Phys 234 with Raffi Budakian

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2026 W

Contents

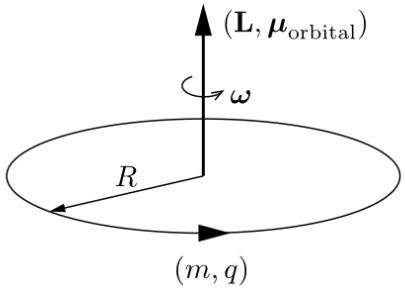
1 Introduction

Lecture 1 - Tuesday, January 06

In our development of quantum theory, we will focus on a set of experiments performed by Otto Stern and Walther Gerlach in 1922, which revealed the electron possesses an intrinsic magnetic moment that is quantized. The series of experiments that have come to be known as the Stern-Gerlach experiments were some of the first measurements that demonstrated the foundational concepts of quantum theory.

1.1 A Classical Description of Orbital Magnetic Moment

Before introducing the S-G experiments, let's look at the interaction of a magnetic moment with an external magnetic field.



Consider the motion of a charged particle with mass m and charge q moving in a circular orbit or radius R. From the laws of classical mechanics, we know that the particle has an angular momentum given by

$$\mathbf{L} = I\omega \tag{1}$$

where $I = mR^2$ is the moment of inertia of the particle, and ω is the angular velocity.

We also know from the laws of electricity and magnetism that a circulating loop of current produces a magnetic moment

$$\mu_{\text{orbital}} = i\ \mathbf{A} \tag{2}$$

where i is the electrical current and $\mathbf{A}$ is the area vector, whose magnitude corresponds to the area enclosed by the current, and whose direction is normal to the plane of the orbit.

If we express equations (1, 2) in terms of the circular orbit, then we can find a simple expression for the magnetic moment in terms of the angular momentum.

$$\mathbf{L} = mR^2\omega \tag{3}$$

$$\begin{aligned} \boldsymbol{\mu}_{\mathbf{orbital}} &= \left(\frac{\Delta q}{\Delta t}\right)\pi R^2\hat{\mathbf{z}} \\ &= \frac{\omega q}{2\pi}\pi R^2\hat{\mathbf{z}} \end{aligned} \tag{4}$$

where the direction $\hat{\mathbf{z}}$ is taken to be normal to the plane of the orbit.

1.1.1 Interaction of a Magnetic Moment with Magnetic Fields

$$\begin{aligned}\mu_{\textbf{orbital}} &= \frac{\omega q R^2}{2}\hat{\mathbf{z}} \\ &= \left(\frac{q}{2m}\right)\mathbf{L}\end{aligned}$$

$$\boxed{\mu_{\text{orbital}} = \left(\frac{q}{2m}\right)\mathbf{L}} \tag{5}$$

1.1.2 Intrinsic Magnetic Moment (Spin)

We see that from a purely classical description, a charged particle with angular momentum also has magnetic moment. Interestingly, the ratio of the angular momentum and the orbital magnetic moment is proportional only the charge-to-mass ratio, and does not involve quantities, such as the radius, that are particular to the orbit of the particle.

The connection between angular momentum and magnetic moment, in fact is very deep. It turns out that elementary particles, such as the proton, electron, neutron, muon, etc. have an intrinsic angular momentum and a magnetic moment. The name given to the intrinsic magnetic moment is "spin"— the name motivated by the classical notion of a rotating charged object, having both angular momentum and magnetic moment.

Note 1.1. Though the term spin implies a rotating body, the particle is not physically spinning. Spin is a fundamental property of a particle, like its mass or charge.

The intrinsic or spin magnetic moment is expressed as

$$\mu_{\text{spin}} = g\left(\frac{q}{2m}\right)\mathbf{S}$$

Comment 1.1. The factor g, known as the "g-factor" is a multiplicative factor, that modifies the classical result we found earlier in eq.(5). For classical orbital motion $g = 1$.

- In 1928, Paul Dirac showed that for certain class of particles, such as electrons, $g = 2$, if quantum theory is made consistent with special relativity.

  Comment 1.2. The relativistic quantum theory also predicted antimatter.

- In 1933, Dirac and Schrödinger were awarded the Nobel Prize in Physics for "For the discovery of new productive forms of atomic theory."

- In 1965, Feynman, Schwinger, and Tomonaga were awarded the Nobel Prize in Physics for their theory of Quantum Electrodynamics (QED), which unified electricity and magnetism and quantum mechanics.

Using QED, it possible to calculate corrections to $g = 2$. For an electron the g-factor has been calculated to be

$$g \approx 2.00231930436256(35)$$

Comment 1.3. This is the most precise constant of nature known.

Comment 1.4. The calculated and measured values of the electron g-factor agree to 35 parts in 10^{14}. This is the equivalent of measuring the diameter of the earth to the precision of the width of a hair. This remarkable agreement is a triumph of quantum theory.

Discovery 1.1. You may have heard of the g-2 experiment in Fermi Lab, whose goal is to measure the g-factor of the muons – a heavier cousin of the electron.
The aim of these experiments is to probe the extent to which experiment and theory agree in predicting the muon g-factor. Discrepancies could point to theories that lie outside of the Standard Model – our best theory describing elementary particles and forces.

For the rest of this section, I will refer to μ_{orbital} as μ.

In the presence of a uniform magnetic field $\mathbf{B}$, a magnetic moment μexperiences a torque that tries to make $\mathbf{B} \| \mu$. The torque acts in a direction that tries to lower the potential energy of μ. Thus, we can express a conservative potential energy $U(\theta)$.

$$\begin{aligned} U(\theta) &= -\mu \cdot \mathbf{B} \\ &= -|\mu||\mathbf{B}| \cos\theta \end{aligned} \tag{6}$$

with

$$\frac{dU}{d\theta} = |\tau| = |\mu||\mathbf{B}| \sin\theta \tag{7}$$

Comment 1.5. In vector form,

$$\tau = \mu \times \mathbf{B} \tag{8}$$

$$|\tau| = |\mu||\mathbf{B}| \sin\theta \tag{9}$$

where θ is the interior angle made between μ and $\mathbf{B}$.

Because U is a conservative potential, its spatial derivatives are equal to the force on μ.

$$\mathbf{F} = -\nabla U = \nabla(\mu \cdot \mathbf{B}) \tag{10}$$

Note 1.2. A magnetic moment experiences a torque, and no net force when placed in a uniform magnetic field. If however, the field varies in space, then it will experience a force in the direction of increasing magnetic field.

1.2 Stern-Gerlach Experiment

The S-G experiments were done to test the Bohr model of the atom, which predicted that the negatively charged electrons moved in discrete orbits around a positively charged nucleus. Classically, a charged object

moving in a circular motion will generate a magnetic moment. This magnetic moment will interact with an external magnetic field that varies as a function of space to produce a force. The deflection of atoms in a magnetic field gradient would test of the Bohr model.

Lecture 2 - Thursday, January 08

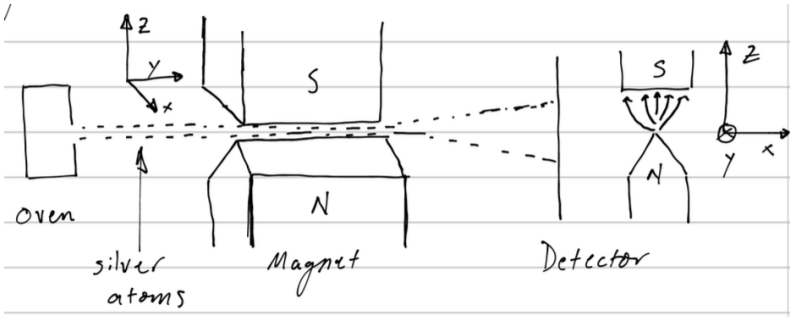


Figure 1: S-G apparatus

In their measurements, Stern and Gerlach used a beam of silver atoms produced by evaporating silver metal from an oven. The beam of neutral atoms exited from a small aperture and were sent through the poles of a permanent magnet that was designed to produce a strong component of the magnetic field gradient in the z-direction. A schematic of the experiment is shown above.

Between the poles of the magnet, the spins experience a force given body

$$F_z = (\mu \cdot \hat{z}) \left(\frac{\partial B_z}{\partial z} = |\mu| \cos\theta \left(\frac{\partial B_z}{\partial z} \right) \right) \tag{11}$$

Classically, we would expect a uniform distribution of θ for the silver atoms exiting the oven. That is, there should be no preferred orientation of silver atoms with respect to any direction in space.

If θ is sampled uniformly over the range $\theta \in \{0, 2\pi\}$, then we expect the distribution like the one shown in the figure below, with a peak at $\theta = 90°$ (See Eq.11.)

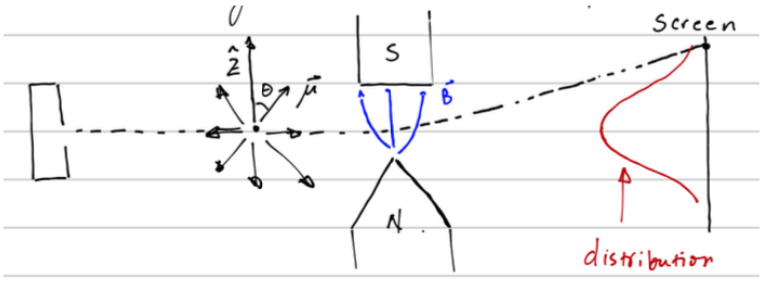


Figure 2: Classical distribution

Instead, of a continuous peak having a $\cos\theta$ distribution, S-G observed two distinct peaks. (See figure below)

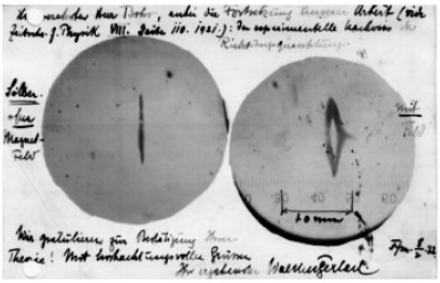


Figure 3: Two peaks

Discovery 1.2. The results were not consistent with the Bohr model, which predicted a continuous distribution of silver atoms.

Corollary 1.1. The spatial quantization of angular momentum was later understood by Ulenbeck and Goudsmit in 1925 as a consequence of the intrinsic "spin" angular momentum of the electron. Furthermore, it was recognized much later that the silver atom as an unpaired electron in the outer $5s$ orbital. Since s orbitals do not have an orbital angular momentum, the total angular momentum of the electron is from the spin.

$$\mu_{\text{total}} = \mu_{\text{spin}} = g\left(\frac{q}{2m}\right)\mathbf{S} \tag{12}$$

This meant that the direction of μ_{spin} had only 2 values, which could only be true if the intrinsic angular momentum of the electron was quantized, having only two values. A measurement of the spin angular momentum for the electron along any axis, yields two distinct values:

$$S_z = \pm\frac{\hbar}{2} \tag{13}$$

Comment 1.6. The z-subscript refers to the measurement axis. The choice is arbitrary.

Definition 1.1. **[Planck's Constant]**

The unit of angular momentum is called Planck's constant:

$$\hbar = \frac{h}{2\pi} = 1.0546 \times 10^{-34}\mathbf{J.s}$$

Theorem 1.1.

For an electron:

$$|mu_{\text{spin}}| \approx \frac{\hbar e}{2m} = 9.27 \times 10^{-24}\frac{\mathbf{J}}{\mathbf{T}} \tag{14}$$

Definition 1.2. **[Spin-$\frac{1}{2}$ Particles]**

We refer to particles with $|S_z| = \frac{\hbar}{2}$ as **spin-$\frac{1}{2}$ particles**.

Note 1.3. Since our choice of coordinates is arbitrary, this means that the outcome of the measurement would be $\pm\frac{\hbar}{2}$ regardless of the direction of the magnetic field.

2 Quantum?

2.1 The Quantum State Vector

Definition 2.1. **[Dirac Notation]**

We write $|+\rangle$ to mean spin-up and $|-\rangle$ to mean spin-down. This notation is called "ket".

Comment 2.1. You will sometimes see these notations, all of which refer to spin-up:

$$|+\rangle = |+\hbar/2\rangle = |\uparrow\rangle = |+\hat{z}\rangle$$

Note 2.1. In general, $|\psi\rangle = a\,|+\rangle + b\,|-\rangle$ where a and b are complex constants.

2.1.1 Postulate 1

Theorem 2.1. Postulate 1

The state a quantum system, including all the information you can know about it, is represented mathematically by ket $|\psi\rangle$.

Following the notation used by McIntyre, we represent the S-G experiment using the following simplified diagram.

