us now specialise to small intervals, $\Delta x = \delta\mathbf{r} \to 0$. Then, the second term in the last equality is of order $\mathcal{O}\left((\delta r)^2\right)$ and can be ignored. Thus, for infinitesimal δr, we write

$$\hat{\mathbf{r}}\,\left(\hat{P}(\delta\mathbf{r})\,|\mathbf{x}\rangle\right) = (\mathbf{x}+\delta\mathbf{r})\;\left(\hat{P}(\delta\mathbf{r})\;|\mathbf{x}\rangle\right) \tag{6.37}$$

This is an eigenvalue equation for the position operator, and we can identify $\hat{P}(\delta\mathbf{r})\;|\mathbf{x}\rangle$ as the position eigenstate with an eigenvalue $(\mathbf{x}+\delta\mathbf{r})$/ We write,

$$\hat{P}(\delta\mathbf{r})\;|\mathbf{x}\rangle = |\mathbf{x}+\delta\mathbf{r}\rangle\;. \tag{6.38}$$

In summary, the operator

$$P(\delta\mathbf{r}) = 1 - \frac{i\mathbf{p}\cdot\delta\mathbf{r}}{\hbar}\,, \tag{6.39}$$

where $\mathbf{p}$ is the momentum operator, is a space translation operator for small intervals $\delta\mathbf{r}$. To perform a large translation $\mathbf{r}_B - \mathbf{r}_A$ from a point A to a point B we divide the translation into infinitesimally small steps,

$$\frac{\mathbf{r}_B - \mathbf{r}_A}{N} = \delta\mathbf{r}, \quad N \to \infty \tag{6.40}$$

and perform an infinite number of very small translations $\delta\mathbf{r}$ in succession:

$$\begin{aligned}
|\mathbf{x} + \mathbf{r}_B - \mathbf{r}_A\rangle &= P(\delta\mathbf{r})^N \\
&= \lim_{N\to\infty}\left(1 - \frac{i\mathbf{p}\cdot\delta\mathbf{r}}{\hbar}\right)^N |\mathbf{x}\rangle \\
&= \lim_{N\to\infty}\left(1 - \frac{i\mathbf{p}\cdot(\mathbf{r}_A - \mathbf{r}_B)}{N\,\hbar}\right)^N |\mathbf{x}\rangle
\end{aligned}$$

which leads to,

$$|\mathbf{x} + \mathbf{r}_B - \mathbf{r}_A\rangle = U(\mathbf{r}_B - \mathbf{r}_A)\,|\mathbf{x}\rangle\,, \tag{6.41}$$

with

$$U(\mathbf{r}) = e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}}\,. \tag{6.42}$$

The exponential of an operator is defined as usual through its Taylor series expansion at all orders,

$$e^X = \sum_{n=0}^{\infty} \frac{X^n}{n!}\,.$$

Due to the hermiticity of the momentum operator, we have that

$$U^\dagger(\mathbf{r})U(\mathbf{r}) = \mathbf{1}\,, \tag{6.43}$$

and the physically intuitive result that

$$U^{-1}(\mathbf{r}) = U(-\mathbf{r})\,. \tag{6.44}$$

6.5 Representation of momentum in position space

Let's act with a small translation operator on an arbitrary state $|a\rangle$

$$\begin{aligned}\left(1 - \frac{i\hat{\mathbf{p}}\cdot\delta\mathbf{r}}{\hbar}\right)|a\rangle &= \left(1 - \frac{i\hat{\mathbf{p}}\cdot\delta\mathbf{r}}{\hbar}\right)\int \mathrm{d}^3\mathbf{x}\;|\mathbf{x}\rangle\,\langle\mathbf{x}|a\rangle \\ &= \int \mathrm{d}^3\mathbf{x}\;|\mathbf{x}+\delta\mathbf{r}\rangle\,\langle\mathbf{x}|a\rangle \\ &= \int \mathrm{d}^3\mathbf{x}\;|\mathbf{x}\rangle\,\langle\mathbf{x}-\delta\mathbf{r}|a\rangle\end{aligned}$$

For small displacements, we can expand up to linear terms in $\delta\mathbf{r}$:

$$\langle\mathbf{x}-\delta\mathbf{r}|a\rangle = \langle\mathbf{x}|a\rangle - \delta\mathbf{r}\cdot\nabla\,\langle\mathbf{x}|a\rangle$$

Substituting above, we have

$$\begin{aligned}\left(1 - \frac{i\hat{\mathbf{p}}\cdot\delta\mathbf{r}}{\hbar}\right)|a\rangle &= \int \mathrm{d}^3\mathbf{x}\;|\mathbf{x}\rangle\,\langle\mathbf{x}|a\rangle - \int \mathrm{d}^3\mathbf{x}\;|\mathbf{x}\rangle\,(\delta\mathbf{r}\cdot\nabla)\,\langle\mathbf{x}|a\rangle \\ &= |a\rangle - \int \mathrm{d}^3\mathbf{x}\;|\mathbf{x}\rangle\,(\delta\mathbf{r}\cdot\nabla)\,\langle\mathbf{x}|a\rangle\end{aligned}$$

Comparing the two sides of the equation, we have

$$\hat{\mathbf{p}}\,|a\rangle = \int \mathrm{d}^3\mathbf{x}\;|\mathbf{x}\rangle\,[-i\hbar\nabla]\,\langle\mathbf{x}|a\rangle \tag{6.45}$$

and,

$$\begin{aligned}\langle \mathbf{r}| \hat{\mathbf{p}} |a\rangle &= \int \mathrm{d}^3\mathbf{x}\ \langle \mathbf{r}|\mathbf{x}\rangle \left[-i\hbar\nabla\right] \langle \mathbf{x}|a\rangle \\ &= \int \mathrm{d}^3\mathbf{x}\ \delta\left(\mathbf{r}-\mathbf{x}\right) \left[-i\hbar\nabla\right] \langle \mathbf{x}|a\rangle\end{aligned} \tag{6.46}$$

which leads to

$$\langle \mathbf{r}| \hat{\mathbf{p}} |a\rangle = \left[-i\hbar\nabla_{\mathbf{r}}\right] \langle \mathbf{r}|a\rangle\,. \tag{6.47}$$

Finally, we obtain the representation of the momentum operator in the position-ket basis by setting $|a\rangle = |\mathbf{r}'\rangle$, a position eigenstate,

$$\langle \mathbf{r}| \hat{\mathbf{p}} |\mathbf{r}'\rangle = \left[-i\hbar\nabla_{\mathbf{r}}\right] \langle \mathbf{r}|\mathbf{r}'\rangle\,, \tag{6.48}$$

we find

$$\langle \mathbf{r}| \hat{\mathbf{p}} |\mathbf{r}'\rangle = \left[-i\hbar\nabla_{\mathbf{r}}\right] \delta\left(\mathbf{r}-\mathbf{r}'\right)\,. \tag{6.49}$$

6.6 Eigenstates of the momentum operator

The eigenstates of the momentum operator satisfy:

$$\hat{\mathbf{p}} |\mathbf{p}\rangle = \mathbf{p} |\mathbf{p}\rangle \tag{6.50}$$

with

$$\langle \mathbf{p}_1|\mathbf{p}_2\rangle = \delta^{(3)}\left(\mathbf{p}_1-\mathbf{p}_2\right)\,. \tag{6.51}$$

The probability that a particle with a momentum $\mathbf{p}$ is found at a position $\mathbf{x}$ is

$$\langle \mathbf{x}|\mathbf{p}\rangle\,.$$

Consider

$$\langle \mathbf{x}| \hat{\mathbf{p}} |\mathbf{p}\rangle = \mathbf{p}\,\langle \mathbf{x}|\mathbf{p}\rangle\,,$$

but also, from the previous section,

$$\langle \mathbf{x}| \hat{\mathbf{p}} |\mathbf{p}\rangle = -i\hbar\nabla\,\langle \mathbf{x}|\mathbf{p}\rangle\,.$$

We have then derived the following differential equation for the requested probability amplitude:

$$-i\hbar\nabla\,\langle \mathbf{x}|\mathbf{p}\rangle = \mathbf{p}\,\langle \mathbf{x}|\mathbf{p}\rangle \tag{6.52}$$

which has a solution

$$\langle \mathbf{x}|\mathbf{p}\rangle = Ne^{\frac{i\mathbf{p}\cdot\mathbf{x}}{\hbar}} \tag{6.53}$$

We compute the normalisation constant as follows:

$$\begin{aligned}\delta^{(3)}(\mathbf{x}-\mathbf{y}) = \langle \mathbf{x}|\mathbf{y}\rangle &= \int \mathrm{d}^3\mathbf{p}\ \langle \mathbf{x}|\mathbf{p}\rangle \langle \mathbf{p}|\mathbf{y}\rangle = \int \mathrm{d}^3\mathbf{p}\ \langle \mathbf{x}|\mathbf{p}\rangle \langle \mathbf{y}|\mathbf{p}\rangle^* \\ &= |N|^2 \int \mathrm{d}^3\mathbf{p}\ e^{i\frac{\mathbf{p}}{\hbar}(\mathbf{x}-\mathbf{y})} = |N|^2 (2\pi\hbar)^3 \delta^{(3)}(\mathbf{x}-\mathbf{y}) \\ \rightsquigarrow |N| &= \frac{1}{(2\pi\hbar)^{3/2}}.\end{aligned}$$

Thus, we can write

$$\langle \mathbf{x}|\mathbf{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}}. \tag{6.54}$$

6.6.1 Position and momentum wave-functions

Let's assume that a particle is in a state $|\phi\rangle$. The probability amplitudes for finding the particle at a position $\mathbf{x}$ or to have a momentum $\mathbf{p}$ are given by the position and momentum wave functions

$$\langle \mathbf{x}|\phi\rangle\,, \quad \langle \mathbf{p}|\phi\rangle$$

respectively. The two amplitudes are related by a Fourier transformation. Indeed,

$$\begin{aligned}\langle \mathbf{x}|\phi\rangle &= \int_{-\infty}^{+\infty} \mathrm{d}^3\mathbf{p}\ \langle \mathbf{x}|\mathbf{p}\rangle \langle \mathbf{p}|\phi\rangle \\ &= \int_{-\infty}^{+\infty} \frac{\mathrm{d}^3\mathbf{p}}{(2\pi\hbar)^{(3/2)}} e^{i\frac{\mathbf{p}}{\hbar}\cdot\mathbf{x}} \langle \mathbf{p}|\phi\rangle\,.\end{aligned} \tag{6.55}$$

Similarly,

$$\begin{aligned}\langle \mathbf{p}|\phi\rangle &= \int_{-\infty}^{+\infty} \mathrm{d}^3\mathbf{x}\ \langle \mathbf{p}|\mathbf{x}\rangle \langle \mathbf{x}|\phi\rangle \\ &= \int_{-\infty}^{+\infty} \frac{\mathrm{d}^3\mathbf{x}}{(2\pi\hbar)^{(3/2)}} e^{-i\frac{\mathbf{x}}{\hbar}\cdot\mathbf{p}} \langle \mathbf{x}|\phi\rangle\,.\end{aligned} \tag{6.56}$$

Chapter 7

The harmonic oscillator

A very simple system in quantum mechanics, which we can solve exactly, is the harmonic oscillator in one space dimension. The Hamiltonian of the oscillator in classical physics is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2, \tag{7.1}$$

where m is the mass of the oscillaing particle and ω the angular frequency of the oscillation. For convenience, we shall set

$$m = \hbar = \omega = 1$$

in this chapter. It will always be easy to recover the full dependence on these parameters with dimensional analysis.

7.1 Quantization

We quantize the harmonic oscillator by promoting the coordinate x and momentum p to operators, satisfying the commutation relation

$$[x, p] = i. \tag{7.2}$$

The Hamiltonian can be cast as

$$H = \frac{(x - ip)}{\sqrt{2}}\frac{(x + ip)}{\sqrt{2}} - i\frac{xp - px}{2}, \tag{7.3}$$

and using the commutation relation above,

$$H = a^\dagger a + \frac{1}{2}, \tag{7.4}$$

with

$$a = \frac{x + ip}{\sqrt{2}}\,, \quad a^\dagger = \frac{x - ip}{\sqrt{2}}\,. \tag{7.5}$$

For reasons to become clear later, the $a, a^\dagger$ operators are called *annihilation* and *creation* operators respectively. Their commutator is

$$\begin{aligned}\left[a, a^\dagger\right] &= \left[\frac{x+ip}{\sqrt{2}}, \frac{x-ip}{\sqrt{2}}\right] = \frac{1}{2}\left([x,-ip]+[ip,x]\right) = -i\,[x,p] \\ &= 1\,.\end{aligned}$$

Exercise 7.1. *Prove that for the operators A, B, C,*

$$[AB, C] = [A, C]\,B + A\,[B, C]\,.$$

We define the so-called *number operator*

$$N \equiv a^\dagger a. \tag{7.6}$$

The commutators of the number operator and the creation or annihilation operators are

$$\left[N, a^\dagger\right] = \left[a^\dagger a, a^\dagger\right] = a^\dagger\left[a, a^\dagger\right] = a^\dagger \tag{7.7}$$

and

$$[N, a] = \left[a^\dagger a, a\right] = \left[a^\dagger, a\right] a = -a. \tag{7.8}$$

The Hamiltonian $H = N + \frac{1}{2}$ and the number operator have common eigenstates $|n\rangle$, since they commute.
If $|n\rangle$ is such an eigenstate with an eigenvalue n,

$$N\,|n\rangle = n\,|n\rangle\,, \tag{7.9}$$

the eigenvalue n cannot be negative. Indeed,

$$0 \le |a\,|n\rangle|^2 = \langle n|\,a^\dagger a\,|n\rangle = \langle n|\,N\,|n\rangle = n. \tag{7.10}$$

Also, the states $a^\dagger\,|n\rangle$ and $a\,|n\rangle$ are eigenstates of N with eigenvalues $n+1$ and $n-1$ respectively:

$$\begin{aligned} N\left(a^\dagger\,|n\rangle\right) &= \left(\left[N, a^\dagger\right] + a^\dagger N\right)|n\rangle = \left(a^\dagger + a^\dagger n\right)|n\rangle \\ &= (n+1)\left(a^\dagger\,|n\rangle\right), \end{aligned} \tag{7.11a}$$

$$\begin{aligned} N\left(a\,|n\rangle\right) &= \left([N, a] + aN\right)|n\rangle = \left(-a + an\right)|n\rangle \\ &= (n-1)\left(a\,|n\rangle\right). \end{aligned} \tag{7.11b}$$

Thus

$$a\,|n\rangle = c_n\,|n-1\rangle\,, \quad a^\dagger\,|n\rangle = d_n\,|n+1\rangle\,.$$

We can fix the normalization factors c_n, d_n by requiring that the states $|n\rangle$ have a unit norm.

$$\begin{aligned} 1 = \langle n+1|n+1\rangle &= \frac{\langle n|\, aa^\dagger\, |n\rangle}{|d_n|^2} = \frac{\langle n|\, [a,a^\dagger] + a^\dagger a\, |n\rangle}{|d_n|^2} \\ &= \frac{\langle n|\, 1+N\, |n\rangle}{|d_n|^2} = \frac{1+n}{|d_n|^2}. \end{aligned} \tag{7.12a}$$

Similarly,

$$\begin{aligned} 1 = \langle n-1|n-1\rangle &= \frac{\langle n|\, a^\dagger a\, |n\rangle}{|c_n|^2} = \frac{\langle n|\, N\, |n\rangle}{|c_n|^2} \\ &= \frac{n}{|c_n|^2}\,. \end{aligned} \tag{7.12b}$$

We can choose $c_n = \sqrt{n}$ and $d_n = \sqrt{n+1}$. We these choices, we have

$$a^\dagger\, |n\rangle = \sqrt{n+1}\, |n+1\rangle\,, \tag{7.13a}$$

and

$$a\, |n\rangle = \sqrt{n}\, |n-1\rangle\,. \tag{7.13b}$$

Notice that for n non-integer, the repeated application of the last equation leads eventually to an eigenstate with a negative eigenvalue, which is inconsistent with the requirement $n \geq 0$. The only allowed values of n, are non-negative integers. Notice that the coefficient in the lhs of Eq. 7.13b vanishes for $n = 0$, thus preventing to obtain a state $|-1\rangle$ with a negative eigenvalue. The spectrum of eigenvalues for the number operator and the Hamiltonian is discrete (quantized) with

$$n = 0, 1, 2, 3, \ldots$$

and energy eigenvalues

$$E_n = n + \frac{1}{2}. \tag{7.14}$$

The eigenstates can all be generated from the "ground" state $|0\rangle$ by a repeated

application of the creation operator:

$$\begin{aligned} |1\rangle &= a^\dagger |0\rangle \\ |2\rangle &= \frac{{a^\dagger}^2}{\sqrt{2!}} |0\rangle \\ &\vdots \\ |n\rangle &= \frac{{a^\dagger}^n}{\sqrt{n!}} |0\rangle \\ &\vdots \end{aligned}$$

Let's focus on the ground state for which we shall compute the expecation values

$$\langle x\rangle, \langle p\rangle, \langle x^2\rangle, \langle p^2\rangle.$$

We recall that

$$a = \frac{x+ip}{\sqrt{2}}, \quad a^\dagger = \frac{x-ip}{\sqrt{2}},$$

which, by inverting, yield

$$x = \frac{a+a^\dagger}{\sqrt{2}}, \quad p = \frac{a-a^\dagger}{\sqrt{2}i}. \tag{7.15}$$

We shall need that

$$a|0\rangle = 0, \quad \langle 0| a^\dagger = 0,$$

and

$$aa^\dagger |0\rangle = \underbrace{\left[a, a^\dagger\right]}_{1} |0\rangle + a^\dagger \underbrace{a|0\rangle}_{0} = |0\rangle$$

It is then easy to compute that

$$\langle 0| x |0\rangle = \langle 0| p |0\rangle = 0, \tag{7.16}$$

and

$$\langle 0| x^2 |0\rangle = \langle 0| p^2 |0\rangle = \frac{1}{2}. \tag{7.17}$$

In the ground state, the product of the uncertainties in position and momentum is therefore minimal:

$$\left\langle (\Delta x)^2 \right\rangle \left\langle (\Delta p)^2 \right\rangle = \frac{1}{4}$$

Exercise 7.2. *Show that for the $|n\rangle$ state, the product of uncertainties is*

$$\left\langle (\Delta x)^2 \right\rangle_n \left\langle (\Delta p)^2 \right\rangle_n = \left(n + \frac{1}{2} \right)^2 . \tag{7.18}$$

We shall now determine the wave function in the ground state:

$$\psi_0(x) \equiv \langle x|0\rangle ,$$

where

$$\hat{x}\,|x\rangle = x\,|x\rangle$$

and

$$a\,|0\rangle = 0.$$

We have

$$\begin{aligned} 0 = \langle x|\, a\,|0\rangle = \langle x|\, \frac{\hat{x} + i\hat{p}}{\sqrt{2}}\,|0\rangle = \frac{x}{\sqrt{2}}\,\langle x|0\rangle + \frac{i}{\sqrt{2}}\,\langle x|\,\hat{p}\,|0\rangle \\ = \frac{x}{\sqrt{2}}\,\langle x|0\rangle + \frac{i}{\sqrt{2}} \left(-i \frac{\mathrm{d}}{\mathrm{d}x} \right) \langle x|0\rangle . \end{aligned} \tag{7.19}$$

We have thus derived the following differential equation for the wave-function in the ground state:

$$\left(x + \frac{\mathrm{d}}{\mathrm{d}x} \right) \psi_0(x) = 0 . \tag{7.20}$$

The solution of the above is

$$\psi_0(x) = A e^{-\frac{x^2}{2}} . \tag{7.21}$$

We can fix the normalization by requiring,

$$\begin{aligned} 1 = \langle 0|0\rangle = \int_{-\infty}^{\infty} \langle 0|x\rangle\,\langle x|0\rangle = \int_{-\infty}^{\infty} \mathrm{d}x\ |\psi_0(x)|^2 \\ = |A|^2 \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-x^2} \\ \rightsquigarrow |A| = \left(\int_{-\infty}^{\infty} \mathrm{d}x\, e^{-x^2} \right)^{-1/2} . \end{aligned} \tag{7.22}$$

The integral is

$$I = \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-x^2} = \sqrt{\pi},$$

We obtain this result as follows:

$$I^2 = \left(\int_{-\infty}^{\infty} \mathrm{d}x\, e^{-x^2}\right)^2 = \int_{-\infty}^{\infty} \mathrm{d}x\mathrm{d}y\, e^{-x^2-y^2}\,, \tag{7.23}$$

subistituting $x = r\cos\theta, y = r\sin\theta$ gives

$$\begin{aligned} I^2 &= \int_0^{\infty} \mathrm{d}r\, re^{-r^2} \int_0^{2\pi} \mathrm{d}\theta = 2\pi \int_0^{\infty} \mathrm{d}r\, re^{-r^2} = 2\pi \int_0^{\infty} \mathrm{d}r\, \frac{-1}{2}\frac{\mathrm{d}}{\mathrm{d}r} e^{-r^2} \\ &= -\pi\, e^{-r^2}\Big|_{r=0}^{\infty} = \pi\,. \end{aligned} \tag{7.24}$$

We thus have that

$$\langle x|0\rangle = \frac{1}{\pi^{1/4}} e^{-x^2/2}. \tag{7.25}$$

We compute the wave-functions of all energy eigenstates recursively.

$$\begin{aligned} \langle x|n\rangle &= \langle x|\, \frac{a^\dagger}{\sqrt{n}}\, |n-1\rangle \\ &= \frac{1}{\sqrt{n}} \int \mathrm{d}y\ \langle x|\, a^\dagger\, |y\rangle\, \langle y|n-1\rangle \\ &= \frac{1}{\sqrt{2n}} \int \mathrm{d}y\ \langle x|\, x - ip\, |y\rangle\, \langle y|n-1\rangle \\ &= \frac{1}{\sqrt{2n}} \left(x - \frac{\mathrm{d}}{\mathrm{d}x}\right) \langle x|n-1\rangle\,. \end{aligned} \tag{7.26}$$

Iterating, we obtain

$$\langle x|n\rangle = \frac{1}{\sqrt{2^n n!}} \left(x - \frac{\mathrm{d}}{\mathrm{d}x}\right)^n \langle x|0\rangle \tag{7.27}$$

The solutions for $n = 0, 1, 2, 3$ can be seen in Fig. 7.1.