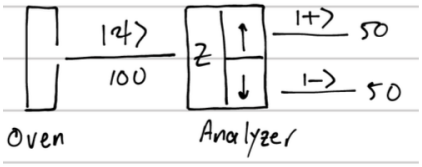
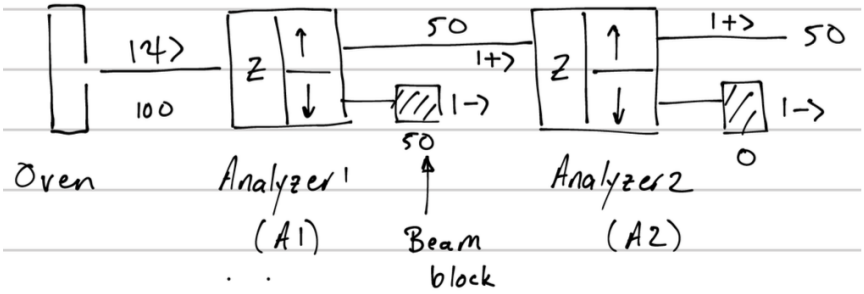


Figure 4: S-G apparatus diagram

Explaination: The diagram refers to a measurement made with the magnet oriented in the z-direction, and 2 outcomes: $S_z = \pm\hbar/2$, corresponding to the states $|+\rangle$ and $|-\rangle$. There is a 50/50 probability of measuring either state.

Comment 2.2. The order of events measured at the output of the Analyzer is completely random.

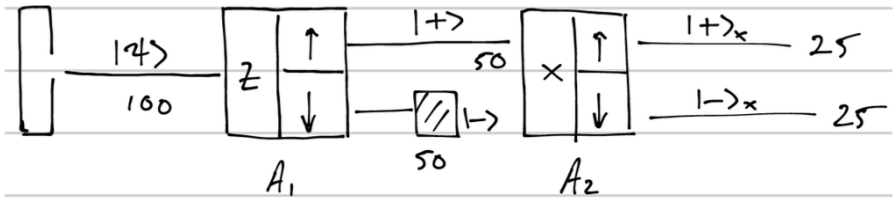
2.1.2 Stern-Gerlach Experiment #1



Analyzer 1 prepares the beam in the $|+\rangle$ state with respect to the z-axis.

Discovery 2.1. If a second analyzer is placed, having the same orientation as the first, at the output of the first analyzer, then the state of the particles is not affected by passing through the second analyzer.

2.1.3 Stern-Gerlach Experiment #2

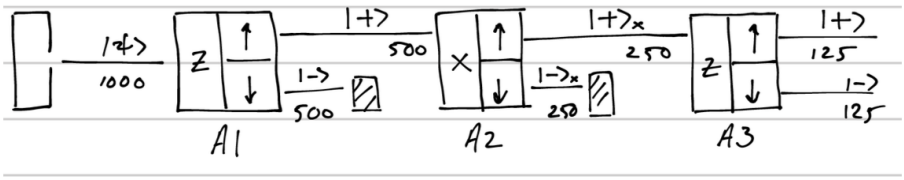


Here, we prepare the state in the $|+\rangle$ state and rotate the measurement analyzer by 90° so that it's orientation is along the x-axis.

Discovery 2.2. We again find a 50/50 chance of measuring either $|+\rangle_x$ or $|-\rangle_x$. We use the x-subscript to indicate the measurement axis.

Note 2.2. We would get the same 50/50 distribution if we used the lower port ($|-\rangle$) of Analyzer 1.

2.1.4 Stern-Gerlach Experiment #3



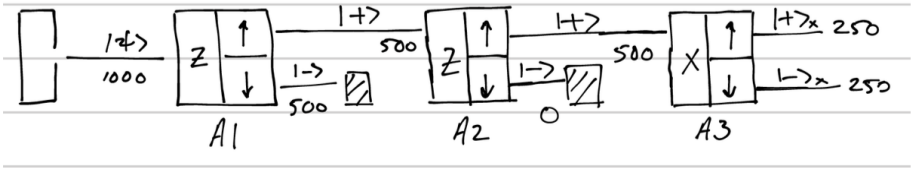
Classically, you might expect that the output of A3 should be 100% polarized in the $|+\rangle$ state.

Discovery 2.3. However, we see that the spins that exit A2 retain no information of having been polarized in the $|+\rangle$ state by A1.
This is because the measurement of S_x disturbs our knowledge of S_z.

Theorem 2.2.

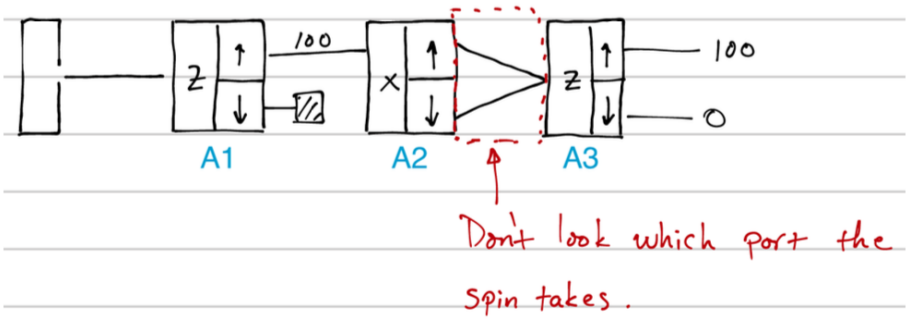
In quantum mechanics, we cannot simultaneously know S_x and S_z. Measurement of different orthogonal components of S are incompatible, i.e., a measurement of one component of S disturbs the outcome of the measurement of the other component.

Suppose we repeat Experiment 3, this time switching the order of the last two analyzers.



All measurements are compatible with themselves. Classical measurements do not disturb the state of the system. Therefore, we get the same outcome regardless of the order in which the measurements are performed. For quantum measurements, in contrast, the order can determine the outcome, provided some of the measurements are incompatible.

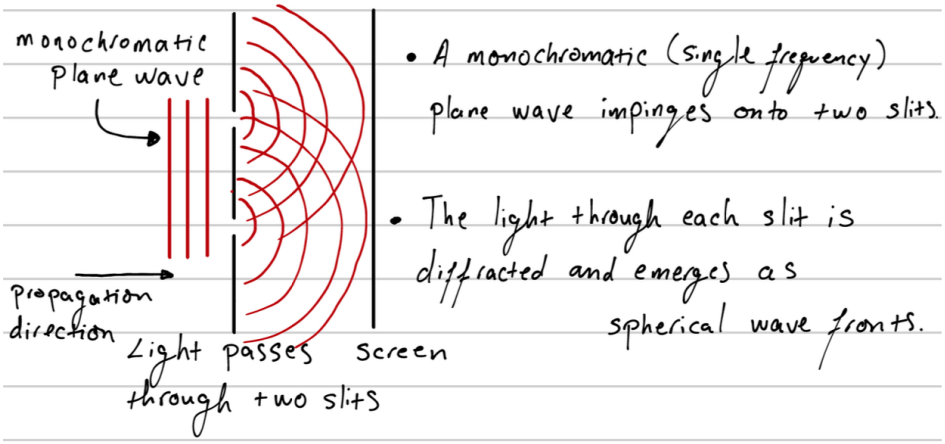
2.1.5 Stern-Gerlach Experiment #4



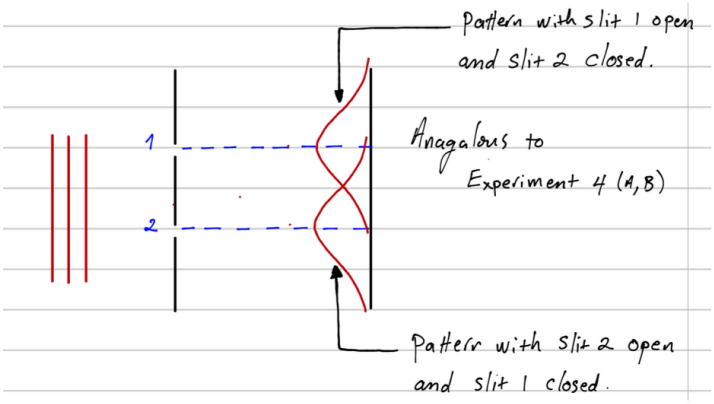
Note 2.3. We did not make measurement. You don't make measurement, you don't disturb the state.

This behaviour has no classical analog. However, this behaviour is consistent with the interference phenomenon observed for waves. In particular, the fact that no particles are observed in the lower port ($|-\rangle$) of A3 in S-G Exp.4 reminds us of two waves of equal amplitude that interfere destructively to produce zero amplitude.

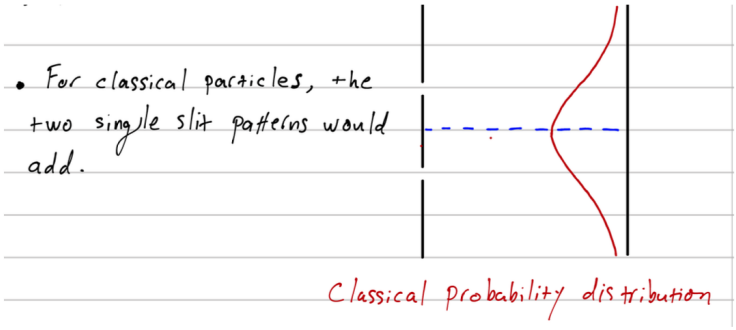
2.2 Young's Double Slit Interference Experiment



If we cover one slit at a time, and allow the light from only one of the slits to fall on the screen, the resulting intensity pattern will look the one shown below.

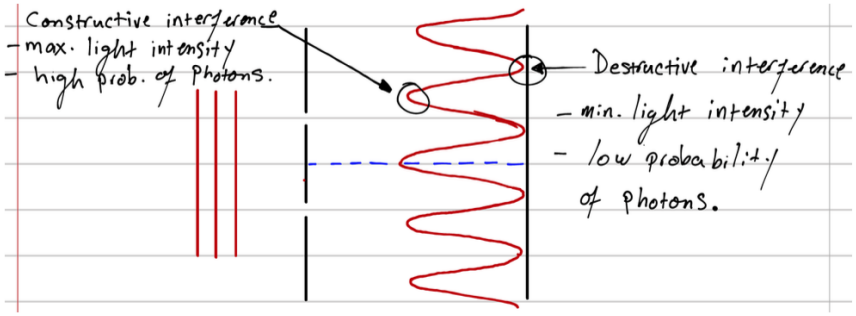


Each pattern by itself resembles what we would expect for a classical distribution of particles arriving from the individual slits. If both slits are opened, then for classical particles, we would expect a distribution like the one shown below.



Comment 2.3. For classical particles, the two single-slit intensity patterns would add.

Discovery 2.4. However, we observe that the waves from the two slits interfere.

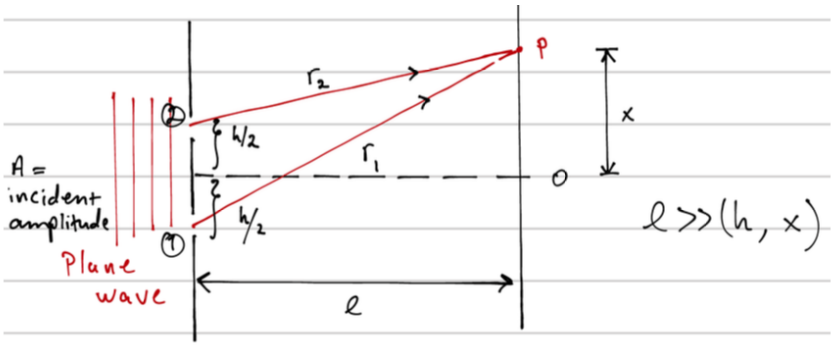


Comment 2.4. The key difference between classical particles and waves is the interference phenomenon observed for waves.

Physically, we interpret the intensity as being proportional to the probability of observing a photon. The interference intensity is calculate by squaring the sum of the field amplitudes from the two slits.

The S-G Experiment 4 exhibits an identical interference phenomenon as observed in Young's double slit experiment. This implies that the spins that take the upper and lower paths through A2 (x-analyzer) interfere constructively to produce all $|+\rangle$ spins through A3 (z-analyzer).

2.2.1 2-Slit Pattern Calculation



1/2 of the incident wave amplitude exits from slits (1) and (2). The waves exiting each slit have a travelling wave solution given by

$$a_{(1,2)}(r_{(1,2)}, t) = \left(\frac{A}{2}\right) e^{i(kr_{(1,2)} - \omega t)} \tag{15}$$

where the wavenumber $k = 2\pi/k$, $\omega/k = c$, and

$$r_1 = \sqrt{l^2 + \left(\frac{h}{2} + x\right)^2}, \quad r_2 = \sqrt{l^2 + \left(\frac{h}{2} - x\right)^2}$$

The wave amplitude at point P is

$$a(x) = \frac{A}{2}\left(e^{ikr_1} + e^{ikr_2}\right) e^{-i\omega t} \tag{16}$$

The wave intensity at point P is proportional to the magnitute square of the total wave amplitude at P.

$$I(x) = \left(\frac{A^2}{4}\right)\left|e^{ikr_1} + e^{ikr_2}\right|^2 \tag{17}$$

$$= \left(\frac{A^2}{2}\right)[1 + \cos(k[r_1 - r_2])] \tag{18}$$

We have

$$r_1 - r_2 \approx \frac{hx}{l}, \qquad l \gg (h, x)$$

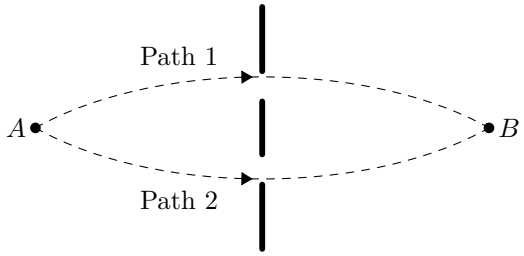
so

$$I(x) = \left(\frac{A^2}{2}\right)\left[1 + \cos\left(\frac{2\pi h}{\lambda l}x\right)\right]$$

Lecture 3 - Tuesday, January 13

We can turn down the light level low enough so that there is only one photon going through the double slit device at any given time.

According to our classical notion of reality, we think of a photon taking either one of two the paths to reach the screen. However, according to the laws of quantum mechanics, each particle takes both paths.



If a photon (or any quantum particle) can take multiple paths to go between points A and B, the probability to go from A to B is calculated by summing the probability amplitudes for each of the possible paths, and calculating the square of the sum of the amplitudes. This is contrary to the classical way of calculating probability, where we add the probability of each event separately.

Classical way of adding probabilies:

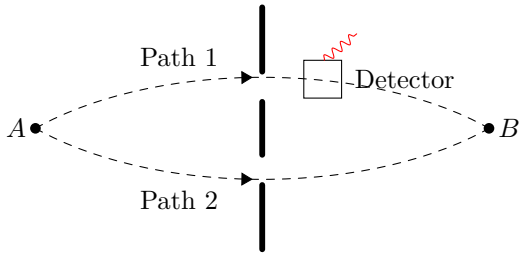
$$P_{\text{classical}} = \left|a_1 e^{i\phi_1}\right|^2 + \left|a_2 e^{i\phi_2}\right|^2$$
$$= a_1^2 + a_2^2$$

Quantum mechanical way of adding probabilies:

$$P_{\text{quantum}} = \left|a_1 e^{i\phi_1} + a_2 e^{i\phi_2}\right|$$
$$= (a_1 e^{-i\phi_1} + a_2 e^{-i\phi_2})(a_1 e^{i\phi_1} + a_2 e^{i\phi_2})$$
$$= a_1^2 + a_2^2 + \underbrace{2a_1 a_2 \cos(\phi_1 - \phi_2)}_{\text{interference term}}$$

If we place a device between A and B that can tell us which path the particle takes, then we don't observe interference, and instead recover the classical probability distribution. The act of observation

localizes the particle to the path where the particle was observed to be. The particle can no longer exist in both paths, and therefore no interference takes place. This behaviour is sometimes referred to as the "collapse of the wavefunction". The notion of the wavefunction will be developed later in the course.



2.3 Quantum State Vectors

We use the notation $|\psi\rangle$ to mathematically represent the state of the system, where $|\psi\rangle$ is in a Hilbert space.

2.3.1 Hilbert Space

Definition 2.2. **[Hilbert Space]**

A **Hilbert space** is a space such that

1. it is a linear vector space (an example would be the Euclidean space);
2. it is a complex vector space;
3. it is a complete vector space, so the distance between points are defined.

Definition 2.3. **[Dimension]**

We define the **dimension** of a Hilbert space corresponding to a particual quantum system the number of possible measurement outcomes for that quantum system.

Example 2.1. Suppose the quantum system is spin-$\frac{1}{2}$, and we measure along x, y, and z. The dimension of spin-$\frac{1}{2}$ is 2.

Definition 2.4. **[Inner Product]**

Given two vectors $|\psi\rangle$ and $|\phi\rangle$, we define the **inner product** of them to be

$$\langle\phi|\psi\rangle \coloneqq \langle\phi|\,|\psi\rangle$$

where $\langle\phi| \coloneqq (|\phi\rangle)^\dagger$ is the conjugate transpose (Hermitian conjugate).

Theorem 2.3. Orthonormality of Base Vectors

Bases vectors are orthonormal. i.e.,

$$\langle +|+\rangle = \langle -|-\rangle = 1, \qquad \langle +|-\rangle = \langle -|+\rangle = 0$$

Discovery 2.5. We have

$$(a\,|\psi\rangle)^\dagger = a^*\,\langle\psi|$$

Discovery 2.6. We write $|\psi\rangle = a\,|+\rangle + b\,|-\rangle$ and $|\phi\rangle = c\,|+\rangle + d\,|-\rangle$, so

$$\begin{aligned}\langle\phi|\psi\rangle &= (c\,|+\rangle + d\,|-\rangle)^\dagger(a\,|+\rangle + b\,|-\rangle)\\ &= (c^*\,|+\rangle + d^*\,|-\rangle)(a\,|+\rangle + b\,|-\rangle)\\ &= c^*a\langle+|+\rangle + c^*b\langle+|-\rangle + d^*a\langle-|+\rangle + d^*b\langle-|-\rangle\\ &= c^*a + d^*b\end{aligned}$$

Discovery 2.7. Now suppose $|\psi\rangle = a\,|+\rangle + b\,|-\rangle$, then its projection on one of the base vectors is simply:

$$\langle +|\psi\rangle = \langle +|\,(a\,|+\rangle + b\,|-\rangle) = a$$

where (a, b) is called the probability amplitudes. We also find that

$$\begin{aligned}\langle\psi|+\rangle = (\langle+|\psi\rangle)^\dagger &= (a^*\,\langle+| + b^*\,\langle-|)\,|+\rangle\\ &= a^*\langle+|+\rangle + b^*\langle-|+\rangle = a^*\end{aligned}$$

2.3.2 Postulate 4 for a Spin-1/2 System

Theorem 2.4. Postulate 4 (Spin-1/2 System)

The probability of obtaining $\pm\frac{\hbar}{2}$ in a measurement of the observable S_z of a system in the state $|\psi\rangle$ is

$$\text{Prob}\left(\pm\frac{\hbar}{2}\right) = |\langle\pm|\psi\rangle|^2$$

Comment 2.5. If you think back to Young's double slit experiment, we can make a correspondence with the probability amplitude and the complex field amplitude of an electromagnetic wave.

$$E_0 e^{i\phi} \iff a$$

The intensity of an electromagnetic wave is proportional to the square of the magnitude of the electric field amplitude. If you recall, we said that the probability of a photon hitting the screen at a given position is proportional to the intensity of light at that position.

$$I = |E|^2 = E_0^2 \iff |a|^2$$

Now we have a way of calculating the probabilities, we note that it must be the case that

$$P\left(+\frac{\hbar}{2}\right) + P\left(-\frac{\hbar}{2}\right) = 1$$

Moreover, we know that

$$P\left(+\frac{\hbar}{2}\right) = |a|^2, \qquad P\left(-\frac{\hbar}{2}\right) = |b|^2$$

This implies that our state must be normalized.

Example 2.2. Given $|\psi\rangle = 3\,|+\rangle + 2\,|-\rangle$, we note that $|\psi\rangle$ is not normalized, the way we normalize it is by solving

$$\langle\psi'|\psi'\rangle = 1$$

where $|\psi'\rangle = c\,|\psi\rangle$ for some constant c. We solve for it and obtain c is such that $|c| = 1/\sqrt{13}$. However, it could be the case that

$$c = \frac{1}{\sqrt{13}} e^{i\theta}$$

where $e^{i\theta}$ is known as the phase vector. Although in mathematics this factor matter as different values of phase vector changes the value of our vector, it does not have any effect on the measurement we make. In particular,

$$\begin{aligned}
\text{Prob} = |\langle a|\psi'\rangle|^2 &= \left| \frac{1}{\sqrt{13}} e^{i\theta} \langle a| \underbrace{3\,|a\rangle + 3\,|b\rangle}_{|\psi\rangle} \right| \\
&= \frac{1}{13} \left| e^{i\theta} \underbrace{\langle a|\psi\rangle}_{d} \right|^2 \\
&= \frac{1}{13} \left(e^{i\theta} d\right)\left(e^{-i\theta} d\right) = \frac{1}{13}|d|^2
\end{aligned}$$

Lemma 2.1. Multiplying a state vector by an overall phase factor $e^{i\theta}$ does not change the probability of a measurement.

2.3.3 Matrix Notation

We represent a ket as a column matrix and a bra as a row matrix.

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\langle + | = \begin{pmatrix} 1 & 0 \end{pmatrix}, \qquad \langle - | = \begin{pmatrix} 0 & 1 \end{pmatrix}$$

Unit Norm:

$$\langle + | + \rangle = \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1, \qquad \langle - | - \rangle = \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 1$$

Orthogonality:

$$\langle + | - \rangle = \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0, \qquad \langle - | + \rangle = \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0$$

Comment 2.6. In other words, $|+\rangle$ and $|-\rangle$ form an orthonormal basis.

A general state $|\psi\rangle = a\,|+\rangle + b\,|-\rangle$ can be represented in matrix form as

$$|\psi\rangle = a \begin{pmatrix} 1 \\ 0 \end{pmatrix} + b \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix}.$$

The corresponding bra $\langle\psi|$ is

$$\langle \psi | = (|\psi\rangle)^\dagger = \begin{pmatrix} a^* & b^* \end{pmatrix}.$$

The inner product in matrix form is thus

$$\langle \psi | \psi \rangle = \begin{pmatrix} a^* & b^* \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = |a|^2 + |b|^2.$$

The inner product $\langle\psi|\psi\rangle$ is a measure of the square of the magnitude of the quantum state vector $|\psi\rangle$.

2.4 Representation and Change of Basis

Lecture 4 - Tuesday, January 20

2.4.1 Basis States of the Observable S_x

Given an arbitrary state $|\psi\rangle$, we know that

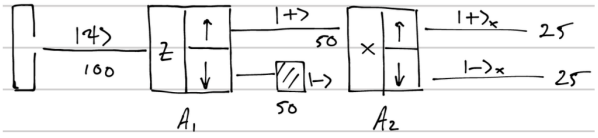
$$|\psi\rangle = a\,|+\rangle + b\,|-\rangle$$
$$|\psi\rangle = a'\,|+\rangle + b'\,|-\rangle$$

where (a, b, a', b') are constants.

Question 2.1.

How do I represent $|\pm\rangle_x$ in terms of $|\pm\rangle$?