7.2 Time evolution

We now consider the position and momentum operators in the Heisenberg picture. They satisfy the Heisenberg equations of motion (remember $\hbar = 1$)

$$\begin{aligned} i\frac{\partial}{\partial t} x &= [x, H] = \left[x, \frac{x^2+p^2}{2}\right] = \left[x, \frac{p^2}{2}\right] = [x,p]\,\frac{p}{2} + \frac{p}{2}\,[x,p] \\ &= ip\,. \end{aligned} \tag{7.28}$$

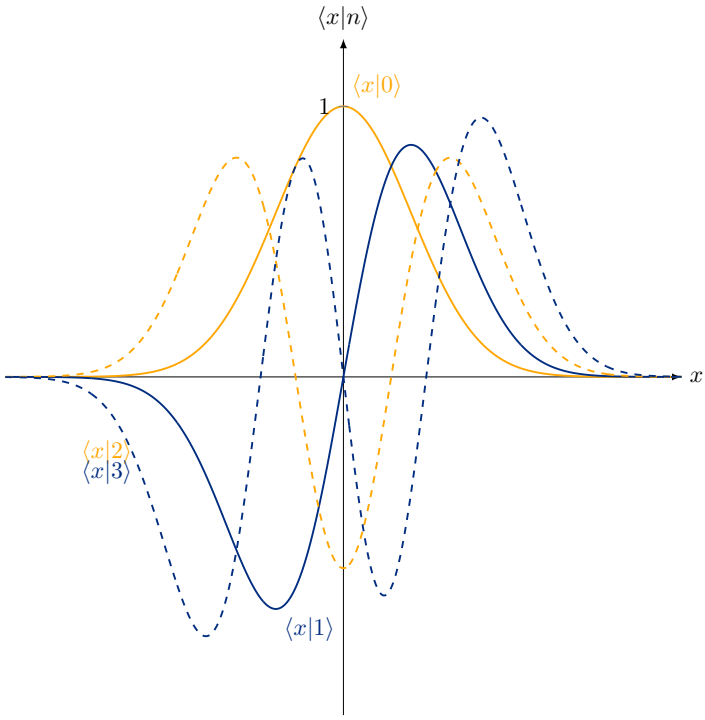


Figure 7.1: The wavefunctions of the energy levels $n = 0, 1, 2, 3$ of the quantum harmonic oscillator.

Similarly,

$$i\frac{\partial}{\partial t}p = [p, H] = \left[p, \frac{x^2+p^2}{2}\right] = \left[p, \frac{x^2}{2}\right] = [p, x]\,\frac{x}{2} + \frac{x}{2}\,[p, x] \qquad (7.29)$$
$$= -ix\,,$$

with

$$[A, BC] = [A, B]\,C + B\,[A, C]\,. \qquad (7.30)$$

Thus

$$\frac{\partial x(t)}{\partial t} = p(t)\,, \qquad \frac{\partial p(t)}{\partial t} = -x(t)\,. \qquad (7.31)$$

The solution of these equations is

$$x(t) = x(0)\cos t + p(0)\sin t \tag{7.32a}$$
$$p(t) = -x(0)\sin t + p(0)\cos t \tag{7.32b}$$

The above are all operator equations. Notice that for any energy eigenstate, the expectation values of the momentum and position operators vanish. Indeed,

$$\langle n|\, a^\dagger \,|n\rangle = \langle n|\, a \,|n\rangle = 0 \tag{7.33}$$

and

$$x(0) = \frac{a + a^\dagger}{\sqrt{2}}\,, \quad p(0) = \frac{a - a^\dagger}{\sqrt{2}i} \tag{7.34}$$

and therefore,

$$\langle n|\, x(t) \,|n\rangle = \langle n|\, p(t) \,|n\rangle = 0\,. \tag{7.35}$$

Unlike the position and momentum of a classical harmonic oscillator, the expectation values of their analogue quantum operators do not oscillate in an energy eigenstate.

7.3 Coherent states

Are there quantum states in which the expectation values of the position and momentum operators oscillate as in the classical system? Yes. These states are called coherent states. Consider a state $|\lambda\rangle$ which is an eigenstate of the annihilation operator a:

$$a\,|\lambda\rangle = \lambda\,|\lambda\rangle\,. \tag{7.36}$$

We can write a coherent state as a superposition of energy eigenstates:

$$|\lambda\rangle = \sum_{n=0}^{\infty} f(n)\,|n\rangle\,. \tag{7.37}$$

Then

$$\begin{aligned} a\,|\lambda\rangle &= \sum_{n=1}^{\infty} f(n)\sqrt{n}\,|n-1\rangle \\ &= \sum_{n=0}^{\infty} f(n+1)\sqrt{n+1}\,|n\rangle \end{aligned}$$

Substituting into Eq. 7.36 we find:

$$\sum_{n=0}^{\infty} \left[f(n+1)\sqrt{n+1} - \lambda f(n) \right] |n\rangle = 0. \tag{7.38}$$

Since the set of $|n\rangle$ eigenstates is a complete basis of Hilbert space, we must have the recurrence identity:

$$f(\ell+1) = f(\ell)\frac{\lambda}{\sqrt{1+\ell}}, \quad \ell = 0, 1, 2, \ldots \tag{7.39}$$

We can solve this recurrence identity easily:

$$\begin{aligned} \prod_{i=0}^{n-1} f(\ell+1) &= \prod_{\ell=0}^{n-1} f(\ell)\frac{\lambda}{\sqrt{1+\ell}} \\ \rightsquigarrow f(n)\left(\prod_{\ell=1}^{n-1} f(\ell)\right) &= f(0)\left(\prod_{\ell=1}^{n-1} f(\ell)\right)\frac{\lambda^n}{\sqrt{n!}} \\ \rightsquigarrow f(n) &= f(0)\frac{\lambda^n}{\sqrt{n!}}\,. \end{aligned} \tag{7.40}$$

Therefore, the coherent state $|\lambda\rangle$ is

$$|\lambda\rangle = f(0)\sum_{n=0}^{\infty}\frac{\lambda^n}{\sqrt{n!}}|n\rangle\,. \tag{7.41}$$

We fix the constant $f(0)$ by normalizing the state

$$\begin{aligned} 1 = \langle\lambda|\lambda\rangle &= |f(0)|^2 \sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{\lambda^n}{\sqrt{n!}}\frac{(\lambda^*)^m}{\sqrt{m!}}\langle m|n\rangle \\ &= |f(0)|^2 \sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{\lambda^n}{\sqrt{n!}}\frac{(\lambda^*)^m}{\sqrt{m!}}\delta_{nm} \\ &= |f(0)|^2 \sum_{n=0}^{\infty}\frac{(|\lambda|^2)^n}{n!} \\ &= |f(0)|^2 e^{|\lambda|^2} \\ \rightsquigarrow f(0) &= e^{-|\lambda|^2/2} \end{aligned} \tag{7.42}$$

Therefore, the normalized coherent state takes the form (up to a choice of an overall phase):

$$|\lambda\rangle = e^{-|\lambda|^2/2}\sum_{n=0}^{\infty}\frac{\lambda^n}{\sqrt{n!}}|n\rangle\,. \tag{7.43}$$

The probability that a particle in a coherent state $|\lambda\rangle$ is measured to have an energy $E_n = n + \frac{1}{2}$ is,

$$P\left(|\lambda\rangle \to |n\rangle\right) = |\langle n|\lambda\rangle|^2 = e^{-|\lambda|^2} \frac{\left(|\lambda|^2\right)^n}{n!} \tag{7.44}$$

which is a Poisson distribution with a mean value

$$\begin{aligned} \langle n\rangle &= \langle\lambda| N |\lambda\rangle \\ &= |\lambda|^2 . \end{aligned} \tag{7.45}$$

Notice that for $\lambda = 0$ in Eq. 7.44 the coherent state becomes the ground state (first energy eigenstate) of the harmonic oscillator:

$$|\lambda = 0\rangle = |n = 0\rangle . \tag{7.46}$$

We can work further on Eq. 7.44,

$$\begin{aligned} |\lambda\rangle &= e^{-|\lambda|^2/2} \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{n!}} |n\rangle \\ &= e^{-|\lambda|^2/2} \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{n!}} \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle \\ &= e^{-|\lambda|^2/2} \left(\sum_{n=0}^{\infty} \frac{(\lambda a^\dagger)^n}{n!} \right) |0\rangle \end{aligned}$$

leading to

$$|\lambda\rangle = e^{-|\lambda|^2/2} e^{\lambda a^\dagger} |0\rangle . \tag{7.47}$$

The expectation value of the energy in a coherent state is:

$$\begin{aligned} \langle\lambda| H |\lambda\rangle &= \langle\lambda| a^\dagger a |\lambda\rangle + \langle\lambda| \frac{1}{2} |\lambda\rangle \\ &= |a|\lambda\rangle|^2 + \frac{1}{2} \\ &= |\lambda|\lambda\rangle|^2 + \frac{1}{2} \\ \rightsquigarrow \langle\lambda| H |\lambda\rangle &= |\lambda|^2 + \frac{1}{2}. \end{aligned} \tag{7.48}$$

The expectation value of the position operator in a coherent state is:

$$\begin{aligned} \langle\lambda| x |\lambda\rangle &= \langle\lambda| \frac{a + a^\dagger}{\sqrt{2}} |\lambda\rangle \cos t + \langle\lambda| \frac{a - a^\dagger}{i\sqrt{2}} |\lambda\rangle \sin t \\ &= \frac{\lambda + \lambda^*}{\sqrt{2}} \cos t + \frac{\lambda - \lambda^*}{i\sqrt{2}} \sin t \end{aligned} \tag{7.49}$$

For

$$\lambda = |\lambda| \, e^{i\theta} = |\lambda| \, (\cos\theta + i \sin\theta) \, ,$$

we obtain:

$$\langle\lambda| \, x \, |\lambda\rangle = \sqrt{2} \, |\lambda| \cos(t - \theta). \tag{7.50}$$

The expectation value of the position in a coherent state oscillates exactly as the position in a classical harmonic oscillation with amplitude $\sqrt{2} \, |\lambda|$. Performing a similar computation, we find for the expectation value of the momentum:

$$\langle\lambda| \, p \, |\lambda\rangle = -\sqrt{2} \, |\lambda| \sin(t - \theta). \tag{7.51}$$

Carrying on to the second powers of the position and momentum operators we find (**exercise**) the following results:

$$\langle\lambda| \, x^2 \, |\lambda\rangle = \frac{1}{2} + 2 \, |\lambda|^2 \cos^2(t - \theta), \tag{7.52}$$

$$\langle\lambda| \, p^2 \, |\lambda\rangle = \frac{1}{2} + 2 \, |\lambda|^2 \sin^2(t - \theta), \tag{7.53}$$

For the uncertainties in position and momentum we have:

$$\left\langle (\Delta x)^2 \right\rangle = \langle\lambda| \, x^2 \, |\lambda\rangle - \langle\lambda| \, x \, |\lambda\rangle^2 = \frac{1}{2} \tag{7.54}$$

and

$$\left\langle (\Delta p)^2 \right\rangle = \langle\lambda| \, p^2 \, |\lambda\rangle - \langle\lambda| \, p \, |\lambda\rangle^2 = \frac{1}{2}. \tag{7.55}$$

The product of the uncertainties in position and momentum for a particle in a coherent state is therefore exactly the minimum allowed by Heisenberg's uncertainty principle:

$$\left\langle (\Delta x)^2 \right\rangle \left\langle (\Delta p)^2 \right\rangle = \frac{1}{4}. \tag{7.56}$$

Schrödinger's wave equation

Consider a particle in a quantum state $|\psi, t\rangle$ and subject to the Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}), \tag{8.1}$$

where $\mathbf{p}, \mathbf{r}$ are the position and momentum operators. The time evolution of the particle's state is determined by Schrödinger's equation,

$$i\hbar \frac{\partial}{\partial t} |\psi, t\rangle = H |\psi, t\rangle . \tag{8.2}$$

The traditional *Schrödinger's wave equation* is the application of the above to the position-representation of the state $|\psi, t\rangle$:

$$\psi(\mathbf{r}, t) = \langle \mathbf{r} | \psi, t \rangle ,$$

called the wave-function. We have:

$$\begin{aligned} \langle \mathbf{r}| \, i\hbar \frac{\partial}{\partial t} |\psi, t\rangle &= \langle \mathbf{r}| \, H \, |\psi, t\rangle \\ \rightsquigarrow i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) &= \langle \mathbf{r}| \, \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) \, |\psi, t\rangle \\ \rightsquigarrow i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) &= \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}, t) . \end{aligned} \tag{8.3}$$

Eq. 8.3 is Schrödinger's wave equation.

The time evolution of energy eigenstates is particularly simple for time-independent Hamiltonians.

$$H |\psi_E, t = 0\rangle = E |\psi_E, t = 0\rangle , \tag{8.4}$$

then

$$\begin{aligned} |\psi_E, t\rangle &= e^{-iEt/\hbar} |\psi_E, t = 0\rangle \\ \rightsquigarrow \langle \mathbf{r} | \psi_E, t\rangle &= e^{-iEt/\hbar} \langle \mathbf{r} | \psi_E, t = 0\rangle \\ \rightsquigarrow \psi_E(\mathbf{r}, t) &= e^{-iEt/\hbar} \psi_E(\mathbf{r}) \end{aligned} \tag{8.5}$$

Substituting into Eq. 8.3 we obtain:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi_E(\mathbf{r}) = E\psi_E(\mathbf{r}) \tag{8.6}$$

This is Schrödinger's time independent wave equation.

Exercise 8.1. *Solve Eq. 8.6 for the wavefunctions of the energy eigenstates of the harmonic oscillator.*

8.1 Probability density and probability current

Consider a particle in a state $|\psi, t\rangle$ at a time t. The probability amplitude that the particle is found at a position $\mathbf{r}$ is the wave-function:

$$\psi(\mathbf{r}, t) = \langle \mathbf{r}|\psi, t\rangle \,.$$

From the normalization of the state we have:

$$\begin{aligned} 1 = \langle\psi, t|\psi, t\rangle &= \int \mathrm{d}^3\mathbf{r}\ \langle\psi, t|\mathbf{r}\rangle \langle\mathbf{r}|\psi, t\rangle \\ &= \int \mathrm{d}^3\mathbf{r}\ |\psi(\mathbf{r}, t)|^2 \end{aligned} \tag{8.7}$$

We can interpret the quantity:

$$\rho(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2 \,, \tag{8.8}$$

as the probability density for the particle to be found at the position $\mathbf{r}$.
From the wave equation 8.3 of Schrödinger, we can derive

$$i\hbar\psi^*\partial_t\psi = -\frac{\hbar^2}{2m}\psi^*\nabla^2\psi + V(\mathbf{r})\,|\psi|^2 \tag{8.9}$$

$$i\hbar\psi\partial_t\psi^* = \frac{\hbar^2}{2m}\psi\nabla^2\psi^* - V(\mathbf{r})\,|\psi|^2 \tag{8.10}$$

Adding the two equations we obtain:

$$\begin{aligned} \partial_t(\psi^*\psi) &= -\frac{\hbar}{2mi}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right) \\ &= -\nabla\cdot\left[\frac{\hbar}{2mi}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)\right] \end{aligned} \tag{8.11}$$

We have derived a *continuity equation* for the probability density $\rho = |\psi|^2$,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0, \tag{8.12}$$

with a probability current:

$$\mathbf{j} = \frac{\hbar}{2mi} \left[\psi^* \nabla \psi - \psi \nabla \psi^*\right]. \tag{8.13}$$

Let's now rewrite

$$\psi(\mathbf{r}, t) = \sqrt{\rho(\mathbf{r}, t)} \cdot e^{iF(\mathbf{r},t)/\hbar}, \tag{8.14}$$

where the function $F(\mathbf{r}, t)$ is real. Then,

$$\psi^* \nabla \psi - \psi \nabla \psi^* = \frac{2i}{\hbar} \rho \nabla F. \tag{8.15}$$

The probability current is then

$$\mathbf{j}(\mathbf{r}, t) = \rho(\mathbf{r}, t) \frac{\nabla F(\mathbf{r}, t)}{m}. \tag{8.16}$$

We can regard $\nabla F/m$ as a "velocity".
Integrating the probability current over all space we find that it is equal to the expectation value of the momentum divided by the mass:

$$\begin{aligned} \int \mathrm{d}^3\mathbf{r}\, \mathbf{j}(\mathbf{r}, t) &= \int \mathrm{d}^3\mathbf{r}\, \frac{1}{2m} \left[\psi^*(-i\hbar\nabla)\psi + \psi(i\hbar\nabla)\psi^*\right] \\ &= \int \mathrm{d}^3\mathbf{r}\, \frac{1}{2m} \left[\langle\psi, t|\mathbf{r}\rangle \langle\mathbf{r}| \mathbf{p} |\psi, t\rangle + \langle\psi, t| \mathbf{p} |\mathbf{r}\rangle \langle\mathbf{r}|\psi, t\rangle\right] \\ &= \frac{1}{m} \langle\psi, t| \mathbf{p} |\psi, t\rangle. \end{aligned} \tag{8.17}$$

8.2 Quantized energy levels

One of the biggest triumphs of quantum mechanics is the prediction of bound states, where particles are restricted to small regions of space (atoms, molecules) and have a discrete energy spectrum. In this section, we shall try to understand these phenomena qualitatively from the wave equation of Schrödinger. Consider a well-potential (i.e. a potential which can trap a particle as in Fig 8.1) in one space-dimension. Schrödinger's equation can be written in the form

$$\frac{\psi''}{\psi} = \frac{2m\,(V(x) - E)}{\hbar^2} \tag{8.18}$$

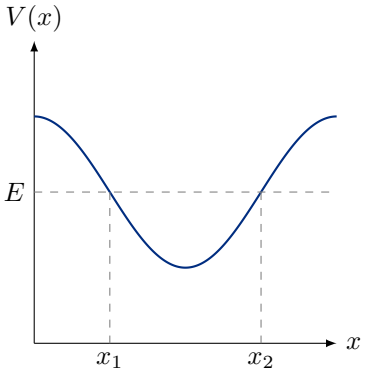


Figure 8.1: A well-potential.