Recall the experiment:



We don't know yet the form of $|\pm\rangle_x$, however completeness requires that we can express $|\pm\rangle_x$ as a linear superposition of S_z-basis eigenvectors $|\pm\rangle$.

$$|+\rangle_x = a\,|+\rangle + b\,|-\rangle$$
$$|-\rangle_x = c\,|+\rangle + d\,|-\rangle$$

To find the set of coefficients $\{a, b, c, d\}$, we need to analyze the outcome of the measurements. In qunatum mechanics, we can only measure probabilities, not the probability amplitudes.

$$|\langle +|+\rangle_x|^2 = \frac{1}{2} \quad |\langle +|-\rangle_x|^2 = \frac{1}{2}$$
$$|\langle -|+\rangle_x|^2 = \frac{1}{2} \quad |\langle -|-\rangle_x|^2 = \frac{1}{2}$$

Now we have

$$|\langle +\,|\,(a|+\rangle + b|-\rangle)|^2 = |a|^2 = \frac{1}{2}$$
$$|\langle -\,|\,(a|+\rangle + b|-\rangle)|^2 = |b|^2 = \frac{1}{2}$$
$$|\langle +\,|\,(c|+\rangle + d|-\rangle)|^2 = |c|^2 = \frac{1}{2}$$
$$|\langle -\,|\,(c|+\rangle + d|-\rangle)|^2 = |d|^2 = \frac{1}{2}$$
$$|a| = |b| = |c| = |d| = \frac{1}{\sqrt{2}}$$

The states $|\pm\rangle_x$ must be normalized, thus

$$|\,{}_x\langle +|+\rangle_x|^2 \;\Rightarrow\; |a|^2 + |b|^2 = 1$$
$$|\,{}_x\langle -|-\rangle_x|^2 \;\Rightarrow\; |c|^2 + |d|^2 = 1$$

The states $|\pm\rangle_x$ must also be orthogonal, thus

$${}_x\langle +|-\rangle_x \;=\; {}_x\langle -|+\rangle_x \;=\; 0 \quad\Rightarrow\quad \big(a^*\langle +| + b^*\langle -|\big)\big(c|+\rangle + d|-\rangle\big) = 0$$
$$a^*c + b^*d = 0$$
$$ac^* + bd^* = 0$$

The most general way of expressing the probability amplitudes is

$$a = |a|e^{i\alpha}, \qquad b = |b|e^{i\beta}$$

$$c = |c|e^{i\gamma}, \qquad d = |d|e^{i\delta}.$$

Using the orthogonality relationships, we find

$$\frac{1}{2}\left(e^{i(\gamma-\alpha)} + e^{i(\delta-\beta)}\right) = 0.$$

Note 2.4. Only the relative phase between the terms matters. The choice of phases is not unique, therefore we must adopt a convention for picking phases. The convention used is to make the coefficient of the $|+\rangle$ real and positive. Let $\alpha = \gamma = 0 \;\Rightarrow\; \frac{1}{2}\left(1 + e^{i(\delta-\beta)}\right) = 0$. Let $\beta = 0$ and $\delta = \pi$ (again by convention).

$$\Rightarrow \quad |+\rangle_x = \frac{1}{\sqrt{2}}\left(|+\rangle + |-\rangle\right) \qquad |-\rangle_x = \frac{1}{\sqrt{2}}\left(|+\rangle - |-\rangle\right).$$

Exercise 2.1. Following the same steps and show that

$$|+\rangle_y = \frac{1}{\sqrt{2}}(|+\rangle + i\,|-\rangle), \qquad |-\rangle_y = \frac{1}{\sqrt{2}}(|+\rangle - i\,|-\rangle)$$

2.4.2 Change of Basis

Because the eigenvectors of S_z and S_x form a complete basis, we can represent an arbitrary state $|\psi\rangle$ using either basis.

- $|\psi\rangle$ represented in the S_z basis:
$$|\psi\rangle = a\,|+\rangle + b\,|-\rangle\,.$$
- $|\psi\rangle$ represented in the S_x basis:
$$|\psi\rangle = a'\,|+\rangle_x + b'\,|-\rangle_x\,.$$
- Solve for coefficients $\{a', b'\}$ in terms of $\{a, b\}$:

$$a' = {}_x\langle +|\,\psi\rangle = {}_x\langle +|\,\left(a\,|+\rangle + b\,|-\rangle\right), \qquad b' = {}_x\langle -|\,\psi\rangle = {}_x\langle -|\,\left(a\,|+\rangle + b\,|-\rangle\right).$$

Discovery 2.8. We can organize the above into a matrix equation:

$$\begin{pmatrix} a' \\ b' \end{pmatrix} = \underbrace{\begin{pmatrix} {}_x\langle +|+\rangle & {}_x\langle +|-\rangle \\ {}_x\langle -|+\rangle & {}_x\langle -|-\rangle \end{pmatrix}}_{U} \begin{pmatrix} a \\ b \end{pmatrix}.$$

Definition 2.5. **[Transformation Matrix]**

The matrix U is referred to as a *transformation matrix*. Using

$$|+\rangle_x = \frac{1}{\sqrt{2}}\big(|+\rangle + |-\rangle\big), \qquad |-\rangle_x = \frac{1}{\sqrt{2}}\big(|+\rangle - |-\rangle\big),$$

We compute:

$$\begin{aligned}
U_{11} &= {}_x\langle +|+\rangle = \frac{1}{\sqrt{2}}\big(\langle +| + \langle -|\big)\,|+\rangle = \frac{1}{\sqrt{2}},\\
U_{12} &= {}_x\langle +|-\rangle = \frac{1}{\sqrt{2}}\big(\langle +| + \langle -|\big)\,|-\rangle = \frac{1}{\sqrt{2}},\\
U_{21} &= {}_x\langle -|+\rangle = \frac{1}{\sqrt{2}}\big(\langle +| - \langle -|\big)\,|+\rangle = \frac{1}{\sqrt{2}},\\
U_{22} &= {}_x\langle -|-\rangle = \frac{1}{\sqrt{2}}\big(\langle +| - \langle -|\big)\,|-\rangle = -\frac{1}{\sqrt{2}}.
\end{aligned}$$

Lemma 2.2. $U_{z\to x}$ transforms a vector from the z-basis to the x-basis.

$$U_{z\to x} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

Example 2.3. Given the normalized state vector

$$|\psi\rangle = \frac{1}{\sqrt{26}}\big(5\,|+\rangle + |-\rangle\big)$$

in the S_z basis, calculate $|\psi\rangle$ in the S_x basis.

$$\begin{pmatrix} a' \\ b' \end{pmatrix} = \frac{1}{\sqrt{26}} \cdot \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 5 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} a' \\ b' \end{pmatrix} = \frac{1}{\sqrt{52}}\begin{pmatrix} 6 \\ 4 \end{pmatrix} = \frac{1}{\sqrt{13}}\begin{pmatrix} 3 \\ 2 \end{pmatrix}$$

$$|\psi\rangle = \frac{1}{\sqrt{13}}\Big(3\,|+\rangle_x + 2\,|-\rangle_x\Big).$$

2.4.3 Transformation Matrix

Let $|\psi\rangle$ be a quantum state that belongs to a Hilbert space H. Let $\{|a_n\rangle\}$ and $\{|b_n\rangle\}$ be two complete orthonormal bases that span H. We can represent the state $|\psi\rangle$ in both bases:

$$|\psi\rangle = \sum_n \langle a_n|\psi\rangle\ |a_n\rangle = \sum_n A_n\,|a_n\rangle\,,$$

$$|\psi\rangle = \sum_n \langle b_n|\psi\rangle \; |b_n\rangle = \sum_m B_m \, |b_m\rangle \, ,$$

where $A_n = \langle a_n|\psi\rangle$ and $B_n = \langle b_n|\psi\rangle$ are the coefficients of the basis vectors in the a- and b-bases, respectively. We seek to find the transformation matrix $U_{a\to b}$ that transforms $|\psi\rangle$ from the a-basis to the b-basis.

Note 2.5. We note that the inner product $\langle\psi|\psi\rangle$ is independent of the choice of basis.

Let us express $\langle\psi|\psi\rangle$ by expanding the bra $|\psi\rangle$ in the b-basis and the ket $|\psi\rangle$ in the a-basis:

$$\langle\psi|\psi\rangle = \sum_m \sum_n \big(\langle b_m|\psi\rangle\big)^* \langle a_n|\psi\rangle \, \langle b_m|a_n\rangle = \sum_m \sum_n A_n \, B_m^* \, \langle b_m|a_n\rangle.$$

We can organize the above expression in matrix form:

$$\langle\psi|\psi\rangle = \begin{pmatrix} B_1^* & B_2^* & \cdots \end{pmatrix} \underbrace{\begin{pmatrix} \langle b_1|a_1\rangle & \langle b_1|a_2\rangle & \cdots \\ \langle b_2|a_1\rangle & \langle b_2|a_2\rangle & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}}_{U_{a\to b}} \begin{pmatrix} A_1 \\ A_2 \\ \vdots \end{pmatrix}.$$

$$\boxed{\underbrace{|\psi\rangle}_{b\text{-basis}} = U_{a\to b} \; \underbrace{|\psi\rangle}_{a\text{-basis}}}$$

Note 2.6. The transformation matrix $U_{a\to b}$ allows us to compute the representation of the state $|\psi\rangle$ in the b-basis, given that we know $|\psi\rangle$ in the a-basis.

Likewise, we can also compute $|\psi\rangle$ in the a-basis starting from the b-basis by calculating the inverse of $U_{a\to b}$:

$$U_{a\to b}^{-1} \underbrace{|\psi\rangle}_{b\text{-basis}} = U_{a\to b}^{-1} U_{a\to b} \; \underbrace{|\psi\rangle}_{a\text{-basis}} .$$

$$\underbrace{|\psi\rangle}_{a\text{-basis}} = U_{a\to b}^{-1} \underbrace{|\psi\rangle}_{b\text{-basis}} := U_{b\to a} \; \underbrace{|\psi\rangle}_{b\text{-basis}} .$$

$$\therefore \quad \boxed{U_{b\to a} = U_{a\to b}^{-1}}$$

Discovery 2.9. Conservation of probability requires that $\langle\psi|\psi\rangle$ is independent of the choice of basis. Therefore

$$\underbrace{\langle\psi|\psi\rangle}_{a\text{-basis}} = \underbrace{\langle\psi|\psi\rangle}_{b\text{-basis}}.$$

$$\implies \quad \underbrace{\langle\psi|\psi\rangle}_{a\text{-basis}} = \big(U_{b\to a}\,|\psi\rangle\big)^\dagger \big(U_{b\to a}\,|\psi\rangle\big) = \langle\psi| \; U_{b\to a}^\dagger U_{b\to a} \; |\psi\rangle \, .$$

For the above equality to hold, we require that

$$U^\dagger_{b\to a} U_{b\to a} = 1.$$

In general, transformation matrices are *unitary*, by which we mean that they preserve the norm of the state vector and satisfy:

$$UU^\dagger = 1, \qquad U^\dagger U = 1.$$

Since $UU^\dagger = 1$, $U^\dagger$ must also satisfy

$$U^\dagger = U^{-1}.$$

2.5 Generalized Quantum Systems

Lecture 5 - Thursday, January 22

2.5.1 Postulates 2 and 3

Theorem 2.5. Postulate 2

A physical observable is represented mathematically by an operator $\{\hat{S}_x, \hat{S}_y, \hat{S}_z\}$, in general, an operator $\hat{A}$ that acts on kets.

Theorem 2.6. Postulate 3

The only possible result of a measurement of an observable is one of the eigenvalues corresponding to the operator $\hat{A}$.

Comment 2.7. Note the ($\hat{}$) superscript notation is used to signify that the mathematical object is an operator. Most of the time, we will suppress this notation.

2.5.2 Properties of Operators Corresponding to Observables

Physical observables are represented by Hermitian matrices.

Definition 2.6. **[Hermitian Matrix]**

A **Hermitian matrix** $\hat{A}$ is a square matrix that satisfies the condition

$$\hat{A} = \hat{A}^\dagger$$

Recall that $(\hat{A}^\dagger)_{ij} = A^*_{ji}$.

Lemma 2.3. Hermitian matrices have real eigenvalues.

Proof. Consider the quantity $\hat{A}\,|a_n\rangle = a_n\,|a_n\rangle$

$$\langle a_m|\,\hat{A}\,|a_n\rangle - \langle a_m|\,\hat{A}^\dagger\,|a_n\rangle = 0.$$

This statement is true by the definition of a Hermitian matrix.

$$\underbrace{\langle a_m|\,\hat{A}\,|a_n\rangle}_{a_n\langle a_m|a_n\rangle} - \underbrace{\langle a_m|\,\hat{A}^\dagger\,|a_n\rangle}_{(\hat{A}|a_m\rangle)^\dagger = a_m^*\langle a_m|} = 0$$

$$\implies \quad (a_n - a_m^*)\langle a_m|a_n\rangle = 0.$$

Consider the case $m = n$.

$$(a_n - a_n^*)\langle a_n|a_n\rangle = 0$$

Because $\langle a_n|a_n\rangle \neq 0$, we must have $(a_n - a_n^*) = 0$. Hence $a_n = a_n^*$, which implies that $a_n \in \mathbb{R}$. □

Comment 2.8. Physically, all measurement outcomes corresponding to an observable must be real. This property of Hermitian matrices ensures real outcomes.

Lemma 2.4. All eigenvectors with distinct eigenvalues are orthonormal.

Proof. The eigenvalues $\{a\}$ of a Hermitian matrix are real. We showed that

$$\begin{aligned} & (a_n - a_m^*)\langle a_m|a_n\rangle = 0 \\ \Rightarrow \quad & (a_n - a_m)\langle a_m|a_n\rangle = 0 \end{aligned}$$

If $a_n \neq a_m$, then $\langle a_m|a_n\rangle = 0$. □

Let $\{|a\rangle\}$ be the set of eigenvectors (I will also refer to them as eigenkets) corresponding to operator $\hat{A}$ and $\{a\}$ be the corresponding set of eigenvalues.

$$|\psi\rangle = \sum_m c_m\,|a_m\rangle$$

where $\{c\}$ are the set of probability amplitudes. The eigenvectors $\{|a\rangle\}$ form an orthonormal set, with

$$\langle a_n|a_m\rangle = \delta_{nm}$$

We can use the above equation to calculate the probability of being in the state $|a_n\rangle$.

$$P_n = \big|\langle a_n|\psi\rangle\big|^2 = \left|\sum_m c_m\langle a_n|a_m\rangle\right|^2 = |c_n|^2.$$

Based on Postulate 3 (2.6), we seek to find the representation of $\hat{A}$ in the eigenbasis $\{|a\rangle\}$

$$\hat{A}\,|a_n\rangle = a_n\,|a_n\rangle$$

The operator $\hat{A}$ acting on an eigenvector $|a_n\rangle$ returns the eigenvector $|a_n\rangle$ scaled by the corresponding eigenvalue a_n. The matrix element are given by

$$A_{nm} := \langle a_n|\hat{A}|a_m\rangle = \langle a_n|(\hat{A}|a_m\rangle) = a_m\langle a_n|a_m\rangle = a_m\delta_{nm}.$$

We see from the form of the above equation that the matrix representation of an operator is diagonal when expressed in its eigenbasis, with the diagonal elements being the eigenvalues of the operator.

Example 2.4. Let $\hat{A}$ be an operator corresponding to an observable in a 2-dimensional Hilbert space.

$$\hat{A}\,|a_1\rangle = a_1\,|a_1\rangle \qquad \hat{A}\,|a_2\rangle = a_2\,|a_2\rangle$$

$$\hat{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

$$A_{11} = a_1 \qquad A_{12} = A_{21} = 0 \qquad A_{22} = a_2$$

$$\hat{A} = \begin{pmatrix} a_1 & 0 \\ 0 & a_2 \end{pmatrix}$$

2.5.3 Representation of the Operators S_x, S_y and S_z

As an example, consider the representation of the three components of the angular momentum operator for a spin-1/2 particle.

In this example, we choose the S_z–basis to represent the three operators. By Postulate 3, we know that $\pm\frac{\hbar}{2}$ are the two eigenvalues for each operator.

Representation of S_z in the S_z–basis: We know that the eigenvectors corresponding to S_z are $|\pm\rangle$. We've also seen that eigenvectors are unit vectors if represented in their own basis. Therefore, in the S_z basis, we have

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

We know that the states $|\pm\rangle$ are eigenstates of S_z, with eigenvalues $\pm\frac{\hbar}{2}$.

$$S_z|\pm\rangle = \pm\frac{\hbar}{2}\,|\pm\rangle.$$

We find the matrix elements of S_z.

$$(S_z)_{11} = \langle +|S_z|+\rangle = \frac{\hbar}{2}, \qquad (S_z)_{12} = \langle +|S_z|-\rangle = 0,$$

$$(S_z)_{21} = \langle -|S_z|+\rangle = 0, \qquad (S_z)_{22} = \langle -|S_z|-\rangle = -\frac{\hbar}{2}.$$

$$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Representation of S_x in the S_z–basis: We need to evaluate the matrix elements $\langle +|S_x|+\rangle$, $\langle +|S_x|-\rangle$, $\langle -|S_x|+\rangle$ and $\langle -|S_x|-\rangle$. This requires that we know how the operator S_x acts on the states $|\pm\rangle$. It's not immediately obvious how to compute this, since $|\pm\rangle$ are not eigenstates of the operator S_x. We do know however how S_x acts on $|\pm\rangle_x$, since these are its eigenstates.

$$S_x|\pm\rangle_x = \pm\frac{\hbar}{2}\,|\pm\rangle_x.$$

We further know how to represent the states $|\pm\rangle_x$ in the S_z–basis.

$$|+\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}, \qquad |-\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}.$$

To evaluate the matrix elements of S_x, however, we need to know how to represent the S_z–eigenstates $|\pm\rangle$ in terms of the eigenstates in the S_x–basis. We can apply a change of basis to represent $|\pm\rangle$ in the S_x–basis. See Lecture 5 for details.

$$|+\rangle = {}_x\langle + \mid +\rangle\,|+\rangle_x + {}_x\langle - \mid +\rangle\,|-\rangle_x, \qquad |-\rangle = {}_x\langle + \mid -\rangle\,|+\rangle_x + {}_x\langle - \mid -\rangle\,|-\rangle_x.$$

$$|+\rangle = \frac{1}{\sqrt{2}}\big(|+\rangle_x + |-\rangle_x\big), \qquad |-\rangle = \frac{1}{\sqrt{2}}\big(|+\rangle_x - |-\rangle_x\big).$$

Calculate the matrix elements of S_x:

$$\begin{aligned}
\langle +|S_x|+\rangle &= \frac{1}{2}\Big({}_x\langle +| + {}_x\langle -|\Big)\,S_x\Big(|+\rangle_x + |-\rangle_x\Big)\\
&= \frac{1}{2}\Big({}_x\langle +| + {}_x\langle -|\Big)\left(\frac{\hbar}{2}|+\rangle_x - \frac{\hbar}{2}|-\rangle_x\right)\\
&= 0,\\
\langle +|S_x|-\rangle &= \frac{1}{2}\Big({}_x\langle +| + {}_x\langle -|\Big)\,S_x\Big(|+\rangle_x - |-\rangle_x\Big)\\
&= \frac{1}{2}\Big({}_x\langle +| + {}_x\langle -|\Big)\left(\frac{\hbar}{2}|+\rangle_x + \frac{\hbar}{2}|-\rangle_x\right)\\
&= \frac{\hbar}{2},\\
\langle -|S_x|+\rangle &= \frac{1}{2}\Big({}_x\langle +| - {}_x\langle -|\Big)\,S_x\Big(|+\rangle_x + |-\rangle_x\Big)\\
&= \frac{1}{2}\Big({}_x\langle +| - {}_x\langle -|\Big)\left(\frac{\hbar}{2}|+\rangle_x - \frac{\hbar}{2}|-\rangle_x\right)\\
&= \frac{\hbar}{2},\\
\langle -|S_x|-\rangle &= \frac{1}{2}\Big({}_x\langle +| - {}_x\langle -|\Big)\,S_x\Big(|+\rangle_x - |-\rangle_x\Big)\\
&= \frac{1}{2}\Big({}_x\langle +| - {}_x\langle -|\Big)\left(\frac{\hbar}{2}|+\rangle_x + \frac{\hbar}{2}|-\rangle_x\right)\\
&= 0.
\end{aligned}$$

Therefore, $S_x = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$.

Exercise 2.2. Show that $S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$.

3 Projection Operators

Lecture 6 - Tuesday, January 27

We seek an operator formalism for calculating the outcome of a measurement of a quantum system.

Prior to a measurement, the state of the system can in general be described by the ket $|\psi\rangle$ that is a linear superposition of eigenvectors of an observable $\hat{A}$.

$$|\psi\rangle = \sum_n c_n |a_n\rangle \qquad \text{where} \qquad c_n = \langle a_n|\psi\rangle .$$

Recall that $\{|a\rangle\}$ is the set of eigenkets of operator $\hat{A}$. Substitute in c_n, we obtain that

$$\begin{aligned} |\psi\rangle &= \sum_n \langle a_n|\psi\rangle \ |a_n\rangle \\ &= \sum_n |a_n\rangle \left(\langle a_n|\psi\rangle \right) = \sum_n \Big(\underbrace{|a_n\rangle \langle a_n|}_{\hat{P}_n} \Big) |\psi\rangle . \end{aligned}$$

3.1 Representation of Projection Operator

Hence, we define the projection operator

$$\hat{P}_n := |a_n\rangle \langle a_n| \tag{19}$$

Consider the action of $\hat{P}_n$ on a state $|\psi\rangle$.

$$\hat{P}_n |\psi\rangle = |a_n\rangle \langle a_n|\, \psi\rangle = c_n |a_n\rangle .$$

Comment 3.1. How do we represent the projection operator? We have seen that the inner product, defined as $\langle\psi|\psi\rangle$, is a scalar. What is $|\psi\rangle \langle\psi|$? — It is the outer product.

Definition 3.1. **[Outer Product]**

If v is a $n \times 1$ complex vector, then the **outer product** w is an $n \times n$ tensor.

$$\hat{w} := |v\rangle \langle v| = v \otimes v = vv^\dagger$$

defined as $w_{ij} = v_i v_j^*$.

Example 3.1. Find the projection operators for the S_z operator.

$$\hat{P}_+ = |+\rangle \langle +| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\hat{P}_- = |-\rangle \langle -| = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Discovery 3.1. We note an interesting fact: the sum of all projection operators corresponding to S_z is identity.

Theorem 3.1. Completeness

We have

$$\sum_{\text{states } n} \hat{P}_n = \sum_{\text{states } n} |a_n\rangle \langle a_n| = \mathbb{1}$$

Proof. Consider the quantity $\langle\psi|\psi\rangle$.

$$\begin{aligned}\langle\psi|\psi\rangle &= \sum_n \sum_m c_n^* c_m \underbrace{\langle a_n|a_m\rangle}_{\delta_{nm}} = \sum_n |c_n|^2 \\ &= \sum_n \langle\psi|\hat{P}_n|\psi\rangle = \langle\psi| \sum_n \hat{P}_n |\psi\rangle\end{aligned}$$

so $\sum_n \hat{P}_n = \mathbb{1}$. □

We can use completeness to represent operators corresponding to observables in terms of their projection operators.

$$\hat{A}\,\mathbb{1} = \sum_n \hat{A}\ |a_n\rangle \langle a_n| = \sum_n a_n\ |a_n\rangle \langle a_n|\,.$$

$$\boxed{\hat{A} = \sum_n^{\text{all states}} a_n\ |a_n\rangle \langle a_n|} \qquad (*)$$

Comment 3.2. Eq. (*) is referred to as **spectral decomposition** of operator $\hat{A}$.

To see how the spectral decomposition of an operator $\hat{A}$ works, consider the action of $\hat{A}$ on an arbitrary state $|\psi\rangle$.

$$|\psi\rangle = \sum_n \langle a_n|\psi\rangle\, |a_n\rangle = \sum_n c_n\, |a_n\rangle\,.$$

We have

$$\begin{aligned}\hat{A}\,|\psi\rangle &= \sum_n \sum_m a_m c_n\ |a_m\rangle \langle a_m|a_n\rangle \\ &= \sum_n \sum_m a_m c_n \underbrace{\langle a_m|a_n\rangle}_{\delta_{nm}} |a_m\rangle \\ &= \sum_n c_n a_n\, |a_n\rangle\,.\end{aligned}$$

Note 3.1. $\hat{A}\,|\psi\rangle$ corresponds to a different state vector $|\psi'\rangle$.

$$|\psi'\rangle = \sum_n c'_n\,|a_n\rangle$$

with $c'_n = c_n a_n$. We note that if $|\psi\rangle$ represents an arbitrary quantum state, then in general

$$\hat{A}\,|\psi\rangle = |\psi'\rangle \neq \text{const.}\;|\psi\rangle\,.$$

Discovery 3.2. Therefore, an arbitrary superposition of eigenstates of an operator is not an eigenstate of the operator.

Let the initial quantum state prior to measurement be given by

$$|\psi_i\rangle = \sum_n c_n\,|a_n\rangle\,.$$

The measurement produces one of the possible eigenstates $|a_n\rangle$. We say that a measurement of $\hat{A}$ that yields a measurement result a_n, "collapses" or "projects" $|\psi_i\rangle$ to $|\psi_f\rangle = |a_n\rangle$. All subsequent measurements using observable $\hat{A}$ yield the state $|a_n\rangle$ with 100% probability, i.e.

$$\hat{A}\,|\psi_f\rangle = \hat{A}\,|a_n\rangle = a_n\,|a_n\rangle\,.$$

We express the measurement process using the projection operator corresponding to state $|a_n\rangle$.

$$|\psi_f\rangle = \frac{\hat{P}_n\,|\psi_i\rangle}{\sqrt{|\langle a_n|\psi_i\rangle|^2}} = \frac{|a_n\rangle\,\langle a_n|\,\psi_i\rangle}{|\langle a_n|\psi_i\rangle|} = \frac{\langle a_n|\psi_i\rangle\;|a_n\rangle}{|\langle a_n|\psi_i\rangle|} \tag{!}$$

The denominator in eq. (!) ensures that the coefficient of $|a_n\rangle$ is normalized to be 1, up to an overall phase factor. If we express the inner product

$$\langle a_n|\psi_i\rangle = |\langle a_n\psi_i\rangle|\,e^{i\alpha},$$

then eq. (!) may be written as

$$|\psi_f\rangle = e^{i\alpha}\,|a_n\rangle\,.$$

Up to an overall phase factor, eq. (!) projects the state $|\psi_i\rangle$ to the state $|a_n\rangle$. Since a quantum state can at most be defined up to an overall phase factor, the states $|a_n\rangle$ and $e^{i\alpha}\,|a_n\rangle$ are equivalent as far as any measurements are concerned.