The second derivative of the wave-function is proportional to the difference of the potential and the energy of the particle. Geometrically, the second derivative represents the rate of change of the slope of the wave-function.

i) If $V(x) > E$ then ψ'' and ψ must have the *same* sign. In that case, the wave function is concave *away* from the axis (as depicted in Fig. 8.2)

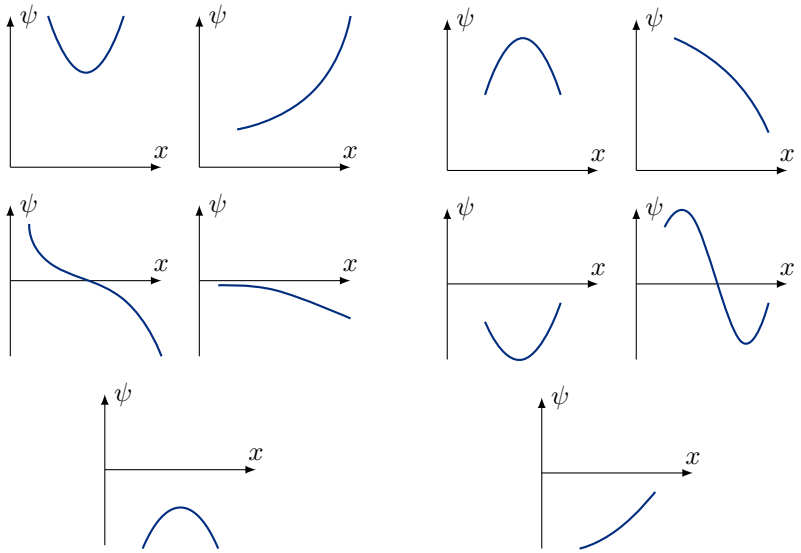
ii) If $V(x) < E$ then ψ'' and ψ must have the *opposite* sign. In that case, the wave function is concave *towards* the axis (as depicted in the right picture of Fig. 8.2)

Let us apply the above qualitative principles to a bound state, where

$$\psi(-\infty) = 0\,. \tag{8.19}$$

Drawing wave-functions with the above rules starting from $x = -\infty$ and guessing the wave-function all the way up to $x = +\infty$, we realize that it is not easy to end up with a wave-function which is bound at $x = +\infty$ (see Fig. 8.3).

In order to get a physical solution with finite probabilities it is necessary to tune the energy very precisely. Only for a selected number of energy values we are able to get physical solutions like in Fig. 8.4. The difficulty in the matching of a physical wave-function over the full range of space explains the quantization of energy. As we increase the energy level of the bound particle the wave-function for $V(x) > E$ oscillates stronger and over a larger range. Higher energy levels lead to more crossings of the wavefunction and the x-axis (Fig. 8.5).



(a) In regions of x where the potential energy is higher than the energy of the particle the wave-function is concave *away* from the x-axis.

(b) Otherwise it is concave *towards* the axis.

Figure 8.2: Examples of Schrödinger wave-functions.

8.3 Semiclassical approximation

In this section we shall develop an approximation method in order to compute the wave-function of a particle in a static system. This means that we demand that the probability of finding the particle at a certain region is the same irrespectively of the time that we performed our experiment. For such a system, we must have:

$$\frac{\partial \rho}{\partial t} = 0. \tag{8.20}$$

The continuity equation 8.12 gives that

$$\nabla \cdot \mathbf{j} = 0. \tag{8.21}$$

For simplicity, we will restrict our discussion to one-dimensional systems. Writing the wave-function in the form

$$\psi(x) = \sqrt{\rho(x)} e^{iS(x)/\hbar}\,, \tag{8.22}$$

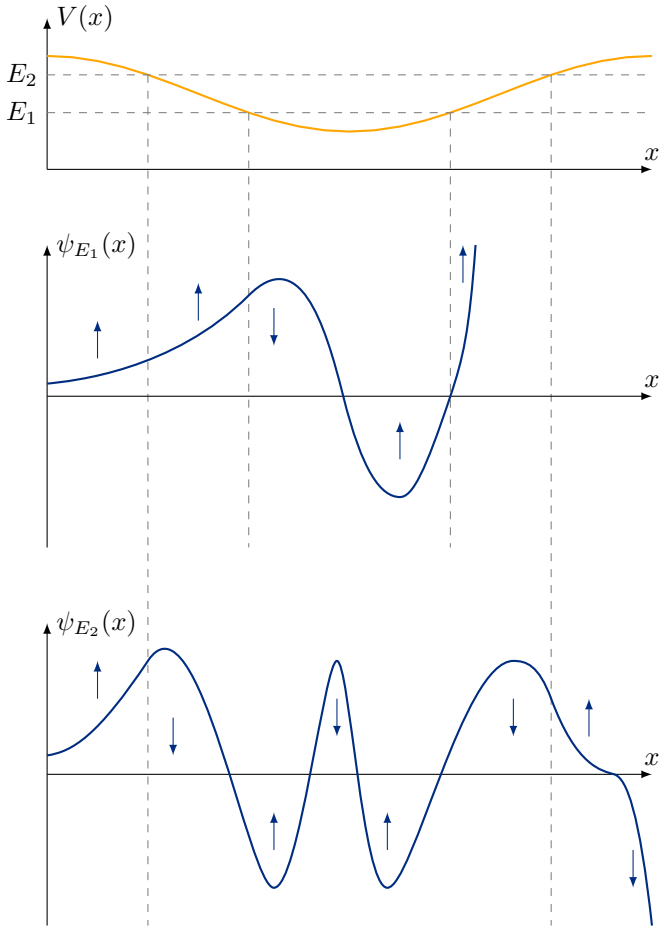


Figure 8.3: A few failed attempts to arrive at a vanishing wave-function as $x \to +\infty$ starting from a physical behavior at $x = -\infty$.

with a probability current

$$j(x) = \rho(x) \frac{\frac{\partial}{\partial x} S(x)}{m}, \tag{8.23}$$

we have from Eq. 8.21 that:

$$\frac{\partial}{\partial x} \left(\rho \frac{\partial S}{\partial x} \right) = 0$$

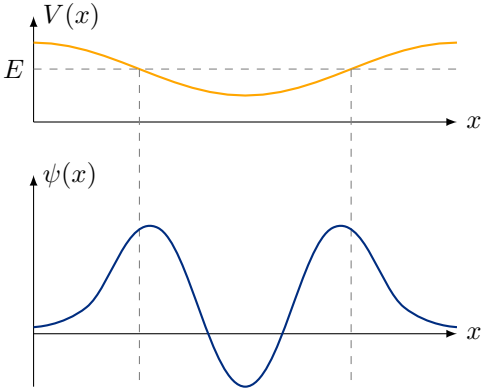


Figure 8.4: Only for selected (quantized) values of the energy we are able to match a physical behavior of the wave-function at $x \to +\infty$ with a physical behavior at $x = -\infty$.

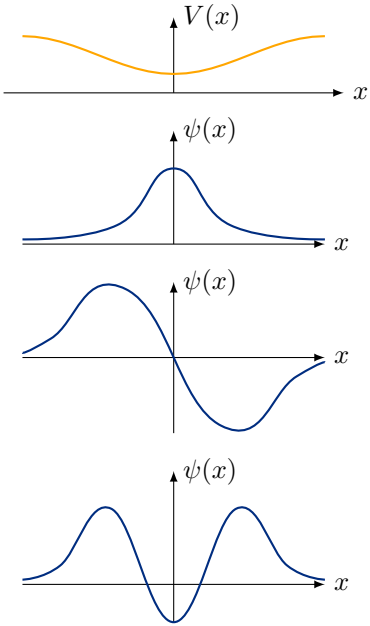


Figure 8.5: Higher energy levels correspond to wave-functions with more crossings with the x-axis.

$$\rightsquigarrow \rho S' = \text{const}$$
$$\rightsquigarrow \rho = \frac{\text{const}}{S'} \,. \tag{8.24}$$

Let's assume that $\hbar$ is a small parameter ($\hbar \to 0$ corresponds to the classical limit) and expand:

$$S = S_0 + \hbar S_1 + \hbar^2 S_2 + \dots \tag{8.25}$$

Notice that the derivatives of the wave-function are proportional to the wave-function itself (by taking the derivative Eq. 8.22):

$$\psi' = \psi \left[\frac{\sqrt{\rho}'}{\sqrt{\rho}} + i\frac{S'}{\hbar} \right] \tag{8.26}$$

$$\psi'' = \psi \left[\left(\frac{\sqrt{\rho}'}{\sqrt{\rho}} + i\frac{S'}{\hbar} \right)^2 + \left(\frac{\sqrt{\rho}'}{\sqrt{\rho}} \right)' + i\frac{S''}{\hbar} \right] \tag{8.27}$$

Substituting our expansion ansatz for ψ of Eq. 8.25 into Eq. 8.18 and keeping the leading order term in $\hbar$ (semiclassical approximation), we obtain the following differential equation:

$$\left(S_0'\right)^2 = -2m\left(V(x) - E\right). \tag{8.28}$$

For the regions of x where $V(x) > E$ we have

$$S_0'(x) = \pm i\sqrt{2m(V(x) - E)} \tag{8.29}$$

and, thus,

$$\psi_{(V(x)>E)} \approx \frac{\text{const}}{\left[2m\left(V(x) - E\right)\right]^{\frac{1}{4}}} \exp\left(\pm \int_{x_0}^{x} \mathrm{d}y \, \frac{\sqrt{2m\left(V(y) - E\right)}}{\hbar} \right) \tag{8.30}$$

Similarly, for $V(x) < E$, we find an approximate solution:

$$S_0'(x) = \pm\sqrt{2m(E - V(x))} \tag{8.31}$$

and, thus,

$$\psi_{(V(x)<E)} \approx \frac{\text{const}}{\left[2m(E - V(x))\right]^{\frac{1}{4}}} \exp\left(\pm i \int_{x_0}^{x} \mathrm{d}y \, \frac{\sqrt{2m\left(E - V(y)\right)}}{\hbar} \right) \tag{8.32}$$

Obviously, non of the two solutions is a good approximation for values of the potential close to the energy $V(x) \sim E$. For these regions, we can find an explicit solution expanding the potential around the region $x = x_{sp}$ for which $V(x_{sp}) = E$. We write:

$$\begin{aligned} V(x) &\approx V(x_{sp}) + (x - x_{sp})V'(x_{sp}) + \dots \\ &= E + (x - x_{sp})V'(x_{sp}) + \dots \end{aligned} \tag{8.33}$$

The Hamiltonian becomes

$$H \approx \frac{\hat{p}^2}{2m} + E + (\hat{x} - x_{sp})V'(x_{sp}) \tag{8.34}$$

and we need to solve the eigenvalue problem:

$$\begin{aligned} H\,|\psi_E\rangle &= E\,|\psi_E\rangle \\ \rightsquigarrow \left[\frac{\hat{p}^2}{2m} + (\hat{x} - x_{sp})V'(x_{sp})\right]|\psi_E\rangle &= 0\,. \end{aligned} \tag{8.35}$$

The linear potential problem can be solved exactly, as we shall see in the next section.

Having approximate solutions for the three distinct regions $V(x) < E$, $V(x) > E$ and $V(x) \approx E$ we can construct an approximate solution for all values of x. It is required that the solutions are the same for the regions where more than one approximations are valid. This leads to "matching" conditions which, for bound states, leads to quantization conditions of the energy levels.

8.4 Linear potential

In this section we shall solve Schrödinger's energy eigenstate problem for a linear potential:

$$\left[\frac{\hat{p}^2}{2m} + a\hat{x} + b\right]|\psi\rangle = 0. \tag{8.36}$$

It is easier to solve this problem in momentum space. Recall that

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}. \tag{8.37}$$

It is easy to verify that this amplitude satisfies the correct momentum eigenstate equation:

$$\begin{aligned} \langle x|\,\hat{p}\,|p\rangle &= -i\hbar\frac{\partial}{\partial x}\langle x|p\rangle = -i\hbar\frac{\partial}{\partial x}\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar} \\ &= p\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar} = p\,\langle x|p\rangle\,. \end{aligned} \tag{8.38}$$

For two momentum states, $|p\rangle, |q\rangle$, we have

$$\begin{aligned}\langle p|\,\hat{x}\,|q\rangle &= \int \mathrm{d}y\ \langle p|\,\hat{x}\,|y\rangle\,\langle y|q\rangle = \int \mathrm{d}y\, y\,\langle p|y\rangle\,\langle y|q\rangle \\ &= \int \mathrm{d}y\ \langle p|y\rangle \left(-i\hbar\frac{\partial}{\partial q}\right)\frac{1}{\sqrt{2\pi\hbar}}e^{iqy/\hbar} \\ &= \left(-i\hbar\frac{\partial}{\partial q}\right)\int \mathrm{d}y\ \langle p|y\rangle\,\langle y|q\rangle \\ &= \left(-i\hbar\frac{\partial}{\partial q}\right)\langle p|q\rangle = \left(-i\hbar\frac{\partial}{\partial q}\right)\delta(p-q). \end{aligned} \tag{8.39}$$

Also,

$$\begin{aligned}\langle p|\,\hat{x}\,|\psi\rangle &= \int \mathrm{d}q\,\langle p|\,\hat{x}\,|q\rangle\,\langle q|\psi\rangle \\ &= -i\hbar\frac{\partial}{\partial p}\int \mathrm{d}q\,\delta(q-p)\,\langle q|\psi\rangle \\ \rightsquigarrow \langle p|\,\hat{x}\,|\psi\rangle &= -i\hbar\frac{\partial}{\partial p}\,\langle p|\psi\rangle\,. \end{aligned} \tag{8.40}$$

Thus,

$$\begin{aligned}&\langle p|\,\frac{\hat{p}^2}{2m} + a\hat{x} + b\,|\psi\rangle = 0 \\ &\quad\rightsquigarrow i\hbar a\frac{\partial}{\partial p}\,\langle p|\psi\rangle = \left(\frac{p^2}{2m}+b\right)\langle p|\psi\rangle \\ &\quad\rightsquigarrow \langle p|\psi\rangle = N\exp\left(\frac{\frac{p^3}{6m}+pb}{i\hbar a}\right) \end{aligned} \tag{8.41}$$

The wavefunction in $x-$space can be found as:

$$\begin{aligned}\langle x|\psi\rangle &= \int_{-\infty}^{\infty}\mathrm{d}p\,\langle x|p\rangle\,\langle p|\psi\rangle \\ &= N\int_{-\infty}^{\infty}\frac{\mathrm{d}p}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}\exp\left(\frac{\frac{p^3}{6m}+pb}{i\hbar a}\right) \end{aligned} \tag{8.42}$$

The solution is an Airy function. It is defined through its integral representation

$$\mathrm{Ai}(z) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}t\,\exp\left[i\left(\frac{t^3}{3}+zt\right)\right] \tag{8.43}$$

and can be computed numerically for all values of z.

Chapter 9

Particle in a constant electromagnetic field

The Hamiltonian for a charged particle in a time-independent electromagnetic field is

$$H = \frac{(\mathbf{p} - q\mathbf{A})^2}{2m} + q\Phi, \tag{9.1}$$

where $\mathbf{A} = \mathbf{A}(\mathbf{r})$ and $\Phi = \Phi(\mathbf{r})$ are the vector and scalar potential respectively. Working in the Heisenberg picture, we find that the velocity operator is (**exercise**):

$$\frac{\mathrm{d}r_i}{\mathrm{d}t} = -\frac{i}{\hbar}\left[r_i, H\right] = \frac{p_i - qA_i}{m} \tag{9.2}$$

and the operator analogue of the classical momentum is then

$$\mathbf{\Pi} = m\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = \mathbf{p} - q\mathbf{A}. \tag{9.3}$$

We call $\mathbf{\Pi}$ the kinetic momentum and $\mathbf{p}$ the canonical momentum. For the commutator of kinetic momenta we find,

$$[\Pi_i, \Pi_j] = i\hbar q\left(\partial_i A_j - \partial_j A_i\right). \tag{9.4}$$

Recalling that the magnetic field is given by

$$B_i = \epsilon_{ijk}\partial_j A_k, \tag{9.5}$$

we have that

$$\epsilon_{ijk}B_k = \left(\partial_i A_j - \partial_j A_i\right). \tag{9.6}$$

We then write,

$$[\Pi_i, \Pi_j] = i\hbar q\epsilon_{ijk}B_k. \tag{9.7}$$

We now compute the commutator

$$\begin{aligned}[\Pi_i, H] &= \left[\Pi_i, \frac{\Pi_j \Pi_j}{2m} + q\Phi\right] \\ &= i\hbar q \left(-\partial_i \Phi + \epsilon_{ijk} \frac{1}{2m} \left[\Pi_j B_k - B_j \Pi_k\right]\right)\end{aligned}$$

We then obtain for the quantum operator corresponding to the classical force,

$$m\frac{\mathrm{d}^2\mathbf{r}}{\mathrm{d}t^2} = \frac{1}{i\hbar}\left[m\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}, H\right] = q\left[-\nabla\Phi + \frac{1}{2}\left(\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} \times \mathbf{B} - \mathbf{B} \times \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}\right)\right]. \tag{9.8}$$

9.1 Wave-function for a particle in an electromagnetic field

The time-evolution of a state is determined by Schrödinger's equation, which in the case of a particle in a constant electromagnetic field takes the form:

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi, t\right\rangle = \left(\frac{\Pi^2}{2m} + q\Phi\right)\left|\psi, t\right\rangle. \tag{9.9}$$

For the wave-function

$$\psi(\mathbf{r}, t) = \langle \mathbf{r} | \psi, t\rangle,$$

we obtain

$$i\hbar\frac{\partial\psi(\mathbf{r}, t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\left(\nabla - \frac{i}{\hbar}qA\right)\left(\nabla - \frac{i}{\hbar}qA\right) + q\Phi\right]\psi(\mathbf{r}, t) \tag{9.10}$$

We define a "covariant" gradient operator:

$$\nabla_c \equiv \nabla - \frac{i}{\hbar}qA \tag{9.11}$$

We then rewrite Schrödinger's equation as

$$i\hbar\frac{\partial\psi(\mathbf{r}, t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla_c^2 + q\Phi\right]\psi(\mathbf{r}, t) \tag{9.12}$$

Maxwell equations are invariant under a gauge transformation, which in the case of steady fields takes the form:

$$\mathbf{A}(\mathbf{r}) \to \mathbf{A}(\mathbf{r}) + \nabla\Lambda(\mathbf{r}). \tag{9.13}$$

Under this transformation, Schrödinger's equation becomes:

$$i\hbar\frac{\partial\psi_\Lambda(\mathbf{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}(\nabla_c - \nabla\Lambda)^2 + q\Phi\right]\psi_\Lambda(\mathbf{r},t) \tag{9.14}$$

We would now like to compare the solutions of the Schrödinger equation before and after the gauge transformation. We can verify easily that if $\psi(\mathbf{r},t)$ is a solution of Eq. 9.12 then also the function

$$\psi_\Lambda(\mathbf{r},t) = e^{\frac{iq}{\hbar}\Lambda(\mathbf{r})}\psi(\mathbf{r},t) \tag{9.15}$$

is a solution. Indeed,

$$\left(\nabla - \frac{iq\mathbf{A}}{\hbar} - \frac{iq\nabla\Lambda}{\hbar}\right)e^{\frac{iq}{\hbar}\Lambda(\mathbf{r})} = e^{\frac{iq}{\hbar}\Lambda(\mathbf{r})}\left(\nabla - \frac{iq\mathbf{A}}{\hbar}\right) \tag{9.16}$$

and

$$\left(\nabla_c - i\frac{q}{\hbar}\nabla\Lambda\right)^2 e^{\frac{iq}{\hbar}\Lambda(\mathbf{r})}\psi(\mathbf{r},t) = e^{\frac{iq}{\hbar}\Lambda(\mathbf{r})}\nabla_c^2\psi(\mathbf{r},t). \tag{9.17}$$

Therefore, a gauge transformation results in the wave-function being multiplied with an overall phase.