3.1.1 Postulate 5 of QM

Theorem 3.2. Postulate 5

After a measurement of observable $\hat{A}$ that yields the result a_n, the quantum system is in a new state that is the normalized projection of the original system ket onto the ket(s) corresponding to the result of the measurement:

$$|\psi_f\rangle = \frac{\hat{P}_n |\psi_i\rangle}{\sqrt{\langle\psi_i|\hat{P}_n|\psi_i\rangle}}.$$

3.1.2 Expectation Value of an Operator

We introduce the expectation value of an operator $\hat{A}$, which returns the average or "expected" value of the operator corresponding to the state $|\psi\rangle$. Consider an arbitrary state $|\psi\rangle$ expressed in the $\hat{A}$ basis.

$$|\psi\rangle = \sum_n^{\text{all states}} c_n |a_n\rangle \qquad \text{where} \qquad c_n = \langle a_n|\psi\rangle.$$

where

$$\hat{A} = \sum_n a_n |a_n\rangle \langle a_n| .$$

Definition 3.2. **[Expectation]**

The expectation value of $\hat{A}$ for the state $|\psi\rangle$ is given by

$$\begin{aligned}\langle\psi|\hat{A}|\psi\rangle &= \sum_n a_n \langle\psi|a_n\rangle\langle a_n|\psi\rangle \\ &= \sum_n a_n |\langle a_n|\psi\rangle|^2 = \sum_n a_n |c_n|^2.\end{aligned}$$

We see that the expectation value returns the eigenvalues of operator $\hat{A}$ weighted by the probabilities. Thus, it corresponds to the average value of the operator for a given state $|\psi\rangle$.

3.2 Analysis of S-G Experiment 3 & 4 Using Projection Operators

We can view output ports of a S-G analyzer as projection operators that act on the input state.

The act of going through the S-G analyzer does not constitute a measurement. The measurement process would involve putting a detector on one or both ports of the S-G analyzer to obtain information about the state of the atom. If we place a detector on one of the ports and register the presense of an atom, then we know the state of that atom with %100 certainty.

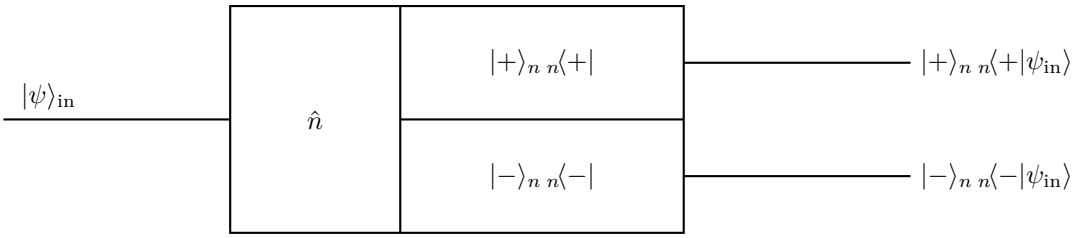
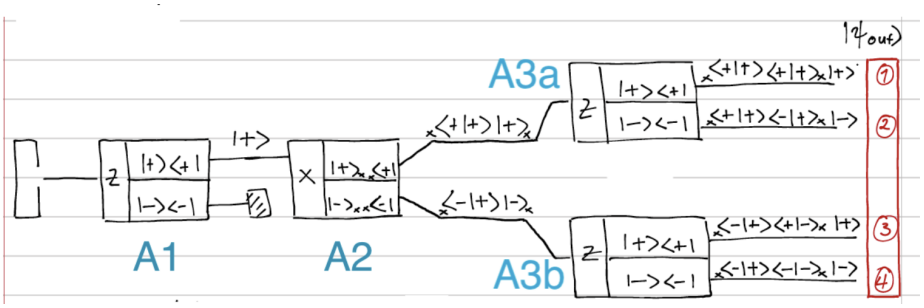


Fig. S-G Analyzer oriented in an arbitrary direction $\hat{\mathbf{n}}$.

3.2.1 Analysis of S-G Experiment 3 Using Projection Operators

Consider S-G Experiment 3:



Output of $|+\rangle$ port of Analyzer 1:

$$|\psi_1\rangle = |+\rangle\ \langle+|\psi\rangle_{\text{oven}} = |+\rangle$$

> **Comment 3.3.** The prefactor $\langle+|\psi\rangle_{\text{oven}}$ is proportional to the number of spins in the $|+\rangle$ state that come out of the oven. We will set the prefactor to 1 to simplify the math.

- Output of $|+\rangle_x$ port of Analyzer 2:

$$\begin{aligned}|\psi_{2+}\rangle &= |+\rangle_x\ {}_x\langle+|\psi_1\rangle \\ &= {}_x\langle+|+\rangle\ |+\rangle_x\end{aligned}$$

- Output of $|-\rangle_x$ port of Analyzer 2:

$$\begin{aligned}|\psi_{2-}\rangle &= |-\rangle_x\ {}_x\langle-|\psi_1\rangle \\ &= {}_x\langle-|+\rangle\ |-\rangle_x\end{aligned}$$

- Output of $|+\rangle$ port of Analyzer 3a:

$$\begin{aligned}|\psi_{\text{out}}\rangle_1 &= |+\rangle\,\langle+|\psi_{2+}\rangle \\ &= |+\rangle\,\langle+|\Big({}_x\langle+|+\rangle\ |+\rangle_x\Big) \\ &= {}_x\langle+|+\rangle\,\langle+|+\rangle_x\ |+\rangle \\ &= \big|\langle+|+\rangle_x\big|^2\ |+\rangle = \frac{1}{2}\,|+\rangle\end{aligned}$$

• Output of $|-\rangle$ port of Analyzer 3a:

$$\begin{aligned}|\psi_{\text{out}}\rangle_2 &= |-\rangle\langle -|\psi_{2+}\rangle \\ &= |-\rangle\langle -|\Big({}_x\langle +|+\rangle\ |+\rangle_x\Big) \\ &= {}_x\langle +|+\rangle\langle -|+\rangle_x\ |-\rangle = \frac{1}{2}|-\rangle\end{aligned}$$

• Output of $|+\rangle$ port of Analyzer 3b:

$$\begin{aligned}|\psi_{\text{out}}\rangle_3 &= |+\rangle\langle +|\psi_{2-}\rangle \\ &= |+\rangle\langle +|\Big({}_x\langle -|+\rangle\ |-\rangle_x\Big) \\ &= {}_x\langle -|+\rangle\langle +|-\rangle_x\ |+\rangle \\ &= \left|\langle +|-\rangle_x\right|^2\ |+\rangle = \frac{1}{2}|+\rangle\end{aligned}$$

• Output of $|-\rangle$ port of Analyzer 3b:

$$\begin{aligned}|\psi_{\text{out}}\rangle_4 &= |-\rangle\langle -|\psi_{2-}\rangle \\ &= |-\rangle\langle -|\Big({}_x\langle -|+\rangle\ |-\rangle_x\Big) \\ &= {}_x\langle -|+\rangle\langle -|-\rangle_x\ |-\rangle = -\frac{1}{2}|-\rangle\end{aligned}$$

Probabilities of measurement outcomes:

1. Probability to exit in the $|+\rangle$ port of A3a:

$$P_1 = |\langle +|\psi_{\text{out}}\rangle_1|^2 = \frac{1}{4}$$

2. Probability to exit in the $|-\rangle$ port of A3a:

$$P_2 = |\langle -|\psi_{\text{out}}\rangle_2|^2 = \frac{1}{4}$$

3. Probability to exit in the $|+\rangle$ port of A3b:

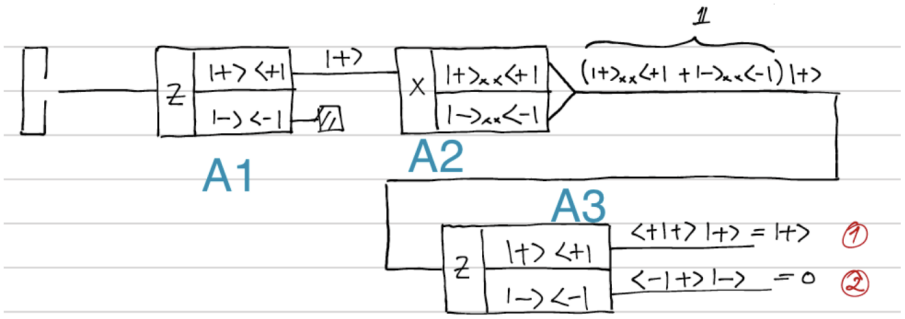
$$P_3 = |\langle +|\psi_{\text{out}}\rangle_3|^2 = \frac{1}{4}$$

4. Probability to exit in the $|-\rangle$ port of A3b:

$$P_4 = |\langle -|\psi_{\text{out}}\rangle_4|^2 = \frac{1}{4}$$

3.2.2 Analysis of S-G Experiment 4 Using Projection Operators

Consider S-G Experiment 4:



If you recall, in S-G Experiment 4, both outputs of A2 are sent into A3. We found that if we did not measure either output of A2, then the probability amplitudes for each of the two paths through A2 added constructively to produce 100% probability of exiting the $|+\rangle$ port of A3.

This result comes out naturally using the projection operator formalism.

- Output of $|+\rangle$ port of Analyzer 1:

$$|\psi_1\rangle = |+\rangle$$

- Output of Analyzer 2:

$$\begin{aligned} |\psi_2\rangle &= \Big(|+\rangle_x \, {}_x\langle +| \; + \; |-\rangle_x \, {}_x\langle -| \Big) \, |\psi_1\rangle \\ &= \underbrace{\Big(|+\rangle_x \, {}_x\langle +| \; + \; |-\rangle_x \, {}_x\langle -| \Big)}_{1} \, |+\rangle \\ &= |+\rangle \end{aligned}$$

> **Comment 3.4.** Note, I've used Completeness in simplifying the above expression.

- Output of $|+\rangle$ port of Analyzer 3:

$$\begin{aligned} |\psi_{3+}\rangle &= |+\rangle \langle +|\psi_2\rangle \\ &= \langle +|+\rangle \; |+\rangle \\ &= |+\rangle \end{aligned}$$

- Output of $|-\rangle$ port of Analyzer 3:

$$\begin{aligned} |\psi_{3-}\rangle &= |-\rangle \langle -|\psi_2\rangle \\ &= \langle -|+\rangle \; |-\rangle \\ &= 0 \end{aligned}$$

Probability of measurement outcomes

1. Probability to exit the $|+\rangle$ port of A3:

$$P_+ = \big|\langle +|+\rangle\big|^2 = 1$$

2. Probability to exit the $|-\rangle$ port of A3:

$$P_- = 0$$

3.3 Expectation Value of Operators

We wish to consider the average value of an observable corresponding to the operator $\hat{A}$ when performed on a particular state $|\psi\rangle$.

We know from Postulate 3 (2.6) of QM that the measurement will yield one of the possible eigenvalues of the observable with probability (Postulate 4 (2.4))

$$P_n = \left|\langle a_n|\psi\rangle\right|^2$$

where $\{|a\rangle\}$ represent the eigenbasis of $\hat{A}$. The new state after measurement will be (Postulate 5 (3.2))

$$|\psi'\rangle = |a_n\rangle$$

Each measurement projects or "collapses" the initial quantum state $|\psi\rangle$ to one of the eigenstates of $\hat{A}$.

Therefore, to determine the original $|\psi\rangle$, we must repeat the measurement many times and determine the probabilities for each outcome. This means we need many identical copies of $|\psi\rangle$ in order to reconstruct it.

From the distribution of measurement outcomes, we can reconstruct the original $|\psi\rangle$ up to some overall phase factor.