We shall now revisit our interpretation of the absolute square of the wave-function as a probability density:

$$\rho(\mathbf{r},t) = |\psi(\mathbf{r},t)|^2 .$$

Taking the time derivative we have,

$$\begin{aligned}\frac{\partial\rho}{\partial t} &= \psi^*\left(\partial_t\psi\right) + \left(\partial_t\psi^*\right)\psi \\ &= i\frac{\hbar}{2m}\left(\psi^*\nabla_c^2\psi - \psi\left(\nabla_c^2\psi\right)^*\right) \\ &= -\nabla\mathbf{J},\end{aligned} \tag{9.18}$$

where

$$\mathbf{J} = -i\frac{\hbar}{2m}\left[\psi^*\nabla_c\psi - \psi\nabla_c^*\psi^*\right], \tag{9.19}$$

and

$$\nabla_c^* = \nabla + \frac{i}{\hbar}qA\,. \tag{9.20}$$

Contrast this current with the one in the absence of the electromagnetic field. It is consistent with the substitution:

$$\nabla \to \nabla_c,$$

or, equivalently, replacing the canonical momentum operator with the kinetic momentum operator,

$$\mathbf{p} \to \mathbf{\Pi}.$$

9.2 Aharonov-Bohm effect

Consider a particle that at $t = 0$ is found at a position $|\mathbf{a}\rangle$. After some time t the state will have evolved according to Schrödinger's equation:

$$i\hbar\partial_t |\mathbf{a}, t\rangle = \left[\frac{\Pi^2}{2m} + q\Phi\right] |\mathbf{a}, t\rangle \,. \tag{9.21}$$

The probability amplitude that the particle is found at a position $\mathbf{r}$ after time t is then

$$\langle \mathbf{r}|\mathbf{a}, t\rangle \,,$$

and it satisfies

$$i\hbar\partial_t \langle \mathbf{r}|\mathbf{a}, t\rangle = \left[-\frac{\hbar^2}{2m}\nabla_c^2 + q\Phi\right] \langle \mathbf{r}|\mathbf{a}, t\rangle \,. \tag{9.22}$$

Let's assume that we can compute the amplitude for the same transition

$$\langle \mathbf{r}|\mathbf{a}, t\rangle_0$$

in the absence of a vector potential $\mathbf{A} = 0 \rightsquigarrow \nabla_c = \nabla$. Then, the amplitude for the transition for $\mathbf{A} \neq 0$ is:

$$\langle \mathbf{r}|\mathbf{a}, t\rangle = \langle \mathbf{r}|\mathbf{a}, t\rangle_0 \exp\left(\frac{iq}{\hbar}\int_{\mathbf{a}}^{\mathbf{r}} \mathrm{d}\mathbf{l}\cdot\mathbf{A}\right) \tag{9.23}$$

Exercise 9.1. *Prove that the above is indeed a solution of Eq. 9.22 and that it satisfies the amplitude "multiplication rule" for two successive transitions:*

$$\mathcal{M}(a \to b)\mathcal{M}(b \to c) = \mathcal{M}(a \to c).$$

where $\mathcal{M}$ *denotes*

$$\mathcal{M}\,(x \to y) = \langle y|x\rangle \,.$$

Now consider a two-slit experiment where in between the two slits inside the wall there is a magnetic field $\mathbf{B}$. The field is contained inside the wall and the particles cannot penetrate it. The transition amplitude from the shooting point to a point on the screen behind the wall is the sum of the amplitude for the particle to go through slit 1 (path Γ_1) and the amplitude to go through slit 2 (path Γ_2).

$$\mathcal{M} = \mathcal{M}_{\Gamma_1} + \mathcal{M}_{\Gamma_2} \,. \tag{9.24}$$

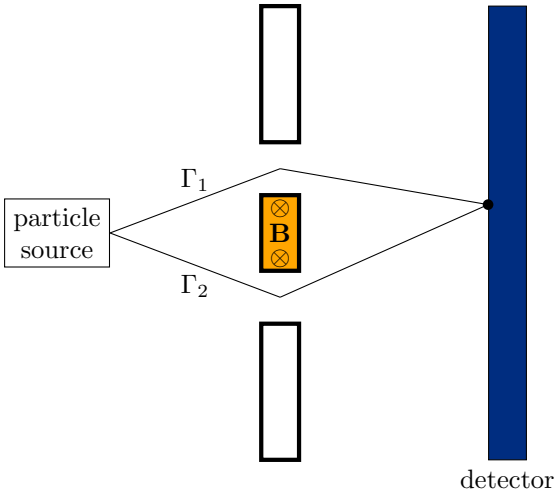


Figure 9.1: Sketch of the setup for the Aharomov-Bohm-effect. Note that the **B**-Field is only within the wall and is enclosed by any path $\Gamma_1 + \Gamma_2$.

According to Eq. 9.23, this is equivalent to:

$$\mathcal{M} = \mathcal{M}_1 \exp\left(\frac{iq}{\hbar}\int_{\Gamma_1} \mathrm{d}\mathbf{l}\cdot\mathbf{A}\right) + \mathcal{M}_2 \exp\left(\frac{iq}{\hbar}\int_{\Gamma_2} \mathrm{d}\mathbf{l}\cdot\mathbf{A}\right) \tag{9.25}$$

The probability of this transition is

$$\begin{aligned} P &= |\mathcal{M}|^2 \\ &= |\mathcal{M}_1|^2 + |\mathcal{M}_2|^2 + 2\Re\left(\mathcal{M}_1^*\mathcal{M}_2 \exp\left(\frac{iq}{\hbar}\oint \mathrm{d}\mathbf{l}\cdot\mathbf{A}\right)\right). \end{aligned} \tag{9.26a}$$

The interference term now depends on the flux of the magnetic field enclosed by the two alternative paths. (Fig. 9.1)

$$\Phi_B = \oint \mathrm{d}\mathbf{l}\cdot\mathbf{A} = \int_{S(\Gamma_1+\Gamma_2)} \mathrm{d}\mathbf{S}\cdot\nabla\mathbf{A} = \int_{S(\Gamma_1+\Gamma_2)} \mathrm{d}\mathbf{S}\cdot\mathbf{B}. \tag{9.26b}$$

$$\rightsquigarrow P = |\mathcal{M}_1|^2 + |\mathcal{M}_2|^2 + 2\Re\left(\mathcal{M}_1^*\mathcal{M}_2 \exp\left(\frac{iq}{\hbar}\Phi_B\right)\right) \tag{9.26c}$$

It is remarkable that the path of the particles lies outside the range of the magnetic field. Nevertheless, the interference pattern is affected by it. This is the Aharonov-Bohm effect.

Chapter 10

Symmetries in Quantum Mechanics

A symmetry changes our way of looking at a physical system without changing the physics of it. In quantum mechanics, symmetry transformations alter quantum states,

$$|\psi\rangle \xrightarrow{T} |\psi'\rangle\,, \quad |\phi\rangle \xrightarrow{T} |\phi'\rangle\,, \tag{10.1}$$

without changing probabilities

$$|\langle\phi'|\psi'\rangle|^2 = |\langle\phi|\psi\rangle|^2\,. \tag{10.2}$$

States can be represented as vectors in Hilbert space. If $\{|a_i\rangle\}$ is a set of base-kets, we can write

$$|\psi\rangle = \sum_i c_i\,|a_i\rangle$$

and we represent $|\psi\rangle$ as a Hilbert space vector

$$|\psi\rangle \doteq \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}.$$

Under the symmetry transformation T, the vector of $|\psi\rangle$ in Hilbert space transforms as

$$\begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix} \xrightarrow{T} \begin{pmatrix} c_1' \\ c_2' \\ \vdots \\ c_N' \end{pmatrix} = \begin{pmatrix} U_{11}(T) & \dots & U_{1N}(T) \\ U_{21}(T) & \dots & U_{2N}(T) \\ \vdots & \ddots & \vdots \\ U_{N1}(T) & \dots & U_{NN}(T) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$$

or, briefly,

$$\underbrace{|\psi'\rangle}_{\text{Hilbert space vector}} \doteq \overbrace{U(T)}^{\text{matrix}}\,\underbrace{|\psi\rangle} \tag{10.3}$$

where the kets in the above equations are the vector representations of the states in Hilbert space and not the states themselves. The matrix $U(T)$ changes for other representation of the states with sets of base states different than $\{|a_i\rangle\}$.

To preserve the probabilities under symmetry transformations, according to Wigner's theorem, we have two options:

i) $U(T)$ is linear and unitary,

$$\begin{aligned} U(a|\psi\rangle + b|\phi\rangle) &= aU|\psi\rangle + bU|\phi\rangle \\ \langle\psi|U^\dagger U|\phi\rangle &= \langle\psi|\phi\rangle\,, \end{aligned}$$

ii) $U(T)$ is anti-linear and anti-unitary,

$$\begin{aligned} U(a|\psi\rangle + b|\phi\rangle) &= a^*U|\psi\rangle + b^*U|\phi\rangle \\ \langle\psi|U^\dagger U|\phi\rangle &= \langle\phi|\psi\rangle\,. \end{aligned}$$

We shall not prove Wigner's theorem here. [1] We will restrict ourselves in verifying the inverse statement. Consider, for example, that U is anti-linear and anti-unitary. For two states,

$$|\phi\rangle\,, \quad |\psi\rangle = a_1|\psi_1\rangle + a_2|\psi_2\rangle\,, \tag{10.4}$$

the probability that $|\psi\rangle$ collapses into $|\phi\rangle$ is transformed to

$$\begin{aligned} \left|\langle\phi'|\psi'\rangle\right|^2 &= \left|\langle\phi|U^\dagger U|\psi\rangle\right|^2 \\ &= \left|\langle\phi|U^\dagger U\left(a_1|\psi_1\rangle + a_2|\psi_2\rangle\right)\right|^2 \\ &= \left|\langle\phi|U^\dagger\left(a_1^*U|\psi_1\rangle + a_2^*U|\psi_2\rangle\right)\right|^2 \\ &= \left|a_1^*\langle\phi|U^\dagger U|\psi_1\rangle + a_2^*\langle\phi|U^\dagger U|\psi_2\rangle\right|^2 \\ &= \left|a_1^*\langle\psi_1|\phi\rangle + a_2^*\langle\psi_2|\phi\rangle\right|^2 \\ &= \left|\left(a_1^*\langle\psi_1| + a_2^*\langle\psi_2|\right)|\phi\rangle\right|^2 \\ &= \left|\langle\psi|\phi\rangle\right|^2 \\ &= \left|\langle\phi|\psi\rangle\right|^2. \end{aligned}$$

[1] A proof can be found in Weinberg's Quantum Theory of Fields, Vol. I

Similarly, if U is linear and unitary,

$$\begin{aligned}
\left|\langle\phi'|\psi'\rangle\right|^2 &= \left|\langle\phi|\, U^\dagger U\,|\psi\rangle\right|^2 \\
&= \left|\langle\phi|\, U^\dagger U\,(a_1\,|\psi_1\rangle + a_2\,|\psi_2\rangle)\right|^2 \\
&= \left|\langle\phi|\, U^\dagger\,(a_1 U\,|\psi_1\rangle + a_2 U\,|\psi_2\rangle)\right|^2 \\
&= \left|a_1\,\langle\phi|\psi_1\rangle + \langle\phi|\psi_2\rangle\right|^2 \\
&= \Big|\langle\phi|\,\big(a_1\,|\psi_1\rangle + a_2\,|\psi_2\rangle\big)\Big|^2 \\
&= \left|\langle\phi|\psi\rangle\right|^2 .
\end{aligned}$$

10.1 Continuous symmetry transformations

Notice that the unit operator is unitary and linear, not anti-unitary and anti-linear. Some symmetry transformations $T(\theta^a)$ are connected to the unity smoothly, such as rotations, translations and Lorentz boosts, via continuous parameters (angles, velocities, etc),

$$T \equiv T(\theta^a), \quad \theta^a \equiv \begin{cases} \theta, \phi & \text{angles} \\ \beta_x, \beta_y, \beta_z & \text{boosts} \\ \varepsilon_1, \varepsilon_2, \varepsilon_3 & \text{space-displacements} \end{cases} \tag{10.5}$$

Such transformations which are related to the unity (no transformation) continuously must have a unitary and linear representation.

$$|\psi'\rangle = U\left(T(\theta^a)\right)|\psi\rangle\,. \tag{10.6}$$

We choose the parameters θ^a of these continuous transformations so that when the parameters of the transformation vanish, $\theta^a = 0$, the system is unchanged:

$$U\left(T(\theta^a = 0)\right) = 1. \tag{10.7}$$

Let as restrict ourselves to unitary and linear transformations $T \equiv T(\theta^a)$ and study their representation $U(T)$. The product of two such transformations is also a transformation,

$$T_3 = T_2 T_1.$$

A state $|\psi\rangle$ transforms as

$$|\psi\rangle \to |\psi'\rangle = U(T_2)U(T_1)\,|\psi\rangle\,,$$

under the T_1 transformation followed by the T_2 transformation. Transforming under $T_3 = T_2T_1$, we obtain

$$|\psi\rangle \to |\psi''\rangle = U(T_3)\,|\psi\rangle = U(T_2T_1)\,|\psi\rangle\,.$$

The states $|\psi'\rangle$ and $|\psi''\rangle$ must be equivalent, describing the same physics. Therefore, they can only differ by a phase:

$$U(T_2)U(T_1)\,|\psi\rangle = e^{i\phi_\psi(T_2,T_1)}U(T_2T_1)\,|\psi\rangle\,. \tag{10.8}$$

We can show that the phase $\phi_\psi(T_2,T_1)$ is independent of the state $|\psi\rangle$. Take a $|\psi\rangle$ which is a superposition of two independent states:

$$|\psi\rangle = |\psi_A\rangle + |\psi_B\rangle\,.$$

Then,

$$\begin{aligned} e^{i\phi_{AB}}U(T_2T_1)\left(|\psi_A\rangle + |\psi_B\rangle\right) &= U(T_2)U(T_1)\left(|\psi_A\rangle + |\psi_B\rangle\right) \\ &= U(T_2)U(T_1)\,|\psi_A\rangle + U(T_2)U(T_1)\,|\psi_B\rangle \\ &= e^{i\phi_A}U(T_2T_1)\,|\psi_A\rangle + e^{i\phi_B}U(T_2T_1)\,|\psi_B\rangle\,. \end{aligned} \tag{10.9}$$

Multiplying both sides with $U^{-1}(T_2T_1)$, we obtain:

$$\begin{aligned} e^{i\phi_{AB}}\left(|\psi_A\rangle + |\psi_B\rangle\right) &= e^{i\phi_A}\,|\psi_A\rangle + e^{i\phi_B}\,|\psi_B\rangle \\ \rightsquigarrow 0 &= \left(e^{i\phi_{AB}} - e^{i\phi_A}\right)|\psi_A\rangle + \left(e^{i\phi_{AB}} - e^{i\phi_B}\right)|\psi_B\rangle \\ \rightsquigarrow e^{i\phi_{AB}} &= e^{i\phi_A} = e^{i\phi_B}. \end{aligned} \tag{10.10}$$

Thus, the phase is the same for all states and we can write:

$$U(T_2)U(T_1) = e^{i\phi(T_2,T_1)}U(T_2T_1). \tag{10.11}$$

For $\phi(T_2,T_1) = 0$, the matrix $U(T)$ furnishes a representation of the symmetry transformation T. For the general $\phi(T_2,T_1) \neq 0$, $U(T)$ is a so-called *projective* representation of the symmetry transformations. It can be shown that we can always enlarge the symmetry group so that projective representations turn into representations with a zero phase. Let's consider the product of the

representations of three symmetry transformations:

$$\begin{aligned} U(T_3)U(T_2)U(T_1) &= U(T_3)\left[U(T_2)U(T_1)\right] \\ &= \left[U(T_3)U(T_2)\right]U(T_1) \end{aligned}$$

$$\begin{aligned} \rightsquigarrow U(T_3)e^{i\phi(T_2,T_1)}U(T_2T_1) &= e^{i\phi(T_3,T_2)}U(T_3T_2)U(T_1) \\ \rightsquigarrow e^{i\phi(T_2,T_1)+i\phi(T_3,T_2T_1)}U(T_3T_2T_1) &= e^{i\phi(T_3,T_2)+i\phi(T_3T_2,T_1)}U(T_3T_2T_1) \\ \rightsquigarrow \phi(T_2,T_1)+\phi(T_3,T_2T_1) &= \phi(T_3,T_2)+\phi(T_3T_2,T_1) \end{aligned} \tag{10.12}$$

This is satisfied if we write the phase ϕ in terms of a function χ as in:

$$\phi(T_a,T_b) = \chi(T_aT_b) - \chi(T_a) - \chi(T_b). \tag{10.13}$$

Defining a representation of an enlarged symmetry transformation as

$$\bar{U}(T) = U(T)e^{i\chi(T)}, \tag{10.14}$$

we see that $\bar{U}(T)$ furnishes a representation (with zero phase)

$$\begin{aligned} \bar{U}(T_b)\bar{U}(T_a) &= U(T_b)U(T_a)e^{i\left(\chi(T_a)+\chi(T_b)\right)} \\ &= U(T_bT_a)e^{i\left(\phi(T_b,T_a)+\chi(T_a)+\chi(T_b)\right)} \\ &= \bar{U}(T_bT_a)e^{i\left(\phi(T_b,T_a)+\chi(T_a)+\chi(T_b)-\chi(T_bT_a)\right)} \\ &= \bar{U}(T_bT_a)\,. \end{aligned} \tag{10.15}$$

For the symmetries of interest we shall take that they have representations with a zero-phase or that they have been enlarged so that this is achieved.

10.2 Lie algebra and generators

We consider a continuous symmetry transformation

$$T(\theta^a)$$

parameterized by a set of continuous parameters

$$\{\theta^a\}, \quad a = 1 \ldots N$$

The symmetry transformations form a Lie group and the product of two such transformations is also a symmetry transformation belonging to the group:

$$T(\theta_1^a)T(\theta_2^a) = T\left(f^a(\theta_1^a,\theta_2^a)\right). \tag{10.16}$$

We arrange that T corresponds to the unit element of the symmetry group if all values of the parameters are zero, $\theta^a = 0$,

$$T(\theta^a = 0) = 1. \tag{10.17}$$

The product rule of Eq. 10.16 and our definition of the unit transformation of Eq. 10.17 yield:

$$\begin{aligned} f^a(0, \theta^a) &= f^a(\theta^a, 0) \\ &= \theta^a \end{aligned} \tag{10.18}$$

Restricting ourselves to small transformations around the unity transformation, we perform a Taylor expansion around $\theta^a = 0$:

$$\begin{aligned} f^a(\theta_1^a, \theta_2^a) = f^a(0,0) &+ \frac{\partial f^a}{\partial \theta_1^b}\theta_1^b + \frac{\partial f^a}{\partial \theta_2^b}\theta_2^b + \frac{1}{2}\frac{\partial^2 f^a}{\partial \theta_1^b \partial \theta_1^c}\theta_1^b\theta_1^c \\ &+ \frac{1}{2}\frac{\partial^2 f^a}{\partial \theta_2^b \partial \theta_2^c}\theta_2^b\theta_2^c + \frac{\partial^2 f^a}{\partial \theta_1^b \partial \theta_2^c}\theta_1^b\theta_2^c + \dots \end{aligned} \tag{10.19}$$

with $b, c = 1, \dots, N$ and Einstein summation convention. Imposing the requirement of Eq 10.18 leads to the form:

$$f^a(\theta_1^a, \theta_2^a) = \theta_1^a + \theta_2^a + f_{bc}^a \theta_1^b \theta_2^c + \dots \tag{10.20}$$

with f_{bc}^a being the second order coefficient of the Taylor expansion of f^a and in this case b, c are dummy indices to sum over.

For an ordinary representation $U(T)$ of the symmetry group,

$$U\left(T(\theta_1^a)\right) U\left(T(\theta_2^a)\right) = U\left(T\left(f^a(\theta_1^a, \theta_2^a)\right)\right). \tag{10.21}$$

For small parameters θ^a, we can expand the representation of the transformation as follows:

$$U\left(T(\theta^a)\right) = 1 + i\theta^a t_a + \frac{1}{2}\theta^b\theta^c t_{bc} + \dots \tag{10.22}$$

where $1, t_a, t_{bc}$ in the above equation are matrices of the same dimensionality as $U\left(T(\theta^a)\right)$ and the matrix t_{bc} is symmetric in b and c:

$$t_{bc} = t_{cb}\,. \tag{10.23}$$

Expanding, using Eq. 10.22, the terms in Eq. 10.21 we have

$$\begin{aligned} &\left(1 + i\theta_1^a t_a + \frac{1}{2}\theta_1^b\theta_1^c t_{bc} + \dots\right)\left(1 + i\theta_2^a t_a + \frac{1}{2}\theta_2^b\theta_2^c t_{bc} + \dots\right) \\ &\quad = 1 + i\left(\theta_1^a + \theta_2^a + f_{bc}^a\theta_1^b\theta_2^c + \dots\right) t_a + \frac{1}{2}\left(\theta_1^b + \theta_2^b + \dots\right)\left(\theta_1^c + \theta_2^c + \dots\right) t_{bc} \end{aligned}$$

where we have neglected θ^a terms of third order and higher. Matching the powers of θ_1^a, θ_2^a, we find that

$$t_{bc} = -t_b t_c - i f_{bc}^a t_a. \tag{10.24}$$

From the symmetry of t_{bc}, we obtain:

$$0 = t_{bc} - t_{cb} = -(t_b t_c - t_c t_b) - i(f_{bc}^a - f_{cb}^a) t_a \tag{10.25}$$

This leads to the commutation relation for the matrices t^a:

$$[t_b, t_c] = i C_{bc}^a t_a. \tag{10.26}$$

where the constants

$$C_{bc}^a = f_{cb}^a - f_{bc}^a \tag{10.27}$$

are antisymmetric in $c \leftrightarrow b$ and are called the *structure constants* of the Lie-group. As you may observe, the structure constants do not depend on the specific representation $U(T(\theta^a))$. Instead, the matrices t_a are specific to the representation and have the same dimensionality. These matrices are known as the *generators* of the representation. Knowing the generators, we can construct the representation of an arbitrary symmetry transformation by using the product property of Eq. 10.21 to assemble large symmetry transformations from many small ones where the expansion of Eq 10.22 is valid. The common commutation relation of Eq. 10.26 satisfied by the generators of all representations of the symmetry group is known as a *Lie algebra*.

Requiring that the representation of a symmetry transformation is unitary, leads to the conclusion that the generators of the transformation are Hermitian operators:

$$U U^\dagger = 1 \rightsquigarrow t_a^\dagger = t_a. \tag{10.28}$$

Therefore, generators are good candidates for physical observables.

In the special case of "Abelian" symmetry groups ,

$$f(\theta_1^a, \theta_2^a) = \theta_1^a + \theta_2^a \,,$$

the generators commute:

$$[t_b, t_c] = 0. \tag{10.29}$$

A representation for general values of the parameters of the symmetry transformation can then be found as:

$$\begin{aligned} U\left(T(\theta^a)\right) &= \lim_{N\to\infty} U\left(T\left(\frac{\theta^a}{N}\right)\right)^N \\ &= \lim_{N\to\infty} \left(1 + i\frac{\theta^a}{N} t_a\right)^N \\ &= \exp\left(i\theta^a t_a\right). \end{aligned} \tag{10.30}$$

10.3 Symmetry and degeneracy

A symmetry transformation T should change a system in the same way irrespective of the time we performed the transformation. Therefore, the following two states must be the same:

$$U(T)\left(e^{iHt/\hbar}\left|\psi\right\rangle\right) = e^{iHt/\hbar}\left(U(T)\left|\psi\right\rangle\right). \tag{10.31}$$

The state of the lhs corresponds to performing the transformation after the system has evolved for time t. The state of the rhs corresponds to performing the transformation at $t = 0$ and then evolving for a time t. Since the above equation is valid for any state $|\psi\rangle$, we must have that the time-evolution operator and the representation of the symmetry commute:

$$\left[U(T), e^{iHt\hbar}\right] = 0. \tag{10.32}$$

Equivalently, the Hamiltonian and the symmetry representations also commute:

$$[U(T), H] = 0. \tag{10.33}$$

For continuous symmetry transformations where

$$U(T) = 1 - i\theta^a t_a + \ldots$$

the generators of the representation commute with the Hamiltonian:

$$[t_a, H] = 0. \tag{10.34}$$

Then, the Hamiltonian and the generators have a common set of eigenstates. Symmetries are associated with a degeneracy in the energy spectrum of a physical system. Consider an energy eigenstate:

$$H\left|E\right\rangle = E\left|E\right\rangle. \tag{10.35}$$

All states,

$$U(T)\left|E\right\rangle,$$

are also eigenstates of the Hamiltonian with the same energy eigenvalue E. Indeed,

$$H\left(U(T)\left|E\right\rangle\right) = U(T)H\left|E\right\rangle = U(T)E\left|E\right\rangle = E\left(U(T)\left|E\right\rangle\right). \tag{10.36}$$

10.4 Rotations and translations

In this section, we should study symmetry transformations corresponding to the change of reference frame. This is the requirement that the laws of quantum mechanics should be the same irrespective of where we are performing our experiment or how we have set up our coordinate system. We should restrict ourselves to Euclidean changes of reference frame, ignoring special relativity effects. These transformations preserve distances,

$$\mathbf{r} = (r_1, r_2, r_3) \to \mathbf{r}' = (r_1', r_2', r_3')$$

with

$$|\mathbf{r}_A - \mathbf{r}_B| = |\mathbf{r}_A' - \mathbf{r}_B'| \tag{10.37}$$

We can prove [2] that *necessarily* such distance preserving transformations $\mathbf{r} \to \mathbf{r}'$ must be linear,

$$r_i' = R_{ij} r_j + a_i \,, \tag{10.38}$$

Notice that the constant (coordinate independent) vector a_i displaces the center of the coordinate system and the constant (coordinate independent) matrix R_{ij} rotates the coordinates. Substituting into Eq. **??**, we find

$$\delta_{k\ell} = \delta_{ij} R_{ik} R_{j\ell} \tag{10.39}$$

. We write this in matrix-notation as

$$RR^T = 1, \quad R_{ij}^T = R_{ji}. \tag{10.40}$$

Taking the determinant of the above we have

$$\det(RR^T) = 1 \quad \rightsquigarrow (\det R)^2 = 1 \quad \rightsquigarrow \det R \neq 0 \,, \tag{10.41}$$

$$\det(RR^T) = 1 \quad \rightsquigarrow (\det R)^2 = 1 \quad \rightsquigarrow \det R \neq 0 \,, \tag{10.42}$$

which proves that there exist the inverse transformation of R. We have

$$\begin{aligned} RR^T &= 1 \\ \rightsquigarrow R^{-1} R R^T &= R^{-1} \\ \rightsquigarrow R_{ij}^{-1} &= R_{ij}^T = R_{ji} \,. \end{aligned} \tag{10.43}$$

[2] see classroom presentation

Making two successive coordinate transformations we have

$$\begin{aligned} r_i'' &= R_{ij} r_j' + a_i \\ &= R_{ij} \left(\bar{R}_{j\ell} r_\ell + \bar{a}_j \right) + a_i \\ &= \left(R\bar{R} \right)_{i\ell} r_\ell + \left[R\bar{a} + a \right]_i \end{aligned} \tag{10.44}$$

Thus, we have the following multiplication rule for the group of coordinate transformations:

$$T(R, a) T(\bar{R}, \bar{a}) = T(R\bar{R}, R\bar{a} + a) \,. \tag{10.45}$$

Notice that rotations alone and translations alone form subgroups:

$$T(R, 0) T(\bar{R}, 0) = T(R\bar{R}, 0) \,. \tag{10.46}$$

and

$$T(1, a) T(1, \bar{a}) = T(1, \bar{a} + a) \,. \tag{10.47}$$

10.4.1 Generators

Consider an infinitesimal transformation:

$$T(\delta_{ij} + \omega_{ij}, \epsilon_i), \quad \omega_{ij}, \varepsilon_i \in \mathbb{R}$$

From Eq. 10.39, keeping only linear terms in ω, we have

$$\begin{aligned} \delta_{k\ell} &= \delta_{ij} R_{ik} R_{j\ell} \\ \rightsquigarrow \omega_{k\ell} &= -\omega_{\ell k} \end{aligned} \tag{10.48a}$$

Let's now look at the transformation of vectors in Hilbert space corresponding to quantum states in a generic representation of the symmetry group:

$$|\psi\rangle \to |\psi'\rangle = U(\omega, \epsilon) \, |\psi\rangle \,. \tag{10.49}$$

Expanding the representation U in the small parameters of the transformation, we have:

$$U(\omega, \epsilon) = 1 + \frac{i}{2} \omega_{ij} J^{ij} - i \epsilon_\rho P^\rho + \ldots \tag{10.50}$$

For $U(\omega, \epsilon)$ to be unitary, we have:

$$U U^\dagger = 1 \rightsquigarrow (J^{k\ell})^\dagger = J^{k\ell}, \; (P^\rho)^\dagger = P^\rho \tag{10.51}$$

Since $\omega_{ij} = -\omega_{ji}$ we can take that

$$J^{k\ell} = -J^{\ell k}. \tag{10.52}$$

We have already identified the *generator*

$$\hbar P^\rho \equiv p^\rho \tag{10.53}$$

as the *operator of momentum*. Similarly, we shall identify the *generators of rotations*

$$\hbar J^{k\ell} \tag{10.54}$$

as *operators of angular momentum*.
How do the expectation values of the generators $J^{k\ell}, P^\rho$ themselves transform under a coordinate transformation? Consider the product

$$U(R,a)U(1+\omega,\epsilon)U^{-1}(R,a) = U\left(R(1+\omega)R^{-1}, R\epsilon - R\omega R^{-1}a\right) \tag{10.55}$$

where

$$U^{-1}(R,a) = U\left(R^{-1}, -R^{-1}a\right) \tag{10.56}$$

and the parameters ω, ϵ of the small transformation are not related to the large transformation parameters R, a. Expanding the lhs and rhs of the above in ω, ϵ we have:

$$\begin{aligned} &U(R,a)U(1+\omega,\epsilon)U^{-1}(R,a) \\ &\quad = U\left(1 + \frac{i}{2}\omega_{k\ell}J^{k\ell} - i\epsilon_\rho P^\rho\right)U^{-1} &(10.57)\\ &\quad = 1 + \frac{i}{2}\omega_{k\ell}UJ^{k\ell}U^{-1} - i\epsilon_\rho UP^\rho U^{-1} &(10.58)\end{aligned}$$

and

$$\begin{aligned} &U\left(R(1+\omega)R^{-1}, R\epsilon - R\omega R^{-1}a\right) \\ &\quad = 1 + \frac{i}{2}\left(R\omega R^{-1}\right)_{k\ell}J^{k\ell} - i\left(R\epsilon - R\omega R^{-1}a\right)_\rho P^\rho \\ &\quad = 1 + \frac{i}{2}\omega_{k\ell}R^{-1}_{km}R^{-1}_{\ell n}\left(J^{mn} - a^m P^n + a^n P^m\right) - i\epsilon_\rho R^{-1}_{\rho k}P^k. &(10.59)\end{aligned}$$

Comparing the two, we obtain:

$$U(R,a)J^{k\ell}U^{-1}(R,a) = R^{-1}_{km}R^{-1}_{\ell n}\left(J^{mn} - a^m P^n + a^n P^m\right) \tag{10.60}$$

and

$$U(R,a)P^\rho U^{-1}(R,a) = R^{-1}_{\rho m}P^m. \tag{10.61}$$

From the above, we can also show that (**exercise**):

$$U^{-1}(R,a)J^{k\ell}U(R,a) = R_{km}R_{\ell n}\left(J^{mn} - a^m P^n + a^n P^m\right) \tag{10.62}$$

and

$$U^{-1}(R,a)P^{\rho}U(R,a) = R_{\rho m}P^{m}. \tag{10.63}$$

The expectation value of the generators transforms as follows with a coordinate symmetry transformation:

$$\langle\psi|\, P^{\rho}\,|\psi\rangle \to \langle\psi|\, U^{-1}P^{\rho}U\,|\psi\rangle = R_{\rho m}\,\langle\psi|\, P^{m}\,|\psi\rangle \tag{10.64}$$

and

$$\langle\psi|\, J^{k\ell}\,|\psi\rangle \to \langle\psi|\, U^{-1}J^{k\ell}U\,|\psi\rangle = R_{km}R_{\ell n}\,\langle\psi|\, J^{k\ell} - a^{m}P^{n} + a^{n}P^{m}\,|\psi\rangle \tag{10.65}$$

Therefore, the expectation value of P^{ρ} transforms as a classical vector and the expectation value of $J^{k\ell}$ transforms as a classical tensor with rotations and translations.

10.4.2 Lie algebra

We now assume further also that the transformation $T(R,a)$ is a small transformation,

$$T(R_{ij}, a_i) = T(\delta_{ij} + \omega'_{ij}, \epsilon'_i). \tag{10.66}$$

and expand Eqs 10.62-10.63 in $\omega'_{ij}, \epsilon'_i$. Matching the coefficients of the expansion, we find the following Lie-algebra for symmetry coordinate transformations:

$$i\left[J^{ij}, J^{k\ell}\right] = \left[\delta_{i\ell}J^{jk} - \delta_{ik}J^{j\ell} + \delta_{jk}J^{i\ell} - \delta_{j\ell}J^{ik}\right]. \tag{10.67a}$$

$$i\left[P^{m}, J^{rs}\right] = \delta_{mr}P^{s} - \delta_{ms}P^{r} \tag{10.67b}$$

$$\left[P^{r}, P^{s}\right] = 0\,. \tag{10.67c}$$

We identify the momentum and angular momentum operators as

$$\mathbf{p} \equiv (p_1, p_2, p_3) \equiv \hbar\left(P^1, P^2, P^3\right) \tag{10.68}$$

and

$$\mathbf{J} \equiv (J_1, J_2, J_3) \equiv \hbar\left(J^{23}, J^{31}, J^{12}\right) \tag{10.69}$$

respectively. In terms of these operators, the Lie algebra takes the form:

$$[J_i, J_j] = i\hbar\epsilon_{ijk}J_k\,, \tag{10.70a}$$

$$[J_i, p_j] = i\hbar\epsilon_{ijk}p_k\,, \tag{10.70b}$$

$$[p_i, p_j] = 0\,. \tag{10.70c}$$

Chapter 11

Representations of angular momentum

In the previous chapter, we identified the generators of rotations with the angular momentum operators. They satisfy the commutation relations,

$$[J_i, J_j] = i\hbar\epsilon_{ijk}J_k. \tag{11.1}$$

11.1 Eigenstates of angular momentum

We observe that the square of the angular momentum vector:

$$J^2 \equiv J_k J_k = J_1^2 + J_2^2 + J_3^2 \tag{11.2}$$

commutes with the generators J_i:

$$\begin{aligned}\left[J^2, J_i\right] &= \left[J_k J_k, J_i\right] = J_k\left[J_k, J_i\right] + \left[J_k, J_i\right] J_k \\ &= i\hbar\epsilon_{ki\ell}\left(J_k J_\ell + J_\ell J_k\right) = 0.\end{aligned} \tag{11.3}$$

Thus we can find common eigenstates $|f, m\rangle$ [1] for J^2 and one of the generators J_i, let's say J_3.

$$J^2 |f, m\rangle = \hbar^2 f |f, m\rangle , \tag{11.4a}$$

$$J_3 |f, m\rangle = \hbar m |f, m\rangle . \tag{11.4b}$$

We have that

$$\begin{aligned}0 &\leq \left|J_1 |f, m\rangle\right|^2 + \left|J_2 |f, m\rangle\right|^2 + \left|J_3 |f, m\rangle\right|^2 \\ &= \langle f, m| J_1^2 + J_2^2 + J_3^2 |f, m\rangle = \langle f, m| J^2 |f, m\rangle \\ &= \hbar^2 f \langle f, m|f, m\rangle \\ \rightsquigarrow & f \geq 0.\end{aligned} \tag{11.5}$$

[1] we shall relabel these states later

Also, the eigenvalue number m of the third component J_3 is bounded:

$$\begin{aligned} 0 \leq \langle f,m|\, J_1^2 + J_2^2 \,|f,m\rangle &= \langle f,m|\, J^2 - J_3^2 \,|f,m\rangle = \hbar^2(f-m^2) \\ \rightsquigarrow -f \leq m &\leq f. \end{aligned} \tag{11.6}$$

We can construct linear combinations of the first two components of angular momentum

$$J_\pm = J_1 \pm iJ_2 \tag{11.7}$$

which are *ladder* operators:

$$[J_3, J_\pm] = \pm\hbar J_\pm. \tag{11.8}$$

Then

$$\begin{aligned} J_3\left(J_\pm\,|f,m\rangle\right) &= \left([J_3,J_\pm] + J_\pm J_3\right)|f,m\rangle \\ &= \left(\pm\hbar J_\pm + J_\pm J_3\right)|f,m\rangle \\ &= \left(\pm\hbar J_\pm + \hbar m J_\pm\right)|f,m\rangle \\ &= \hbar(m\pm 1)\left(J_\pm\,|f,m\rangle\right) \end{aligned} \tag{11.9}$$

Thus, the state $J_\pm\,|f,m\rangle$ is also an eigenstate of J_3 with eigenvalue $\hbar\,(m\pm 1)$. We may write

$$\begin{aligned} J_\pm\,|f,m\rangle &= c_\pm\,|f,m\pm 1\rangle\,, \\ \rightsquigarrow |c_\pm|^2 &= \langle f,m|\, J_\mp J_\pm \,|f,m\rangle \\ &= \langle f,m|\, J_1^2 + J_2^2 \pm i\,[J_1,J_2]\,|f,m\rangle \\ &= \langle f,m|\, J^2 - J_3^2 \mp \hbar J_3 \,|f,m\rangle\,, \\ \rightsquigarrow |c_\pm|^2 &= \hbar^2\left(f - m(m\pm 1)\right). \end{aligned} \tag{11.10a}$$

We then normalize as:

$$J_\pm\,|f,m\rangle = \hbar\sqrt{f-m(m\pm 1)}\,|f,m\pm 1\rangle \tag{11.10b}$$

Assume j being the maximum value of m. Then,

$$J_+\,|f,j\rangle = 0\,, \tag{11.11}$$

$$\rightsquigarrow f - j(j+1) = 0\,, \tag{11.12}$$

$$\rightsquigarrow f = j(j+1)\,. \tag{11.13}$$

Now, assume that $j' < j$ is the minimum value of f.

$$J_-\,|f,j'\rangle = 0\,, \tag{11.14a}$$

$$\rightsquigarrow j(j+1) - j'(j'-1) = 0\,, \tag{11.14b}$$

$$\rightsquigarrow j' = -j\,. \tag{11.14c}$$

The ladder operators span the allowed range $-j \leq m \leq j$ by integer steps. Thus the number $(2j)$ must be an integer and thus:

$$j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}, \dots \tag{11.15}$$

We shall relabel the eigenstates $|f, m\rangle$ of J^2, J_3 with the half-integer j instead of f. The corresponding eigenvalue equations for the angular momentum operators are:

$$J^2 |j, m\rangle = \hbar^2 j(j+1) |j, m\rangle \tag{11.16a}$$
$$J_3 |j, m\rangle = \hbar m |j, m\rangle . \tag{11.16b}$$

where, we have found that the eigenvalue numbers j, m are quantized. For the ladder operators we have found:

$$J_\pm |j, m\rangle = \hbar \sqrt{j(j+1) - m(m \pm 1)} \, |j, m \pm 1\rangle . \tag{11.16c}$$

11.2 spin-$\frac{1}{2}$ representation of angular momentum

The simplest representation of the angular momentum operators J_i is the spin-$\frac{1}{2}$ representation, where the operators act on the states of a two-state system. For the spin-$\frac{1}{2}$ representation of angular momentum we have a base of two angular momentum eigenstates:

$$\left| \frac{1}{2}, \pm\frac{1}{2} \right\rangle \tag{11.17}$$

satisfying

$$J^2 \left| \frac{1}{2}, \pm\frac{1}{2} \right\rangle = \hbar^2 \frac{3}{4} \left| \frac{1}{2}, \pm\frac{1}{2} \right\rangle , \tag{11.18a}$$
$$J_3 \left| \frac{1}{2}, \pm\frac{1}{2} \right\rangle = \pm\hbar \frac{1}{2} \left| \frac{1}{2}, \pm\frac{1}{2} \right\rangle , \tag{11.18b}$$

$$J_+ \left| \frac{1}{2}, \frac{1}{2} \right\rangle = 0, \qquad J_+ \left| \frac{1}{2}, -\frac{1}{2} \right\rangle = \hbar \left| \frac{1}{2}, \frac{1}{2} \right\rangle , \tag{11.19}$$
$$J_- \left| \frac{1}{2}, \frac{1}{2} \right\rangle = \hbar \left| \frac{1}{2}, -\frac{1}{2} \right\rangle , \qquad J_- \left| \frac{1}{2}, -\frac{1}{2} \right\rangle = 0. \tag{11.20}$$

In the representation where

$$\left| \frac{1}{2}, \frac{1}{2} \right\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \qquad \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{11.21}$$

we find:

$$J_3 \doteq \begin{pmatrix} \left\langle \frac{1}{2}, \frac{1}{2} \right| J_3 \left| \frac{1}{2}, \frac{1}{2} \right\rangle & \left\langle \frac{1}{2}, \frac{1}{2} \right| J_3 \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \\ \left\langle \frac{1}{2}, -\frac{1}{2} \right| J_3 \left| \frac{1}{2}, \frac{1}{2} \right\rangle & \left\langle \frac{1}{2}, -\frac{1}{2} \right| J_3 \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \end{pmatrix} \tag{11.22a}$$
$$= \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Similarly,

$$J_- \doteq \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{11.22b}$$

and,

$$J_+ \doteq \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \tag{11.22c}$$

The ladder operators are $J_\pm = J_1 \pm iJ_2$. From the above we obtain:

$$J_1 \doteq \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad J_2 \doteq \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{11.23}$$

The matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{11.24}$$

are known as the *Pauli matrices*.
Notice with an explicit calculation (**exercise**) that

$$[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k \tag{11.25}$$

Therefore the representation of angular momentum as

$$J_i \doteq \hbar \frac{\sigma_i}{2}$$

satisfies the anticipated Lie-algebra of rotations.
Parenthetically, we note the following properties for the Pauli matrices.

$$\{\sigma_i, \sigma_j\} \equiv \sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}\mathbf{1}_{2\times 2}. \tag{11.26}$$

Combining Eq. 11.25 and Eq. 11.26, we obtain that the product of Pauli matrices is:

$$\sigma_i\sigma_j = \delta_{ij}\mathbf{1}_{2\times 2} + \epsilon_{ijk}\sigma_k \tag{11.27}$$