We express the state $|\psi\rangle$ in the eigenbasis of operator $\hat{A}$.

$$|\psi\rangle = \sum_n c_n \, |a_n\rangle \, .$$

We denote the average or "expected" value of the measurement of $\hat{A}$ for the state $|\psi\rangle$ as $\langle\hat{A}\rangle$.

$$\langle\hat{A}\rangle = \sum_n P_n \, a_n \tag{1}$$

The average value of $\hat{A}$ for the state $|\psi\rangle$ is equal to the sum over all eigenvalues $\{a\}$ of $\hat{A}$ multiplied by the corresponding probability of measurement.

$$\langle\hat{A}\rangle = \sum_n a_n \left|\langle a_n|\psi\rangle\right|^2 \tag{2}$$

$$\langle\hat{A}\rangle = \sum_n a_n |c_n|^2 = \sum_n a_n \, \langle\psi|\hat{P}_n|\psi\rangle \tag{3}$$

where $\hat{P}_n = |a_n\rangle \, \langle a_n|$ is the projection operator for state $|a_n\rangle$ (See Page 29). Using spectral decomposition (3.2), we express operator $\hat{A}$ using projection operators.

$$\hat{A} = \sum_n^{\text{all states}} a_n \, |a_n\rangle \, \langle a_n| \tag{4}$$

Inserting eq. (4) into eq. (3), we find that the expectation value of operator $\hat{A}$ for state $|\psi\rangle$ is

$$\langle\hat{A}\rangle = \langle\psi|\hat{A}|\psi\rangle \tag{5}$$

Note 3.2. The expectation value of an operator for a particular state is a physical quantity. Therefore, it cannot depend on our choice of basis for expressing $|\psi\rangle$.

3.3.1 Root-Mean-Square (RMS) Variation of Measurements

Consider the expectation or average values $\langle S_z\rangle$ and $\langle S_x\rangle$ in the $|\pm\rangle$ basis.

$$\begin{aligned}
\langle \pm|S_z|\pm\rangle &= \pm\frac{\hbar}{2}\langle \pm|\pm\rangle = \pm\frac{\hbar}{2}.\\
\langle +|S_x|+\rangle &= \langle +|\left(\frac{\hbar}{2}|+\rangle_x\ {}_x\langle +| - \frac{\hbar}{2}|-\rangle_x\ {}_x\langle -|\right)|+\rangle\\
&= \frac{1}{\sqrt{2}}\left(\frac{\hbar}{2}\right)\langle +|\big(|+\rangle_x - |-\rangle_x\big) = 0\\
\langle -|S_x|-\rangle &= \langle -|\left(\frac{\hbar}{2}|+\rangle_x\ {}_x\langle +| - \frac{\hbar}{2}|-\rangle_x\ {}_x\langle -|\right)|-\rangle\\
&= \frac{1}{\sqrt{2}}\left(\frac{\hbar}{2}\right)\langle -|\big(|+\rangle_x + |-\rangle_x\big) = 0
\end{aligned}$$

Discovery 3.3. We see that the expectation value of S_x for the states $|\pm\rangle$ is zero. We know from S-G exp. 2 that if we prepare a state in a eigenstate of one component of the angular momentum operator, then make a second measurement along an orthogonal direction, we obtain a 50%/50% probability of measuring spin up or down. Therefore, the average value of the second measurements will yield zero.

Lecture 7 - Wednesday, January 28

Definition 3.3. **[Root-Mean-Square (RMS)]**

The RMS value of a set of measurements of operator A is defined as

$$\Delta A = \sqrt{\langle (A - \langle A\rangle)^2\rangle}$$

Proposition 3.1. We have

$$\Delta A = \sqrt{\langle A^2\rangle - \langle A\rangle^2}$$

where $\langle A^2\rangle$ is the expectation value of A^2.

Example 3.2. Consider the RMS deviation for measurements of S_z for the S_z eigenkets $|\pm\rangle$.

$$\langle \pm | S_z^2 | \pm \rangle = \frac{\hbar^2}{4}$$

$$\Rightarrow \quad \Delta S_z = \sqrt{\langle \pm | S_z^2 | \pm \rangle - \big(\langle \pm | S_z | \pm \rangle\big)^2} = 0$$

Recall that ΔS_z is the average distance between a particular measurement of S_z and the average value of S_z for a collection of measurements performed on a the states $|\pm\rangle$. Because, each measurement yields the same result, either $+\frac{\hbar}{2}$ or $-\frac{\hbar}{2}$, the variation between measurements is zero.

$$\langle + | S_z | + \rangle \pm \Delta S_z \;\Rightarrow\; \frac{\hbar}{2} \pm 0$$

$$\langle - | S_z | - \rangle \pm \Delta S_z \;\Rightarrow\; -\frac{\hbar}{2} \pm 0$$

Example 3.3. Consider the RMS deviation of the operators S_x and S_y for the states $|\pm\rangle$. We have found that $\langle \pm | S_x | \pm \rangle = 0$. Likewise, you can also show that $\langle \pm | S_y | \pm \rangle = 0$.
To calculate ΔS_x and ΔS_y, we need to calculate $\langle S_x^2 \rangle$ and $\langle S_y^2 \rangle$.
There are at least two equivalent ways of calculating expectation values. Previously, I used the spectral decomposition of of S_x to calculate $\langle S_x \rangle$. We can use this approach again to calculate S_x^2:

$$\begin{aligned}
S_x &= \frac{\hbar}{2} |+x\rangle \langle +x| - \frac{\hbar}{2} |-x\rangle \langle -x|, \\
S_x^2 &= \left(\frac{\hbar}{2} |+x\rangle \langle +x| - \frac{\hbar}{2} |-x\rangle \langle -x|\right)\left(\frac{\hbar}{2} |+x\rangle \langle +x| - \frac{\hbar}{2} |-x\rangle \langle -x|\right) \\
&= \frac{\hbar^2}{4} |+x\rangle \langle +x|+x\rangle \langle +x| - \frac{\hbar^2}{4} |+x\rangle \langle +x|-x\rangle \langle -x| \\
&\quad - \frac{\hbar^2}{4} |-x\rangle \langle -x|+x\rangle \langle +x| + \frac{\hbar^2}{4} |-x\rangle \langle -x|-x\rangle \langle -x| \\
&= \frac{\hbar^2}{4}\big(|+x\rangle \langle +x| + |-x\rangle \langle -x|\big) = \frac{\hbar^2}{4}\mathbb{1} \qquad \text{(Completeness)}.
\end{aligned}$$

We can also calculate S_x^2 using the matrix representation of the operator:

$$S_x^2 = \frac{\hbar^2}{4}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{\hbar^2}{4}\mathbb{1}.$$

The expectation value $\langle \pm | S_x^2 | \pm \rangle = \frac{\hbar^2}{4}$.

$$\Delta S_x = \sqrt{\langle \pm | S_x^2 | \pm \rangle - \big(\langle \pm | S_x | \pm \rangle\big)^2} = \frac{\hbar}{2}.$$

Example 3.4. We likewise have for the operator S_y

$$S_y^2 = \frac{\hbar^2}{4}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{\hbar^2}{4}\mathbb{1}.$$

The expectation value $\langle \pm | S_y^2 | \pm \rangle = \frac{\hbar^2}{4}$.

$$\Delta S_y = \sqrt{\langle \pm | S_y^2 | \pm \rangle - \left(\langle \pm | S_y | \pm \rangle\right)^2} = \frac{\hbar}{2}.$$

These set of results demonstrate something very basic and profound about QM. Namely, we cannot simultaneously determine measurement outcomes for two non-commuting observable with arbitrary accuracy. If we determine the state of one operator, e.g., S_z with zero uncertainty, then a second measurement in an orthogonal direction, e.g., S_x or S_y is uncertain. In the next lecture, we will derive a rigorous relationship that quantifies this uncertainty relationship

4 The Uncertainty Principle

Lecture 8 - Tuesday, February 03

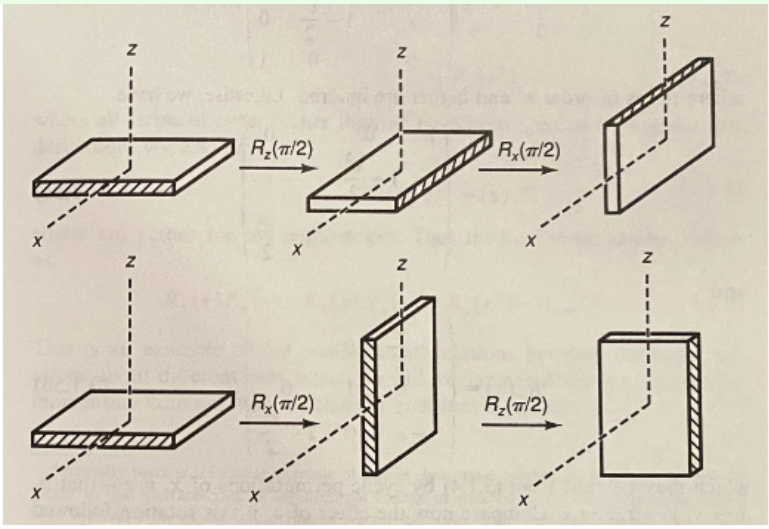
We have seen that we cannot simultaneously determine measurement outcomes for two incompatible observable with arbitrary accuracy. If we determine the state of one operator, e.g., S_z with zero uncertainty, then a second measurement in an orthogonal direction, e.g., S_x or S_y is uncertain.

In this section, we will present a general relationship that quantifies this uncertainty.

We notice that if two observables are incompatible, then the order of measurements produces different outcomes. Recall for example SG-Experiment 3, where switching the order of the second and third x and z analyzers produced different outcomes.

We know from everyday life that certain types of operations do depend on the order in which they are applied. Take for example 3D rotations. You may have noticed that if we rotate an object about two different axes, the final configuration of the object depends on the order of the rotations.

Example 4.1. See the following picture



Consider a rectangular slab which we first rotate by 90° around the z-axis followed by a 90° rotation around the x-axis. Now, compare the final state of the object having first rotated it by 90° around the x-axis followed by a 90° rotation around the z-axis.

Definition 4.1. **[Commute]**

If the order of operations of two operations produces different outcomes, we say that the operations do not **commute**.

Definition 4.2. **[Commutator]**

We quantify the commutativity of operators $\hat{A}$ and $\hat{B}$ by calculating the commutator. Here, for example, $\hat{A}$ and $\hat{B}$ could refer to operators corresponding to rotations around two different axes.

$$[\hat{A}, \hat{B}] := \hat{A}\hat{B} - \hat{B}\hat{A} \tag{1}$$

where the square bracket [ ] is the **commutator**.

Discovery 4.1. Notice that the commutator for the same operator is zero: $[\hat{A}, \hat{A}] = 0$.

Let's calculate the commutation relations for the spin-1/2 operators.

$$\begin{aligned}
[S_x, S_z] &= S_x S_z - S_z S_x \\
&= \frac{\hbar^2}{4}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \frac{\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\
&= \frac{\hbar^2}{4}\left[\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\right] \\
&= -\frac{\hbar^2}{2}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = -i\,\frac{\hbar^2}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\
&= -i\hbar S_y.
\end{aligned}$$

Note 4.1. Notice $[A, B] = -[B, A]$. Therefore $[S_z, S_x] = i\hbar S_y$.

Exercise 4.1. Show taht $[S_x, S_z] = i\hbar S_z$.

Exercise 4.2. Show taht $[S_y, S_z] = i\hbar S_x$.

4.1 The Uncertainty Principle in QM

Theorem 4.1. Uncertainty Principle

$$\Delta A\,\Delta B \geq \frac{1}{2}\,|\langle [A, B]\rangle| \tag{5}$$

where ΔA and ΔB refer the measurement uncertainty obtained for observables A and B for a particular state $|\psi\rangle$. $\langle [A, B]\rangle$ is the expectation value of the commutator $[A, B]$ calculated for the state $|\psi\rangle$.

Example 4.2. Suppose the state $|\psi\rangle = |+\rangle$ is prepared to be in an eigenstate of the operator S_z. We then perform a measurement of either S_x or S_y.
If the particle is in the state $|+\rangle$, then the expectation value of S_z is $\langle +|S_z|+\rangle = \frac{\hbar}{2}$. Because the state $|+\rangle$ is an eigenstate of S_z, there is no uncertainty associated with the measurement of S_z, therefore $\Delta S_z = 0$.
However, for the state $|+\rangle$, the observables S_x and S_y both have uncertainty of measurement outcomes, given by $\Delta S_x = \Delta S_y = \frac{\hbar}{2}$.
For the right hand side, we know that $[S_x, S_y] = i\hbar S_z$, so

$$\begin{aligned}\frac{1}{2}\left|\langle +|\left[S_x, S_y\right]|+\rangle\right| &= \frac{1}{2}\left|i\hbar\langle +|\, S_z\,|+\rangle\right| \\ &= \frac{\hbar}{2}\left(\frac{\hbar}{2}\right)\end{aligned}$$

so the inequality holds as equality.