We shall now use the property of angular momentum operators as generators of rotations. For a rotation of a small angle θ around the $z-$axis, the representation of the transformation reads:

$$\begin{aligned} U(\theta) &= \mathbf{1}_{2\times 2} + \frac{i}{2}\left(\omega_{12}J_{12} + \omega_{21}J_{21}\right) \\ &= \mathbf{1}_{2\times 2} + \theta i\frac{J_3}{\hbar} = \mathbf{1}_{2\times 2} + i\frac{\theta\sigma_3}{2}, \end{aligned} \tag{11.28}$$

where we have used that

$$\omega_{12} = -\omega_{21} = \theta, \quad J_{12} = -J_{21} = \frac{J_3}{\hbar} = \frac{\sigma_3}{2}.$$

For a large angle θ we have

$$U(\theta) = \lim_{N\to\infty}\left[U\left(\frac{\theta}{N}\right)\right]^N = \exp\left(\frac{i\sigma_3\theta}{2}\right). \tag{11.29}$$

The exponential $e^{a\sigma_k}$, where σ_k, $k = 1, 2$ or 3 is a Pauli matrix having the property

$$\sigma^2 = \mathbf{1}_{2\times 2}$$

is given by

$$\begin{aligned} \exp(a\sigma_k) &= \sum_{n=0}^{\infty}\frac{(a\sigma_k)^n}{n!} \\ &= \sum_{k=0}^{\infty}\frac{(a\sigma_k)^{2k}}{(2k)!} + \sum_{k=0}^{\infty}\frac{(a\sigma_k)^{2k+1}}{(2k+1)!} \\ &= 1_{2\times 2}\sum_{k=0}^{\infty}\frac{a^{2k}}{(2k)!} + \sigma_k\sum_{k=0}^{\infty}\frac{a^{2k+1}}{(2k+1)!} \\ &= \mathbf{1}_{2\times 2}\frac{e^a + e^{-a}}{2} + \sigma_k\frac{e^a - e^{-a}}{2} \end{aligned} \tag{11.30}$$

Thus

$$U(\theta) = \exp\left(\frac{i\sigma_3\theta}{2}\right) = \mathbf{1}_{2\times 2}\cos\left(\frac{\theta}{2}\right) + i\sigma_3\sin\left(\frac{\theta}{2}\right)$$

$$= \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) + i\sin\left(\frac{\theta}{2}\right) & 0 \\ 0 & \cos\left(\frac{\theta}{2}\right) - i\sin\left(\frac{\theta}{2}\right) \end{pmatrix}$$

$$= \begin{pmatrix} \exp\left(i\frac{\theta}{2}\right) & 0 \\ 0 & \exp\left(-i\frac{\theta}{2}\right) \end{pmatrix}. \tag{11.31}$$

A general state for a two-state system

$$|\psi\rangle \doteq \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \tag{11.32}$$

under a rotation θ around the $z-$axis will transform as

$$|\psi\rangle \to |\psi'\rangle = U(\theta)\,|\psi\rangle \doteq \begin{pmatrix} e^{i\theta/2}\psi_1 \\ e^{-i\theta/2}\psi_2 \end{pmatrix} \tag{11.33}$$

Notice that a rotation $\theta = 2\pi$ does not bring the system back to the original state, against common intuition:

$$U(2\pi)\,|\psi\rangle = -\,|\psi\rangle\,. \tag{11.34}$$

For spin$-\frac{1}{2}$ systems a rotation of 4π is required in order to return back to the original state.

We can generalize our discussion here for a rotation of an angle θ around any axis $\hat{n}$. We can prove (**exercise)** that the corresponding spin-$\frac{1}{2}$ representation is:

$$U(\hat{n},\theta) = \exp\left(i\frac{\boldsymbol{\sigma}\cdot\hat{n}}{2}\theta\right), \tag{11.35}$$

which can also be written as

$$U(\hat{n}\theta) = \mathbf{1}_{2\times 2}\cos\frac{\theta}{2} + i\boldsymbol{\sigma}\cdot\hat{n}\sin\frac{\theta}{2}, \tag{11.36}$$

where

$$\boldsymbol{\sigma} = (\sigma_1,\sigma_2,\sigma_3)\,. \tag{11.37}$$

To prove the above the following are useful.

$$\boldsymbol{\sigma}\cdot\mathbf{a} = \begin{pmatrix} a_3 & a_1 - ia_2 \\ a_1 + ia_2 & a_3 \end{pmatrix}. \tag{11.38a}$$

$$(\boldsymbol{\sigma}\cdot\mathbf{a})^2 = \mathbf{a}^2, \tag{11.38b}$$

and

$$(\boldsymbol{\sigma}\cdot\mathbf{a})(\boldsymbol{\sigma}\cdot\mathbf{b}) = \mathbf{a}\cdot\mathbf{b} + i(\mathbf{a}\times\mathbf{b})\cdot\boldsymbol{\sigma}. \tag{11.38c}$$

11.3 Orbital angular momentum

In this chapter we study the space-representation of the eigenstates of the angular momentum operators $L_3, L^2 = \sum_i L_i^2$, where we have defined

$$L_i = \epsilon_{ijk}x_j p_k, \tag{11.39}$$

with x_i, p_j being the position and momentum operators. It is straightforward to prove that the operators $\frac{L_i}{\hbar}$ satisfy the Lie algebra of the generators of rotations,

$$\left[\frac{L_i}{\hbar}, \frac{L_j}{\hbar}\right] = i\epsilon_{ijk}\frac{L_k}{\hbar}. \tag{11.40}$$

According to the general theory of the generators for rotations, we anticipate that we can find common eigenstates $|\ell, m\rangle$ for $L^2 = \sum_i L_i^2$ and one of the generators L_i with

$$L^2 |\ell, m\rangle = \hbar^2 \ell(\ell+1) |\ell, m\rangle$$

and

$$L_3 |\ell, m\rangle = \hbar m |\ell, m\rangle .$$

11.3.1 Spherical coordinates

It will be useful to analyze angular momentum using spherical coordinates, where:

$$x_1 = r\sin\theta\sin\phi\,, \tag{11.41a}$$
$$x_2 = r\sin\theta\cos\phi\,, \tag{11.41b}$$
$$x_3 = r\cos\theta\,. \tag{11.41c}$$

For the differentials, we have

$$\partial_r = \sum_i \frac{\partial x_i}{\partial r}\partial_i\,, \tag{11.42a}$$
$$\partial_\theta = \sum_i \frac{\partial x_i}{\partial \theta}\partial_i\,, \tag{11.42b}$$
$$\partial_\phi = \sum_i \frac{\partial x_i}{\partial \phi}\partial_i\,, \tag{11.42c}$$

which in matrix notation gives,

$$\begin{pmatrix}\partial_r\\ \partial_\theta\\ \partial_\phi\end{pmatrix} = \begin{pmatrix}\sin\theta\sin\phi & \sin\theta\cos\phi & \cos\theta\\ r\cos\theta\sin\phi & r\cos\theta\cos\phi & -r\sin\theta\\ r\sin\theta\cos\phi & -r\sin\theta\sin\phi & 0\end{pmatrix}\begin{pmatrix}\partial_1\\ \partial_2\\ \partial_3\end{pmatrix}. \tag{11.43}$$

Inverting, we obtain:

$$\begin{pmatrix}\partial_1\\ \partial_2\\ \partial_3\end{pmatrix} = \begin{pmatrix}\sin\theta\sin\phi & \frac{\cos\theta\sin\phi}{r} & \frac{\cos\phi}{r\sin\theta}\\ \sin\theta\cos\phi & \frac{\cos\phi\cos\theta}{r} & -\frac{\sin\phi}{r\sin\theta}\\ \cos\theta & -\frac{\sin\theta}{r} & 0\end{pmatrix}\begin{pmatrix}\partial_r\\ \partial_\theta\\ \partial_\phi\end{pmatrix}. \tag{11.44}$$

We then calculate, ($\cot\theta = \frac{\cos\theta}{\sin\theta}$)

$$x_2\partial_3 - x_3\partial_2 = \cot\theta\sin\phi\,\partial_\phi - \cos\phi\,\partial_\theta\,, \tag{11.45a}$$
$$x_3\partial_1 - x_1\partial_3 = \cot\theta\cos\phi\,\partial_\phi + \sin\phi\,\partial_\theta\,, \tag{11.45b}$$
$$x_1\partial_2 - x_2\partial_1 = -\partial_\phi\,. \tag{11.45c}$$

The Laplacian operator is,

$$\begin{aligned}\nabla^2 &= \sum_i \partial_i^2 \\ &= \frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right].\end{aligned} \tag{11.46}$$

11.3.2 Orbital angular momentum operators and the Laplacian

Consider the action of an angular momentum operator on a general state $|a\rangle$,

$$L_i\,|a\rangle = \epsilon_{ijk}\hat{x}_i\hat{p}_j\,|a\rangle\,. \tag{11.47}$$

Acting with a position bra $\langle\mathbf{r}| = \langle x_1, x_2, x_3|$, we have

$$\begin{aligned}\langle\mathbf{r}|\,L_i\,|a\rangle &= \epsilon_{ijk}\,\langle\mathbf{r}|\,\hat{x}_j\hat{p}_k\,|a\rangle \\ &= -i\hbar\epsilon_{ijk}x_j\partial_k\,\langle\mathbf{r}|a\rangle\,.\end{aligned} \tag{11.48}$$

For example,

$$\begin{aligned}\langle\mathbf{r}|\,L_3\,|a\rangle &= \langle\mathbf{r}|\,\hat{x}_1\hat{p}_2 - \hat{x}_2\hat{p}_1\,|a\rangle \\ &= -i\hbar(x_1\partial_2 - x_2\partial_1)\,\langle\mathbf{r}|a\rangle\,.\end{aligned} \tag{11.49}$$

Using spherical coordinates introduced in the previous section, we obtain

$$\langle\mathbf{r}|\,L_3\,|a\rangle = i\hbar\,(+\partial_\phi)\,\langle\mathbf{r}|a\rangle\,. \tag{11.50}$$

Similarly,

$$\langle\mathbf{r}|\,L_1\,|a\rangle = -i\hbar\,(\cot\theta\sin\phi\,\partial_\phi - \cos\phi\,\partial_\theta)\,\langle\mathbf{r}|a\rangle\,. \tag{11.51}$$

and

$$\langle\mathbf{r}|\,L_2\,|a\rangle = -i\hbar\,(\cot\theta\cos\phi\,\partial_\phi + \sin\phi\,\partial_\theta)\,\langle\mathbf{r}|a\rangle\,. \tag{11.52}$$

For the *ladder operators*,

$$L_\pm = L_1 \pm iL_2\,, \tag{11.53}$$

we obtain

$$\langle \mathbf{r}| L_\pm |a\rangle = i\hbar \left(e^{\mp i\phi} \left[\partial_\theta \mp i \cot\theta \, \partial_\phi \right] \right) \langle \mathbf{r}|a\rangle \,. \tag{11.54}$$

We can write

$$L^2 = L_3^2 + \frac{1}{2} \left(L_+ L_- + L_- L_+ \right) \tag{11.55}$$

After a little bit of algebra, we arrive at

$$\langle \mathbf{r}| L^2 |a\rangle = -\hbar^2 \left[\frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) \right] \langle \mathbf{r}|a\rangle \,. \tag{11.56}$$

We notice that the representation of the operator L^2 in position-space yields the angular part of the Laplacian operator, which, in turn, represents the square of the momentum. Explicitly,

$$\begin{aligned} \langle \mathbf{r}| p^2 |a\rangle &= -\hbar^2 \nabla^2 \langle \mathbf{r}|a\rangle \\ &= -\hbar^2 \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \right] \langle \mathbf{r}|a\rangle + \frac{1}{r^2} \langle \mathbf{r}| L^2 |a\rangle \,. \end{aligned} \tag{11.57}$$

11.3.3 Spherical harmonics

The eigenstates $|\ell, m\rangle$ of L^2, L_3 satisfy

$$i\hbar \partial_\phi \langle \mathbf{r}|\ell, m\rangle = \hbar m \langle \mathbf{r}|\ell, m\rangle \,, \tag{11.58}$$

and admit the general solution

$$\langle \mathbf{r}|\ell, m\rangle = \eta(r, \theta) e^{-im\phi}. \tag{11.59}$$

For the maximum value ℓ of m, we have that

$$\langle \mathbf{r}| L_+ |\ell, \ell\rangle = 0, \tag{11.60}$$

which yields the differential equation,

$$e^{-i\phi} \left[\partial_\theta - i \cot\theta \, \partial_\phi \right] \eta(r, \theta) e^{-i\ell\phi} = 0 \tag{11.61}$$

$$\rightsquigarrow \left[\partial_\theta - \ell \cot\theta \right] \eta(r, \theta) = 0 \,. \tag{11.62}$$

This admits the solution,

$$\eta(r, \theta) = \psi(r) (\sin\theta)^\ell. \tag{11.63}$$

We then have

$$\langle \mathbf{r}|\ell, \ell\rangle = \psi(r) Y_\ell^\ell(\theta, \phi), \tag{11.64}$$

where

$$Y_\ell^\ell(\theta,\phi) = c_{\ell\ell} e^{-i\ell\phi} (\sin\theta)^\ell \tag{11.65}$$

contains the angular dependence on the variables (θ,ϕ) of $\langle \mathbf{r}|\ell,\ell\rangle$. This function is a so called *spherical harmonic*. We fix the normalization constant as follows,

$$\begin{aligned} 1 &= \langle \ell,\ell|\ell,\ell\rangle \\ &= \int \mathrm{d}^3\mathbf{r}\ \langle \ell,\ell|\mathbf{r}\rangle \langle \mathbf{r}|\ell,\ell\rangle \\ &= \int_0^\infty \mathrm{d}r\, r\, |\psi(r)|^2 \int \mathrm{d}\Omega\ \left|Y_\ell^\ell\right|^2 . \end{aligned} \tag{11.66}$$

We require that the angular integral and the radial integral are normalized to the unity independently:

$$\int_0^\infty \mathrm{d}r\, r\, |\psi(r)|^2 = 1 \tag{11.67}$$

and

$$\int \mathrm{d}\Omega\ \left|Y_\ell^\ell\right|^2 = 1 . \tag{11.68}$$

The angular normalization condition yields,

$$|c_{\ell\ell}|^2 \int_0^{2\pi} \mathrm{d}\phi \int_0^\pi \mathrm{d}\theta\, \sin\theta \left(\sin^2\theta\right)^\ell = 1$$

$$\rightsquigarrow 2\pi B\left(\ell+1,\frac{1}{2}\right) = |c_{\ell\ell}|^{-2} \tag{11.69}$$

$$\sqrt{4\pi \frac{4^\ell(\ell!\,)^2}{(2\ell+1)!}} = |c_{\ell\ell}|^{-1} . \tag{11.70}$$

We can obtain spherical harmonics for $|\ell,m\rangle$ with a lower value of $m < \ell$ by means of the ladder operators. Acting with the L_- operator on a general $|\ell,m\rangle$ state, we obtain

$$\langle \mathbf{r}|\ell,m-1\rangle = \frac{\langle \mathbf{r}|\, L_-\, |\ell,m\rangle}{\sqrt{(\ell+m)(\ell+1-m)}} , \tag{11.71}$$

or equivalently,

$$\langle \mathbf{r}|\ell,m-1\rangle = i\hbar e^{i\phi} \left(\partial_\theta + i\cot\theta\, \partial_\phi\right) \frac{\langle \mathbf{r}|\ell,m\rangle}{\sqrt{(\ell+m)(\ell+1-m)}\hbar} . \tag{11.72}$$

It is obvious that the application of this operator does not mix the radial and angular parts in producing $\langle \mathbf{r}|\ell, m\rangle$ of a different m than ℓ. So, we can decompose

$$\langle \mathbf{r}|\ell, m\rangle = \psi_{\ell m}(r) Y_\ell^m(\theta, \phi). \tag{11.73}$$

The spherical harmonics Y_ℓ^m depend purely on the direction of the vector $\mathbf{r}$. We can think of them as

$$\langle \hat{\mathbf{r}}|\ell, m\rangle = Y_\ell^m(\theta, \phi), \quad \hat{\mathbf{r}} = \frac{\mathbf{r}}{|\mathbf{r}|}\,. \tag{11.74}$$

For the spherical harmonics $Y_\ell^m(\theta, \phi)$, we obtain,

$$Y_\ell^{m-1}(\theta, \phi) = i\left(e^{i\phi}\left[\partial_\theta + i\cot\theta\,\partial_\phi\right]\right)\frac{Y_\ell^m(\theta, \phi)}{\sqrt{(\ell+m)(\ell+1-m)}} \tag{11.75}$$

According to our general theory for the eigenvalues of the generators of rotations, we anticipate that the maximum value ℓ of m is a half-integer and that $m = -\ell, -\ell+1, \ldots, \ell-1, \ell$. Here we shall find a little surprise. While the operators $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ furnish a representation of rotations in Hilbert-space it is not necessary that their eigenvalues take all values permitted by the Lie algebra. In fact, for orbital angular momentum only integer values of ℓ, m are allowed. Assume that $\ell = \frac{1}{2}$. Then, we find that

$$Y_{\frac{1}{2}}^{\frac{1}{2}}(\theta, \phi) = c_{\frac{1}{2}\frac{1}{2}} e^{-i\phi/2}\sqrt{\sin\theta}\,. \tag{11.76}$$

With the application of the lowering operator, we obtain:

$$\begin{aligned} Y_{\frac{1}{2}}^{-\frac{1}{2}}(\theta, \phi) &= i\left(e^{i\phi}\left[\partial_\theta + i\cot\theta\,\partial_\phi\right]\right) c_{\frac{1}{2}\frac{1}{2}} e^{-i\phi/2}\sqrt{\sin\theta} \\ &= i c_{\frac{1}{2}\frac{1}{2}} e^{i\phi/2}\frac{\cos\theta}{\sqrt{\sin\theta}}\,. \end{aligned} \tag{11.77}$$

For a consistent spherical harmonic, we must have that the application of the lowering operator one more time yields zero. Notice also that the derived spherical harmonic gives an infinite value for $\theta = 0$.

Spherical harmonics are only defined for $\ell = 0, 1, 2, 3$ integer values of the indices for the angular momentum eigenvalues. Starting for a generic $m = \ell$ value, repeated application of Eq. 11.75 $\ell - m$ times we can obtain the spherical harmonic Y_ℓ^m. Let's denote the differential operator of Eq. 11.75 as

$$D_- \equiv i\left(e^{i\phi}\left[\partial_\theta + i\cot\theta\,\partial_\phi\right]\right) \tag{11.78}$$

and define

$$\omega_\ell \equiv e^{-i\ell\phi}\sin^\ell\theta. \tag{11.79}$$

We find that

$$\omega_\ell = e^{-i\phi} \sin\theta \, \omega_{\ell-1} \,, \tag{11.80}$$

$$D_- \omega_\ell = (2i\ell \cos\theta)\omega_{\ell-1} \,, \tag{11.81}$$

$$D_- \left(f\left(\theta\right)\right) = -ie^{i\phi} \sin\theta \frac{\mathrm{d}}{\mathrm{d}\left(\cos\theta\right)} f(\theta) \,, \tag{11.82}$$

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}\left(\cos\theta\right)} \left[(\sin\theta)^{2\ell} f(\theta) \right] = &- (\sin\theta)^{2(\ell-1)} \left(2\ell \cos\theta f(\theta) \right. \\ &\left. - \sin^2\theta \frac{\mathrm{d}}{\mathrm{d}\left(\cos\theta\right)} f(\theta) \right) . \end{aligned} \tag{11.83}$$

and that

$$\begin{aligned} D_- \left(f(\theta)\omega_\ell \right) &= f\left(\theta\right) D_- \omega_\ell + \omega_\ell D_- \left(f(\theta) \right) \\ &= \omega_{\ell-1} \frac{-i}{(\sin\theta)^{2(\ell-1)}} \frac{\mathrm{d}}{\mathrm{d}\cos\theta} \left[(\sin\theta)^{2\ell} f(\theta) \right] , \end{aligned} \tag{11.84}$$

where $f(\theta)$ an arbitrary function of the polar angle θ. It is now straightforward to compute the repeated application of the differential operator on ω_ℓ, For example,

$$\begin{aligned} D_-(D_-\omega_\ell) &= 2i\ell D_-(\underbrace{\cos\theta}_{f(\theta)} \omega_{\ell-1}) \\ &= \omega_{\ell-2} \frac{(-i)^2}{(\sin\theta)^{2(\ell-2)}} \frac{\mathrm{d}^2}{\mathrm{d}\left(\cos\theta\right)^2} \left[(\sin\theta)^{2\ell} \right] , \end{aligned} \tag{11.85}$$

and in general,

$$D_-{}^n \omega_\ell = \omega_{\ell-n} \frac{(-i)^n}{(\sin\theta)^{2(\ell-n)}} \frac{\mathrm{d}^n}{\mathrm{d}\left(\cos\theta\right)^n} \left[(\sin\theta)^{2\ell} \right] \tag{11.86}$$

We are now ready to determine the spherical harmonics Y_ℓ^m for positive values of m, using the recurrence identity of Eq. 11.75 on

$$Y_\ell^\ell \left(\theta, \phi\right) = c_{\ell\ell} \omega_\ell \,. \tag{11.87}$$

$\ell - m$ times, we find

$$Y_\ell^m(\theta,\phi) = (-i)^\ell c_{\ell\ell} \sqrt{\frac{(2\ell)!\,(\ell+m)!}{(\ell-m)!}} \frac{e^{-im(\phi-\frac{\pi}{2})}}{(\sin\theta)^m} \frac{\mathrm{d}^{\ell-m}}{\mathrm{d}\left(\cos\theta\right)^{\ell-m}} (\sin\theta)^{2\ell}. \tag{11.88}$$

The normalization $c_{\ell\ell}$ can be determined up to a phase. We conventionally choose this phase to be

$$c_{\ell\ell} = |c_{\ell\ell}| \, (-i)^\ell. \tag{11.89}$$

With this normalization we obtain,

$$Y_\ell^m(\theta,\phi) = \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell+m)!}{(\ell-m)!}}\frac{e^{-im(\phi-\frac{\pi}{2})}}{(\sin\theta)^m}\frac{(-1)^\ell}{2^\ell\ell!}\frac{\mathrm{d}^{\ell-m}}{\mathrm{d}\,(\cos\theta)^{\ell-m}}(\sin\theta)^{2\ell}. \tag{11.90}$$

The derivatives above for the case $m = 0$ are related to the Legendre polynomials, defined as,

$$P_\ell(x) = \frac{(-1)^\ell}{2^\ell\ell!}\frac{\mathrm{d}^\ell}{\mathrm{d}x^\ell}(1-x^2)^\ell. \tag{11.91}$$

As one can check easily, they satisfy the differential equation,

$$\frac{\mathrm{d}}{\mathrm{d}x}\left((1-x^2)\frac{\mathrm{d}}{\mathrm{d}x}P_\ell(x)\right) + \ell(\ell+1)P_\ell(x) = 0. \tag{11.92}$$

For $x = \cos\theta$, we have

$$\frac{\mathrm{d}}{\mathrm{d}\cos\theta}\sin^2\theta\frac{\mathrm{d}}{\mathrm{d}\cos\theta}P_\ell(\cos\theta) + \ell(\ell+1)P_\ell(\cos\theta) = 0. \tag{11.93}$$

or, equivalently,

$$\frac{1}{\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\sin\theta\frac{\mathrm{d}}{\mathrm{d}\theta} + \ell(\ell+1)P_\ell(\cos\theta) = 0. \tag{11.94}$$

For $m = 0$, the spherical harmonics become:

$$Y_\ell^0(\theta,\phi) = \sqrt{\frac{(2\ell+1)}{4\pi}}P_\ell(\cos\theta). \tag{11.95}$$

To obtain the spherical harmonics for negative values of m we have to repeat a completely analogous study starting from Y_l^{-l} as derived from

$$L_-\,|\ell,-\ell\rangle = 0,$$

and using that

$$L_+\,|\ell,m\rangle = \sqrt{(\ell-m)(\ell+m+1)}\,|\ell,m+1\rangle\,.$$

We find that (**exercise**):

$$Y_\ell^{-m}(\theta,\phi) = (-1)^m\left[Y_\ell^m(\theta,\phi)\right]^*. \tag{11.96}$$

11.3.4 Space-representations of rotations

An arbitrary rotation of coordinates $x_i \to x_i' = R_{ij}x_j$ is represented by a unitary operator

$$|\psi\rangle \to U(R)\,|\psi\rangle\,, \tag{11.97}$$

where the operator $U(R)$ is a function of the generators J_i with $i = 1, 2, 3$. Since the square of the angular momentum commutes with all generators J_i, we should also have that

$$\left[J^2, U(R)\right] = 0. \tag{11.98}$$

Thus, the states $|\ell, m\rangle$ and $U(R)\,|\ell, m\rangle$ have the same eigenvalues for the J^2 operator. The $U(R)\,|\ell, m\rangle$ can only be a superposition of $|\ell, m'\rangle$ states with the same value ℓ: In a general decomposition,

$$U(R)\,|\ell, m\rangle = \sum_{\ell' m'} c_{\ell' m'}\,|\ell', m'\rangle \tag{11.99}$$

only the terms with $\ell' = \ell$ are present. We can write that:

$$U(R)\,|\ell, m\rangle = \sum_{m'} c_{m'}\,|\ell, m'\rangle \tag{11.100}$$

Physically, this result is anticipated since a rotation should not change the total angular momentum.

Consider a position state $|\hat{z}\rangle$, corresponding to the unit vector in the $z-$direction. A position state $|\hat{r}\rangle$ with

$$\hat{r} = (\sin\theta\sin\phi, \sin\theta\cos\phi, \cos\theta), \tag{11.101}$$

can be produced by a rotation as for,

$$|\hat{r}\rangle = U(\theta, \phi)\,|\hat{z}\rangle\,. \tag{11.102}$$

We then have

$$\begin{aligned} |\hat{r}\rangle &= \sum_{\ell', m'} U(\theta,\phi)|\ell', m'\rangle\langle\ell', m'|\,|\hat{z}\rangle \\ \rightsquigarrow \langle\ell, m|\hat{r}\rangle &= \sum_{\ell', m'} \langle\ell, m|\,U(\theta,\phi)\,|\ell', m'\rangle\,\langle\ell', m'|\hat{z}\rangle \\ \rightsquigarrow \langle\ell, m|\hat{r}\rangle &= \sum_{m'} \langle\ell, m|\,U(\theta,\phi)\,|\ell, m'\rangle\,\langle\ell, m'|\hat{z}\rangle \end{aligned} \tag{11.103}$$

The matrix-element $\langle\hat{z}|\ell, m\rangle$ is zero unless $m = 0$. Indeed, if $m \neq 0$,

$$L_3\,|\hat{z}\rangle = (\hat{x}_1\hat{p}_2 - \hat{x}_2\hat{p}_1)\,|\hat{z}\rangle = 0,$$

since the position operators $\hat{x}_{1,2}$ yield a zero eigenvalue for a position ket in the orthogonal $z-$direction. Also,

$$0 = \langle \hat{z}| L_3 |\ell, m\rangle = \hbar m \langle \hat{z}|\ell, m\rangle .$$

For $m \neq 0$, we must have that $\langle \hat{z}|\ell, m\rangle = 0$. Therefore,

$$\begin{aligned} \langle \hat{z}|\ell, m\rangle &= \langle \hat{z}|\ell, 0\rangle \, \delta_{0m} = Y_\ell^0(\theta = 0, \phi)\delta_{0m} \\ &= \sqrt{\frac{(2\ell+1)}{4\pi}} \, P_\ell(\cos\theta)|_{\theta=0} \, \delta_{0m} \\ \rightsquigarrow \langle \hat{z}|\ell, m\rangle &= \sqrt{\frac{(2\ell+1)}{4\pi}} \delta_{0m} \end{aligned}$$

Substituting in Eq. 11.103, we obtain:

$$Y_\ell^m(\theta, \phi)^* = \langle \ell, m| \, U(\theta, \phi) \, |\ell, 0\rangle \sqrt{\frac{(2\ell+1)}{4\pi}}. \tag{11.104}$$

11.4 Potentials with spherical symmetry

We have proven that systems with a spherical symmetry have a Hamiltonian which commutes with the generators of rotations. The common eigenstates of J^2 and J_3 should also be eigenstates of the Hamiltonian, satisfying:

$$H \, |E, \ell, m\rangle = E \, |E, \ell, m\rangle \, , \tag{11.105a}$$
$$L^2 \, |E, \ell, m\rangle = \hbar^2 \ell(\ell+1) \, |E, \ell, m\rangle \, , \tag{11.105b}$$
$$L_3 \, |E, \ell, m\rangle = \hbar m \, |E, \ell, m\rangle \, . \tag{11.105c}$$

The Hamiltonian of a particle inside a spherically symmetric potential

$$H = \frac{p^2}{2M} + V(r), \tag{11.106}$$

where the potential $V(r)$ is a function only of the magnitude of a spatial distance, is invariant under rotations. Indeed, we can easily compute that:

$$[r_i, L_j] = i\hbar\epsilon_{ijk} r_k \tag{11.107a}$$
$$[p_i, L_j] = i\hbar\epsilon_{ijk} p_k \tag{11.107b}$$
$$\left[p^2, L_i\right] = 0 \tag{11.107c}$$
$$\left[r^2, L_i\right] = 0 \tag{11.107d}$$

from which we conclude that

$$[H, L_i] = 0. \tag{11.108}$$

Recall that

$$\langle \mathbf{r}|E, \ell, m\rangle = \psi_{E,\ell,m}(r) Y_\ell^m(\theta, \phi)\,. \tag{11.109}$$

and from Eq. 11.57, we also obtain that

$$\langle \mathbf{r}|\, p^2\, |E, \ell, m\rangle = -\hbar^2 \left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) - \frac{\ell(\ell+1)}{r^2}\right] \psi_{E,\ell,m}(r) Y_\ell^m(\theta, \phi). \tag{11.110}$$

From Eq. 11.105a we obtain a differential equation for the radial part of the wave-function

$$\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) - \frac{\ell(\ell+1)}{r^2} - \frac{2M(V(r)-E)}{\hbar^2}\right] \psi_{E,\ell,m}(r) = 0. \tag{11.111}$$

Notice that the "radial" wavefunction does not depend on the eigenvalue m of L_3,

$$\psi_{E,\ell,m}(r) \equiv \psi_{E,\ell}(r)\,. \tag{11.112}$$

We write,

$$\psi_{E,\ell}(r) = \frac{R(r)}{r}\,, \tag{11.113}$$

which yields

$$0 = R''(r) - \left[\frac{\ell(\ell+1)}{r^2} + \frac{2M(V(r)-E)}{\hbar^2}\right] R(r)\,. \tag{11.114}$$

Exercise 11.1. *Solve this equation in the case of a free particle $V(r) = 0$.*

Exercise 11.2. *Solve this equation for a spherical well $V(r) = V_0\Theta(r < r_0)$.*

11.5 The hydrogen atom

We are now in position to discuss a simplified version of the hydrogen atom, where we ignore the spin of the electron. The potential is given by

$$V(r) = -\frac{Ze^2}{r}. \tag{11.115}$$

Exercise 11.3. *Solve Eq. 11.114 for the hydrogen atom potential.*

In this section, we shall determine algebraically the energy spectrum of the hydrogen atom. Consider the operator

$$\mathbf{R} = -\frac{Ze^2\mathbf{r}}{r} + \frac{1}{2m}\left(\mathbf{p}\times\mathbf{L} - \mathbf{L}\times\mathbf{p}\right) \tag{11.116}$$

where

$$\mathbf{L} = \mathbf{r}\times\mathbf{p}.$$

This is the quantum mechanics analogue of the Runge-Lenz vector, a conserved quantity in classical mechanics for the Coulomb potential. Note that

$$\left[r_i, L^2\right] = i\epsilon_{ijk}(L_j r_k - r_j L_k) \tag{11.117a}$$

$$\left[p_i, L^2\right] = i\epsilon_{ijk}(L_j p_k - p_j L_k) \tag{11.117b}$$

or equivalently,

$$\left[\mathbf{r}, L^2\right] = i(\mathbf{L}\times\mathbf{r} - \mathbf{r}\times\mathbf{L}) \tag{11.118a}$$

$$\left[\mathbf{p}, L^2\right] = i(\mathbf{L}\times\mathbf{p} - \mathbf{p}\times\mathbf{L}) \tag{11.118b}$$

We can then rewrite,

$$R_i = -\frac{Ze^2 r_i}{r} + \frac{\left[L^2, p_i\right]}{2mi}. \tag{11.119}$$

The vector operator R_i can be easily shown from above to be Hermitian,

$$R_i^\dagger = R_i.$$

As anticipated from our experience with classical mechanics, it commutes with the Hamiltonian (**exercise**).

$$[H, R_i] = 0, \tag{11.120}$$

with

$$H = \frac{p^2}{2m} - \frac{Ze^2}{r}. \tag{11.121}$$

The Runge-Lenz vector is orthogonal to the angular momentum:

$$\mathbf{L}\cdot\mathbf{R} = \mathbf{R}\cdot\mathbf{L} = 0. \tag{11.122}$$

Also, we can prove the following identities (**exercise**):

$$\mathbf{L} \times \mathbf{p} = -\mathbf{p} \times \mathbf{L} + 2i\hbar\mathbf{p}\,. \tag{11.123a}$$

$$\begin{aligned} \mathbf{r} \cdot (\mathbf{p} \times \mathbf{L}) &= r_i \epsilon_{ijk} p_j L_k \\ &= (\epsilon_{kij} r_i p_j) L_k \\ &= L_k L_k \\ &= \mathbf{L}^2, \end{aligned} \tag{11.123b}$$

$$\begin{aligned} (\mathbf{p} \times \mathbf{L}) \cdot \mathbf{r} &= \epsilon_{ijk} p_j L_k r_i \\ &= \epsilon_{ijk} p_j \left([L_k, r_i] + r_i L_k\right) \\ &= i\hbar \epsilon_{kij} \epsilon_{ki\ell} p_j r_\ell + L^2 \\ &= L^2 + i\hbar 2\delta_{j\ell} p_j r_\ell \\ &= L^2 + 2i\hbar \mathbf{p} \cdot \mathbf{r}\,. \end{aligned} \tag{11.123c}$$

Similarly,

$$(\mathbf{p} \times \mathbf{L})^2 = p^2 L^2\,, \tag{11.124a}$$

$$\mathbf{p} \cdot (\mathbf{p} \times \mathbf{L}) = 0\,, \tag{11.124b}$$

$$(\mathbf{p} \times \mathbf{L}) \cdot \mathbf{p} = 2i\hbar p^2\,, \tag{11.124c}$$

and

$$\left[\frac{r_i}{r}, p_i\right] = \frac{2i\hbar}{r}. \tag{11.125}$$

For the square of the Runge-Lenz vector we find,

$$\begin{aligned} R^2 &= \left(-\frac{Ze^2\mathbf{r}}{r} + \frac{\mathbf{p} \times \mathbf{L}}{m} - \frac{i\hbar}{m}\mathbf{p}\right)^2 \\ &= \dots \\ &= Z^2 e^4 + 2\left(\frac{p^2}{2m} - \frac{Ze^2}{r}\right)\left(\hbar^2 + L^2\right). \end{aligned} \tag{11.126}$$

Thus,

$$R^2 = Z^2 e^4 + \frac{2H}{m}\left(\hbar^2 + L^2\right). \tag{11.127}$$

We can then determine the eigenvalues of the hydrogen-atom Hamiltonian if we know the eigenvalues of R^2. We shall do this by means of an algebraic method.

We find (**exercise**) the following commutation relations:

$$[R_i, R_j] = \frac{-2H}{m} i\hbar \epsilon_{ijk} L_k \tag{11.128a}$$

$$[L_i, R_j] = i\hbar \epsilon_{ijk} R_k\,. \tag{11.128b}$$

We also recall,

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k\,. \tag{11.128c}$$

We now define,

$$A_i^{\pm} = \frac{1}{2}\left(L_i \pm \sqrt{\frac{m}{-2H}}R_i\right) \tag{11.129}$$

The new operators satisfy the algebra,

$$\left[A_i^{\pm}, A_j^{\pm}\right] = i\hbar\epsilon_{ijk}A_k^{\pm} \tag{11.130a}$$

and

$$\left[A_i^{\pm}, A_j^{\mp}\right] = 0\,. \tag{11.130b}$$

which is our familiar algebra of angular momentum. Notice that the operators $A^{\pm}$ are Hermitian if the Hamiltonian has negative eigenvalues, i.e. for negative energies. For the squares $(A^{\pm})^2$, we find that

$$\begin{aligned}(A^{\pm})^2 &= \frac{1}{4}\left[L^2 - \frac{m}{2H}R^2\right],\\ &= \frac{1}{4}\left[L^2 - \frac{m}{2H}\left(Z^2e^4 + \frac{2H}{m}\left(\hbar^2 + L^2\right)\right)\right]\\ \rightsquigarrow (A^{\pm})^2 &= -\frac{\hbar^2}{4} - \frac{m}{8H}Z^2e^4.\end{aligned} \tag{11.131}$$

According to the Lie-algebra for the $A^{\pm}$ operators, the eigenvalues of the $(A^{\pm})^2$ are,

$$\hbar^2 j(j+1), \quad j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots \tag{11.132}$$

Thus, for the energy eigenvalues E, we must have

$$\hbar^2 j(j+1) = -\frac{\hbar^2}{4} - \frac{m}{8E_j}Z^2e^4 \tag{11.133}$$

or, equivalently,

$$E_n = -Z^2\frac{me^4}{2\hbar^2}\frac{1}{n^2} \tag{11.134}$$

with

$$n = (2j+1)^2 = 1, 2, \ldots \tag{11.135}$$

Notice that we have obtained only negative eigenvalues. For states with positive energy eigenvalues, the operators $A_i^{\pm}$ are not Hermitian and our derivation of the selection rules based on the Lie algebra does not go through.

Both $\left(A^{\pm}\right)^2$ operators have a $2j+1 = n$-fold degeneracy which can be revealed by the action of the $A_3^{\pm}$ operators on them. Since the $\left(A^{\pm}\right)^2$ operators are independent, an eigenstate of the Hamiltonian will have a $(2j+1)^2 = n^2-$fold degeneracy.

11.5.1 $SO(4)$ symmetry of hydrogen atom

The Lie algebra for group the group of rotations $SO(N)$ in N dimensions is given by:

$$[J_{ab}, J_{cd}] = -i\hbar\left(\delta_{ad}J_{bc} - \delta_{ac}J_{bd} + \delta_{bc}J_{ad} - \delta_{bd}J_{ac}\right) \tag{11.136}$$

with $a, b, c, d = 1 \ldots N$ and $J_{ab} = -J_{ba}$. Obviously, this group contains rotations in three-dimensions as a subgroup. For $J_{12} \equiv L_3, J_{23} = L_1, J_{31} = L_2$, the commutation relation above takes the familiar form:

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k. \tag{11.137a}$$

where $i, j, k = 1, 2, 3$. For the remaining three generators: J_{14}, J_{24}, J_{34}, the commutation relations yield:

$$[J_{14}, J_{j4}] = i\hbar\epsilon_{ijk}L_k, \quad i, j = 1 \ldots 3\,. \tag{11.137b}$$

and

$$[L_i, J_{j4}] = i\hbar\epsilon_{ijk}J_{k4}\,. \tag{11.137c}$$

Setting,

$$R_i \equiv \sqrt{\frac{-2H}{m}}J_{i4}, \tag{11.138}$$

we recognize the Lie algebra of Eqs (11.128a)-(11.128c). The hydrogen atom has an $SO(4)$ symmetry, which is a larger symmetry than rotation invariance in three dimensions $SO(3)$.

Chapter 12

Addition of angular momenta

A particle such as an electron in an atom, can have more than one type of angular momentum: For example, spin and orbital angular momentum. These two types will be described by *independent* generators of angular momenta living in different representations: J_a, J_b with

$$[J_{ai}, J_{bj}] = 0, \quad i, j = 1 \dots 3\,. \tag{12.1a}$$

As is required for such generators, they satisfy the same Lie algebra:

$$[J_{ai}, J_{aj}] = i\hbar\epsilon_{ijk} J_{ak} \tag{12.1b}$$

$$[J_{bi}, J_{bj}] = i\hbar\epsilon_{ijk} J_{bk} \tag{12.1c}$$

Therefore, there exist common eigenstates of the operators: $J_a^2, J_b^2, J_{a3}, J_{b3}$, with eigenvalues:

$$J_a^2 \left|j_a, m_a, j_b, m_b\right\rangle = \hbar^2 j_a(j_a+1) \left|j_a, m_a, j_b, m_b\right\rangle \tag{12.2a}$$

$$J_b^2 \left|j_a, m_a, j_b, m_b\right\rangle = \hbar^2 j_b(j_b+1) \left|j_a, m_a, j_b, m_b\right\rangle \tag{12.2b}$$

$$J_{a3} \left|j_a, m_a, j_b, m_b\right\rangle = \hbar m_a \left|j_a, m_a, j_b, m_b\right\rangle \tag{12.2c}$$

$$J_{b3} \left|j_a, m_a, j_b, m_b\right\rangle = \hbar m_b \left|j_a, m_a, j_b, m_b\right\rangle \tag{12.2d}$$

12.1 Addition of angular momenta

The sum of the two angular momenta,

$$J_i = J_{ai} + J_{bi}, \tag{12.3}$$

satisfies the same Lie algebra,

$$[J_i, J_j] = i\hbar\epsilon_{ijk} J_k \tag{12.4}$$

Notice that the operators J_a^2 and J_b^2 commute with all the components of the total angular momentum:

$$\left[J_a^2, J_i\right] = \left[J_b^2, J_i\right] = 0 \tag{12.5}$$

We can then find common eigenstates of the J^2, J_3, J_a^2, J_b^2 operators:

$$|j, m, j_a, j_b\rangle$$

with

$$J_a^2 |j, m, j_a, j_b\rangle = \hbar^2 j_a(j_a+1) |j, m, j_a, j_b\rangle \tag{12.6a}$$
$$J_b^2 |j, m, j_a, j_b\rangle = \hbar^2 j_b(j_b+1) |j, m, j_a, j_b\rangle \tag{12.6b}$$
$$J^2 |j, m, j_a, j_b\rangle = \hbar^2 j(j+1) |j, m, j_a, j_b\rangle \tag{12.6c}$$
$$J_3 |j, m, j_a, j_b\rangle = \hbar m |j, m, j_a, j_b\rangle \tag{12.6d}$$

The states $|j, m, j_a, j_b\rangle$ can be written as a linear superposition of states: $|j_a, m_a, j_b, m_b\rangle$:

$$|j, m, j_a, j_b\rangle = \sum_{m_a, m_b} |j_a, m_a, j_b, m_b\rangle \langle j_a, m_a, j_b, m_b|j, m, j_a, j_b\rangle . \tag{12.7}$$

The coefficients

$$\langle j_a, m_a, j_b, m_b|j, m, j_a, j_b\rangle$$

are known as *Clebsch-Gordan coefficients*.
From Eq. 12.7, it is easy to infer that

$$\sum_{m_a, m_b} |\langle j_a, m_a, j_b, m_b|j, m, j_a, j_b\rangle|^2 = 1 . \tag{12.8}$$

From the definition of the total angular momentum, we have that

$$\begin{aligned} 0 &= \langle j_a, m_a, j_b, m_b| J_3 - J_{a3} - J_{b3} |j, m, j_a, j_b\rangle \\ &= (m - m_a - m_b) \langle j_a, m_a, j_b, m_b|j, m, j_a, j_b\rangle . \end{aligned} \tag{12.9}$$

This leads to the conclusion that,

$$\langle j_a, m_a, j_b, m_b|j, m, j_a, j_b\rangle = \langle j_a, m_a, j_b, m_b|j, m, j_a, j_b\rangle \, \delta_{m, m_a+m_b} . \tag{12.10}$$

Finally, we recall that

$$J_\pm = J_1 \pm i J_2 , \tag{12.11a}$$
$$J_{a\pm} = J_{a1} \pm i J_{a2} , \tag{12.11b}$$
$$J_{b\pm} = J_{b1} \pm i J_{b2} , \tag{12.11c}$$

with

$$J_\pm = J_{a\pm} + J_{b\pm} , \tag{12.11d}$$

are *rising/lowering* operators of the m, m_a, m_b eigenvalues respectively. We then obtain, from the last equation,

$$\begin{aligned}\langle j_a, m_a, j_b, m_b | \, J_\pm \, | j, m, j_a, j_b \rangle = \langle j_a, m_a, j_b, m_b | \, J_{a\pm} \, | j, m, j_a, j_b \rangle \\ + \langle j_a, m_a, j_b, m_b | \, J_{b\pm} \, | j, m, j_a, j_b \rangle\end{aligned} \tag{12.12}$$

which yields:

$$\begin{aligned}&\langle j_a, m_a, j_b, m_b | j, m \pm 1, j_a, j_b \rangle \\ &= \sqrt{\frac{j_a(j_a+1) - m_a(m_a \pm 1)}{j(j+1) - m(m \pm 1)}} \, \langle j_a, m_a \pm 1, j_b, m_b | j, m, j_a, j_b \rangle \\ &\quad + \sqrt{\frac{j_b(j_b+1) - m_b(m_b \pm 1)}{j(j+1) - m(m \mp 1)}} \, \langle j_a, m_a, j_b, m_b \pm 1 | j, m, j_a, j_b \rangle\end{aligned} \tag{12.13}$$

The maximum value for j is ,

$$j_{\max} = j_a + j_b$$

and there is only one such state

$$|j = j_a + j_b, m = j_a + j_b, j_a, j_b\rangle = |j_a, m_a = j_a, j_b, m_b = j_b\rangle \, , \quad (\textbf{exercise}) \, .$$

Therefore,

$$\langle j_a, j_a, j_b, j_b | j, m, j_a, j_b \rangle = \delta_{j, j_a + j_b} \delta_{m, j_a + j_b} \, . \tag{12.14}$$

Acting with an J_- on both sides, we obtain a state with $j = j_a + j_b$ and $m = j_a + j_b - 1$,

$$\begin{aligned}|j_a + j_b, j_a + j_b - 1, j_a, j_b\rangle = \sqrt{\frac{j_a}{j_a + j_b}} \, |j_a, j_a - 1, j_b, j_b\rangle \\ + \sqrt{\frac{j_b}{j_a + j_b}} \, |j_a, j_a, j_b, j_b - 1\rangle \, .\end{aligned} \tag{12.15}$$

There is only one more state with $m = j_a + j_b - 1$. This must have $j = j_a + j_b - 1$. Since it has a different quantum number j it must be orthogonal to the previous state:

$$0 = \langle j_a + j_b, j_a + j_b - 1, j_a, j_b | j_a + j_b - 1, j_a + j_b - 1, j_a, j_b \rangle = 0 \tag{12.16}$$

This condition allows us to determine the state (up to a phase):

$$\begin{aligned}|j_a + j_b - 1, j_a + j_b - 1, j_a, j_b\rangle = \sqrt{\frac{j_b}{j_a + j_b}} \, |j_a, j_a - 1, j_b, j_b\rangle \\ - \sqrt{\frac{j_a}{j_a + j_b}} \, |j_a, j_a, j_b, j_b - 1\rangle \, .\end{aligned} \tag{12.17}$$

We can repeat this procedure until it is not possible to create a new state due to exhausting the range of m_a and m_b. We find a number of $(2j_a+1)(2j_b+1)$ and the quantum numbers of the total angular momentum take discrete values in the range: $j = |j_a - j_b| \ldots j_a + j_b, \quad m = -j \ldots j$.
The above conventions lead to real-valued Clebsch-Gordan coefficients. Clebsch-Gordan coefficients are the coefficients for the linear transformation from a complete set of states

$$|j_1, m_1, j_2, m_2\rangle$$

to another complete set

$$|j, m, j_1, j_2\rangle \ .$$

Consider in general two complete sets of states:

$$\{|\psi_i\rangle\} \quad \text{and} \quad \{|\phi_i\rangle\}$$

with

$$\langle\phi_i|\phi_j\rangle = \langle\psi_i|\psi_j\rangle = \delta_{ij} \ ,$$

and the sets are related by a linear transformation with real coefficients:

$$|\phi_i\rangle = \sum_j C_{ij} \, |\psi_j\rangle \, . \tag{12.18}$$

Then

$$\begin{aligned} \delta_{kl} &= \langle\phi_k|\phi_l\rangle \\ &= \sum_{jm} C_{km} C_{lj} \, \langle\psi_j|\psi_m\rangle \\ &= \sum_j C_{kj} C_{lj} \\ &= \sum_j C_{kj} C^T_{jl} \end{aligned} \tag{12.19}$$

which leads to

$$\det C = 1$$

and

$$C^{-1} = C^T \, .$$

From the above,

$$\begin{aligned} C^T C &= 1 \\ \rightsquigarrow \sum_j C_{ji} C_{jk} &= \delta_{ik} \end{aligned}$$

We can then invert Eq 12.18 to read,

$$|\psi_i\rangle = \sum_j C_{ji} |\phi_j\rangle$$

Applying the above for the Clebsch-Gordan coefficients, we derive that:

$$\begin{aligned} &\sum_{j,m} \langle j_1, m_a, j_2, m_b | j, m, j_1, j_2\rangle \langle j_1, m_c, j_2, m_d | j, m, j_1, j_2\rangle \\ &\quad = \delta_{m_a, m_c} \delta_{m_b, m_d}. \end{aligned} \tag{12.20}$$

and we can also invert to write:

$$|j_1, m_1, j_2, m_2\rangle = \sum_{j,m} |j, m, j_1, j_2\rangle \langle j_1, m_1, j_2, m_2 | j, m, j_1, j_2\rangle . \tag{12.21}$$

12.2 Application: Hydrogen atom

The hydrogen atom has an n^2 degeneracy as we have found earlier. The general solution for the wave-function is of the form:

$$\psi(\mathbf{r}) = \frac{R_{n\ell}(r)}{r} Y_\ell^m(\theta, \phi). \tag{12.22}$$

The degeneracy in this form is due to the fact that the energy levels depend only on n but not not ℓ, m. Given that the number of degenerate states is finite, the value of ℓ must be bounded:

$$\ell = 0, \ldots, \ell_{max}.$$

The number of degenerate states is then

$$n^2 = \sum_{\ell=0}^{\ell_{max}} (2\ell + 1) = (\ell_{max} + 1)^2. \tag{12.23}$$

From the above we conclude that the range of ℓ is

$$\ell = 0, \ldots, n - 1. \tag{12.24}$$

The total angular momentum of the electron in the hydrogen atom is the sum of its spin and the orbital angular momentum:

$$J = L + S \tag{12.25}$$

In the ground state, $n = 1$, the orbital angular momentum is zero. The only possibility for j is $j = \frac{1}{2}$. A general hydrogen state is denoted by:

$$n\ell_j,$$

where $\ell = 0, 1, 2, 3, 4, \ldots, n-1$ is represented by the letters

$$s, p, d, f, g, \text{ and then alphabetically.}$$

The hydrogen states are

$$1s_{\frac{1}{2}}, 2p_{\frac{3}{2}}, 2p_{\frac{1}{2}}, 2s_{\frac{1}{2}}, 3d_{\frac{5}{2}}, 3d_{\frac{3}{2}}, 3p_{\frac{3}{2}}, 3p_{\frac{1}{2}}, 3s_{\frac{1}{2}}, \ldots \tag{12.26}$$

The interaction $\mathbf{L} \cdot \mathbf{S}$ splits the energy levels with same n, ℓ but different j. This splitting is known as the fine structure of the hydrogen atom. An even finer splitting (hyperfine splitting) is found by combining the spin of the electron with the spin of the proton and the interaction is due to the magnetic field of the proton.

Chapter 13

Discrete symmetries

In this chapter, we shall discuss symmetry transformations which cannot be connected to the unity by varying a continuous parameter. Such symmetries are *space inversion* (mirror symmetry/parity) and *time reversal*.

This chapter was not taught in 2022. It is recommended as elective reading for the students. It will be taught in the QMII course of 2023.

13.1 Parity

Under a parity transformation in classical physics, the position vector changes sign

$$\mathbf{r} \to -\mathbf{r}\,. \tag{13.1}$$

We would like to preserve this property for the expectation value of the position operator

$$\langle\psi|\,\hat{\mathbf{r}}\,|\psi\rangle \to -\,\langle\psi|\,\hat{\mathbf{r}}\,|\psi\rangle \tag{13.2}$$

Under a parity transformation, a state changes as:

$$|\psi\rangle \to |\psi'\rangle = \Pi\,|\psi\rangle\,, \tag{13.3}$$

which suggest that we can achieve of our requirement of Eq. 13.2 if

$$\Pi^\dagger \hat{\mathbf{r}} \Pi = -\hat{\mathbf{r}}. \tag{13.4}$$

According to the above,

$$\begin{aligned} \hat{\mathbf{r}}\left(\Pi\,|\mathbf{r}\rangle\right) &= -\Pi\left(\hat{\mathbf{r}}\,|\mathbf{r}\rangle\right) \\ &= -\mathbf{r}(\Pi\,|\mathbf{r}\rangle)\,. \end{aligned} \tag{13.5}$$

Therefore, the state $\Pi\,|\mathbf{r}\rangle$ describes the same physics as the state $|-\mathbf{r}\rangle$. We then have:

$$\Pi\,|\mathbf{r}\rangle = e^{i\delta}\,|-\mathbf{r}\rangle\,. \tag{13.6}$$

Conventionally, we shall choose the phase to be zero:

$$\Pi \left|\mathbf{r}\right\rangle = \left|-\mathbf{r}\right\rangle . \tag{13.7}$$

Acting twice on a position state, the parity operator has no effect:

$$\begin{aligned} \Pi^2 \left|\mathbf{r}\right\rangle &= \Pi \left|-\mathbf{r}\right\rangle \\ &= \left|\mathbf{r}\right\rangle . \end{aligned} \tag{13.8}$$

Given that the position eigenkets form a complete basis, we have that:

$$\Pi^2 = 1 . \tag{13.9}$$

Thus, the representation Π of the parity transformation is unitary and hermitian, satisfying

$$\Pi^\dagger = \Pi^{-1} = \Pi . \tag{13.10}$$

Let's consider a space-translation operator

$$U(\Delta\mathbf{r}) = 1 - i\frac{\mathbf{p}\cdot\Delta\mathbf{r}}{\hbar}$$

acting on a position eigenket $\left|\mathbf{r}\right\rangle$. We have

$$\Pi U(\Delta\mathbf{r}) \left|\mathbf{r}\right\rangle = \left|-\mathbf{r}-\Delta\mathbf{r}\right\rangle \tag{13.11}$$

Also,

$$U(-\Delta\mathbf{r})\Pi \left|\mathbf{r}\right\rangle = \left|-\mathbf{r}-\Delta\mathbf{r}\right\rangle . \tag{13.12}$$

Equating the lhs of the last equations we have

$$\Pi U(\Delta\mathbf{r}) = U\left(-\Delta\mathbf{r}\right)\Pi , \tag{13.13}$$

$$\rightsquigarrow \Pi U(\Delta\mathbf{r})\Pi = U(-\Delta\mathbf{r}) . \tag{13.14}$$

This leads to the following transformation for the momentum operator under parity:

$$\Pi\,\hat{\mathbf{p}}\,\Pi = -\hat{\mathbf{p}} . \tag{13.15}$$

We can repeat this analysis for angular momentum, the generators of rotations. An infinitesimal rotation is represented by

$$U(\omega_{ij}) = 1 + \frac{i}{2\hbar}\omega_{ij}J^{ij} \tag{13.16}$$

and

$$U(\omega_{ij}) \left|r_i\right\rangle = \left|r_i + \omega_{ij}r_j\right\rangle . \tag{13.17}$$

We find that

$$\begin{aligned}\Pi U(\omega_{ij})\Pi\,|r_i\rangle &= \Pi U(\omega_{ij})\,|-r_i\rangle \\ &= \Pi\,|-r_i-\omega_{ij}r_j\rangle \\ &= |r_i+\omega_{ij}r_j\rangle \\ &= U(\omega_{ij})\,|r_i\rangle\,.\end{aligned} \tag{13.18}$$

Therefore,

$$\Pi U(\omega_{ij})\Pi = U(\omega_{ij})\,. \tag{13.19}$$

For the angular momentum operators the above equation implies that

$$\Pi\, J_i \Pi = J_i\,. \tag{13.20}$$

(recall that $\hbar J^{12} = J_3, \ldots$).

For a system which is symmetric under parity, the energy eigenstates are also parity eigenstates:

$$\Pi\,|\pi\rangle = \pi\,|\pi\rangle\,. \tag{13.21}$$

The parity operator satisfies,

$$\Pi^2 = 1\,. \tag{13.22}$$

The same identity must be fulfilled by the eigenvalues. Therefore, we have two parity eigenstates $|\pi\rangle = |\pm\rangle$ with eigenvalues ± 1:

$$\Pi\,|\pm\rangle = \pm\,|\pm\rangle\,. \tag{13.23}$$

Multiplying with a position bra, we find

$$\langle\mathbf{r}|\,\Pi\,|\pm\rangle = \pm\,\langle\mathbf{r}|\pm\rangle\,, \tag{13.24}$$

$$\langle -\mathbf{r}|\pm\rangle = \pm\,\langle\mathbf{r}|\pm\rangle\,. \tag{13.25}$$

As we have remarked above in a parity conserving system partity eigenstates are also energy eigenstates. Therefore, the wavefunctions

$$\psi_\pm(\mathbf{r}) \equiv \langle\mathbf{r}|\pm\rangle\,,$$

are either even or odd under $\mathbf{r}\to-\mathbf{r}$:

$$\psi_\pm(\mathbf{r}) = \pm\psi_\pm(-\mathbf{r})\,. \tag{13.26}$$

13.2 Time reversal

Let's consider a system which is symmetric under time reversal:

$$t \to -t\,.$$

In this section, we shall explore the properties of the representation Θ of time-reversal on quantum states:

$$|\psi\rangle \to \Theta\,|\psi\rangle\,.$$

The time translation operator, for infinitessimal time intervals, is:

$$U(\delta t) = 1 - i\frac{H}{\hbar}\delta t \tag{13.27}$$

Acting on a generic state $|\psi, t\rangle$, we have

$$\begin{aligned} \Theta^{-1}U(-\delta t)\Theta\,|\psi, t\rangle &= \Theta^{-1}U(-\delta t)\,|\psi, -t\rangle \\ &= \Theta^{-1}\,|\psi, -t-\delta t\rangle \\ &= |\psi, t+\delta t\rangle \\ &= U(\delta t)\,|\psi, t\rangle\,. \end{aligned} \tag{13.28}$$

Therefore,

$$\Theta^{-1}U(-\delta t)\Theta = U(\delta t)\,. \tag{13.29}$$

Substituting the expression for the operator of an infinitesimaly small time evolution, we have:

$$\Theta^{-1}(-iH)\Theta = iH. \tag{13.30}$$

The representation Θ cannot be unitary and linear. If it were the case, we would derive that

$$\Theta^{-1}H\Theta = -H \tag{13.31}$$

and, equivalently,

$$\Theta H = -H\Theta. \tag{13.32}$$

Assume that there is a state $|E\rangle$ which is an eigenstate of the Hamiltonian:

$$H\,|E\rangle = E\,|E\rangle\,. \tag{13.33}$$

Then, for the state $\Theta\,|E\rangle$, we find that is also an energy eigenstate, however with an energy eigenvalue $-E$:

$$\begin{aligned} H\left(\Theta\,|E\rangle\right) &= -\Theta\left(H\,|E\rangle\right) \\ &= -E\left(\Theta\,|E\rangle\right). \end{aligned} \tag{13.34}$$

This is in contradiction with observations. For free particles it predicts erroneously negative energies.
The above problem is solved if Θ is antilinear and antiunitary. Eq. 13.30 gives

$$\begin{aligned} &\Theta(-iH)\Theta = iH\,. \\ &\rightsquigarrow i\Theta H\Theta = iH \\ &\rightsquigarrow \Theta H\Theta = H \end{aligned} \tag{13.35}$$

Equivalently,

$$\Theta H = H\Theta\,. \tag{13.36}$$

Classically, time reversal changes:

$$\mathbf{r} \to \mathbf{r}\,, \tag{13.37a}$$
$$\mathbf{p} \to -\mathbf{p}\,. \tag{13.37b}$$

The classical transformation rules should also hold for the expectation values of the corresponding quantum operators. Thus, we must have

$$\Theta^{-1}\hat{\mathbf{r}}\Theta = \hat{\mathbf{r}} \tag{13.38}$$

and

$$\Theta^{-1}\hat{\mathbf{p}}\Theta = -\hat{\mathbf{p}} \tag{13.39}$$

This is consistent with the commutation relations:

$$\begin{aligned}
\Theta^{-1}\left[r_i, p_j\right]\Theta &= \Theta^{-1} i\hbar\delta_{ij}\Theta \\
\left[\Theta^{-1} r_i \Theta, \Theta^{-1} p_j \Theta\right] &= -i\hbar\delta_{ij} \\
\left[r_i, -p_j\right] &= -i\hbar\delta_{ij} \\
\left[r_i, p_j\right] &= i\hbar\delta_{ij}\,.
\end{aligned} \tag{13.40}$$

The Lie-algebra of angular momentum is

$$\left[J_i, J_j\right] = i\epsilon_{ijk}J_k\,. \tag{13.41}$$

This leads to

$$\left[-\Theta^{-1}J_i\Theta, -\Theta^{-1}J_j\Theta\right] = i\epsilon_{ijk}\left(-\Theta^{-1}J_k\Theta\right), \tag{13.42}$$

which implies that

$$\Theta^{-1}J_i\Theta = -J_i\,. \tag{13.43}$$