We see that we cannot simultaneously know all three components of the angular momentum. In fact, when we determine one its components, the other two become uncertain.

Although we can only measure one of the components of $\vec{S}$ with certainty, we can determine the magnitude of the vector.

$$S^2 = \vec{S}\cdot\vec{S} = S_x^2 + S_y^2 + S_z^2 \tag{6}$$

We can show that the square of any component of the angular momentum operator is proportional to the identity operator.

$$\begin{aligned} & S_i^2 = \frac{\hbar^2}{4}\mathbb{1}, \qquad i = \{x, y, z\} \\ \Rightarrow \quad & S^2 = \frac{3\hbar^2}{4}\mathbb{1} \\ \therefore \quad & \|\vec{S}\| = \frac{\sqrt{3}\hbar}{2}\mathbb{1}\end{aligned}$$

This yields us that

$$\left[S^2,\, S_i\right] = 0 \tag{7}$$

Note 4.2. The magnitude of the spin angular momentum is longer than its projection that can be measured. We cannot think about the spin-1/2 angular momentum as pointing in a particular direction.

5 Density Operator Done Right

5.1 Pure and Mixed Ensembles in QM

So far, our discussion of QM has dealt with describing particles in a definite quantum state. If we are given a collection, or ensemble of such particles, then we can describe all members of the ensemble with a common state vector. However there are instances where the ensemble is described by a collection of particles in different quantum states. For such ensembles, there is no one state vector that describes the ensemble, therefore we need to expand our formalism to deal with such ensembles.

If you recall, we said that the atoms exiting the oven in the S-G experiment where unpolarized, that is if we sent the beam of particles into a S-G analyzer, we would measure a 50%/50% distribution of spin-up and spin-down particles regardless of the direction in which we oriented the S-G analyzer.

If we place a S-G analyzer in front of the beam exiting the oven, say along the z-direction, then the state of the particles exiting the analyzer is either spin-up ($|+\rangle$) or spin-down ($|-\rangle$).

Definition 5.1. **[Pure Ensemble]**

We refer to ensembles in which all members of the ensemble have a definite polarization as **pure ensembles**.

Definition 5.2. **[Mixed Ensemble]**

Members of the ensemble are represented bt a statistical admixture of states.

In a pure ensemble, all members of the ensemble have a common state vector

$$|\psi\rangle = \sum_n c_n |a_n\rangle$$

Note, with the appropriate unitary transformation, we can always transform to a basis in which the state $|\psi\rangle$ may be expressed in terms of a single ket $|\psi\rangle = |b_n\rangle$ in some other complete basis $\{|b\rangle\}$.

In contrast to pure ensembles, there is no single ket that describes the state of a particles coming out of the oven in the S-G experiment. Such unpolarized states are described as a statistical admixtures of pure ensembles.

Question 5.1.

How do we operationally distinguish mixed ensembles from pure ones?

Imagine we are given a beam of particles of an unknown polarization, and we are asked to identify whether they belong to mixed of pure ensembles. How would we figure this out?
We have a S-G analyzer with which we can measure the state of the particles along any direction in space.

Suppose we orient the analyzer in the x–direction and we find a 50%/50% distribution of spin-up and spin-down particles. This is certainly consistent with having an unpolarized distribution, however the particles can also be in either the $|\pm\rangle$ state, for example and produce the same distribution.

To identify whether the particles belong to a pure or mixed ensemble, we need to rotate the S-G analyzer over

all angles in space. If we find that the there is a direction in which we only get spin-up or spin-down, then the particles belong to a pure ensemble. However, if we find that we get a 50%/50% distribution regardless of the angle, then the particles belong to a mixed ensemble.

Comment 5.1. To be clear, a completely unploarized ensemble is referred to as being fully mixed. In reality, we rarely deal with systems that are fully mixed or completely pure. In real-world experiments, we are usually dealing with ensembles that are a mixture of the two

5.2 Density Operator

A systematic way of working with both types of ensembles is by introducing the density operator $\hat{\rho}$. For the state $|\psi\rangle = \sum_n c_n |n\rangle$, consider the probability of measuring the state $|m\rangle$.

$$\begin{aligned} P_m &= |\langle m|\psi\rangle|^2 \\ &= \langle m|\psi\rangle \langle m|\psi\rangle^* = \langle m| \underbrace{|\psi\rangle\langle\psi|}_{\hat{\rho}} |m\rangle \end{aligned}$$

Definition 5.3. **[Density Operator]**

We define the density operator corresponding to a state $|\psi\rangle$ as $\hat{\rho} := |\psi\rangle\langle\psi|$.

Comment 5.2. For a pure state, the density operator is equivalent to the projection operator.

Lemma 5.1. $\hat{\rho}$ is a Hermitian operator.

Proof. We verify

$$\begin{aligned} \hat{\rho}_{ij} &= \langle i|\hat{\rho}|j\rangle = \langle i|\psi\rangle \langle\psi|j\rangle \\ \hat{\rho}^*_{ji} &= \left(\langle j|\hat{\rho}|i\rangle\right)^* = \left(\langle j|\psi\rangle \langle\psi|i\rangle\right)^* \\ &= \langle j|\psi\rangle^* \langle\psi|i\rangle^* = \langle\psi|j\rangle \langle i|\psi\rangle = \langle i|\psi\rangle \langle\psi|j\rangle = \hat{\rho}_{ij} \end{aligned}$$

as desired. □

Proposition 5.1. The trace of the density operator for a pure ensemble is equal to 1 for any complete basis representation.

Proof. Let $|\psi\rangle$ have normalization $\langle\psi|\psi\rangle = 1$, and $\hat{\rho} = |\psi\rangle\langle\psi|$.

$$\begin{aligned} \mathrm{tr}\{\hat{\rho}\} &= \sum_i \hat{\rho}_{ii} = \sum_i \langle i|\hat{\rho}|i\rangle = \sum_i \langle i|\psi\rangle \langle\psi|i\rangle \\ &= \sum_i \langle\psi|i\rangle \langle i|\psi\rangle \end{aligned}$$

Recall that we know by completeness

$$\sum_i |i\rangle\langle i| = \mathbb{1}$$

Therefore $\text{tr}\{\hat{\rho}\} = \langle\psi|\mathbb{1}|\psi\rangle = \langle\psi|\psi\rangle = 1$. □

Proposition 5.2. For pure states, $\hat{\rho}^2 = \hat{\rho}$.

Proof. The proof is simple, we have

$$\hat{\rho}^2 = |\psi\rangle\langle\psi|\,|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = \hat{\rho}$$

as desired. □

Corollary 5.1. For pure states, $\text{tr}(\hat{\rho}^2) = 1$.

Proposition 5.3. Given a state $|\psi\rangle$, the probability of measuring the state $|\phi\rangle$ is

$$\text{Prob.} = |\langle\phi|\psi\rangle|^2 = \text{tr}\{\hat{P}_\phi\hat{\rho}\}$$

where $\hat{P}_\phi = |\phi\rangle\langle\phi|$ is the projection operator for the state $|\phi\rangle$.

Proof.

$$\begin{aligned}\text{tr}\{\hat{P}_\phi\hat{\rho}\} &= \sum_i \langle i|\hat{P}_\phi\hat{\rho}|i\rangle = \sum_i \langle i|\phi\rangle\langle\phi|\psi\rangle\langle\psi|i\rangle \\ &= \langle\phi|\psi\rangle\sum_i\langle\psi|i\rangle\langle i|\phi\rangle \\ &= \langle\phi|\psi\rangle\langle\psi|\phi\rangle = |\langle\phi|\psi\rangle|^2.\end{aligned}$$

as desired. □

Proposition 5.4. The expectation value of operator $\hat{A}$ for the state $|\psi\rangle$ is

$$\langle\psi|\hat{A}|\psi\rangle = \text{tr}\{\hat{A}\hat{\rho}\}.$$

Proof.

$$\begin{aligned}\langle\psi|\hat{A}|\psi\rangle &= \sum_i \langle\psi|i\rangle\,\langle i|\hat{A}|\psi\rangle \qquad \text{using } \sum_i |i\rangle\langle i| = \mathbb{1} \\ &= \sum_i \langle i|\hat{A}|\psi\rangle\,\langle\psi|i\rangle \\ &= \sum_i \langle i|\hat{A}\hat{\rho}|i\rangle = \text{tr}\{\hat{A}\hat{\rho}\}.\end{aligned}$$

as desired. □

Example 5.1. Use the density matrix formalism to calculate $\langle S_z \rangle$ and $\langle S_y \rangle$ for the states $|\pm\rangle$.

$$\hat{\rho}_+ = |+\rangle\langle +| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\langle +|S_z|+\rangle = \mathrm{Tr}\{S_z \hat{\rho}_+\} = \mathrm{Tr}\left\{ \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \right\} = \mathrm{Tr}\left\{ \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \right\} = \frac{\hbar}{2}$$

$$\hat{\rho}_- = |-\rangle\langle -| = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\langle -|S_z|-\rangle = \mathrm{Tr}\{S_z \hat{\rho}_-\} = \mathrm{Tr}\left\{ \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \right\} = \mathrm{Tr}\left\{ \frac{\hbar}{2} \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix} \right\} = -\frac{\hbar}{2}$$

$$\langle +|S_y|+\rangle = \mathrm{Tr}\{S_y \hat{\rho}_+\} = \mathrm{Tr}\left\{ \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \right\} = \mathrm{Tr}\left\{ \frac{\hbar}{2} \begin{pmatrix} 0 & 0 \\ i & 0 \end{pmatrix} \right\} = 0$$

$$\langle -|S_y|-\rangle = \mathrm{Tr}\{S_y \hat{\rho}_-\} = \mathrm{Tr}\left\{ \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \right\} = \mathrm{Tr}\left\{ \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ 0 & 0 \end{pmatrix} \right\} = 0$$

Note 5.1. When calculating $\mathrm{Tr}\{\hat{A}\hat{\rho}\}$, both $\hat{A}$ and $\hat{\rho}$ must be represented in the same basis.

Exercise 5.1. Calculate $\langle +_y|S_y|+_y\rangle$ using the density operator $\hat{\rho} = |+_y\rangle\langle +_y|$ in the S_z basis.

While density operators can be used to calculate expectation values for pure ensembles, they are especially useful for calculating mixed ensembles. For a mixed ensemble

$$\hat{\rho} = \sum_k P_k \, |\psi_k\rangle\langle\psi_k|$$

where P_k is the probability that a member of the ensemble is in the state $|\psi_k\rangle$, so $\sum_k P_k = 1$. We know that

$$\hat{\rho}_{ij} = \sum_k P_k \, \langle i|\psi_k\rangle\langle\psi_k|j\rangle$$

Hence

$$\begin{aligned} \mathrm{Tr}\{\hat{\rho}\} &= \sum_i \hat{\rho}_{ii} = \sum_i \sum_k P_k \, \langle i|\psi_k\rangle\langle\psi_k|i\rangle \\ &= \sum_k P_k \sum_i \langle\psi_k|i\rangle\langle i|\psi_k\rangle \\ &= \sum_k P_k \underbrace{\langle\psi_k|\psi_k\rangle}_{1} = \sum_k P_k = 1. \end{aligned}$$

Proposition 5.5. For mixed ensembles $\mathrm{tr}\{\hat{\rho}^2\} < 1$.

Proof. We have

$$\begin{aligned}\mathrm{Tr}\{\hat{\rho}^2\} &= \sum_i \sum_k \sum_l P_k P_l \, \langle i|\psi_k\rangle\langle\psi_k|\psi_l\rangle\langle\psi_l|i\rangle \\ &= \sum_k \sum_l P_k P_l \, \langle\psi_k|\psi_l\rangle \underbrace{\sum_i \langle\psi_l|i\rangle\langle i|\psi_k\rangle}_{(\langle\psi_k|\psi_l\rangle)^*} \\ &= \sum_k \sum_l P_k P_l \, |\langle\psi_k|\psi_l\rangle|^2\end{aligned}$$

From the Cauchy-Schwarz inequality, we know

$$\underbrace{\langle\psi_k|\psi_k\rangle}_{1}\,\underbrace{\langle\psi_l|\psi_l\rangle}_{1} \;\geq\; |\langle\psi_k|\psi_l\rangle|^2 \qquad \Rightarrow \qquad |\langle\psi_k|\psi_l\rangle|^2 \leq 1$$

$$\therefore \quad \sum_k \sum_l P_k P_l \, |\langle\psi_k|\psi_l\rangle|^2 \leq 1 \qquad \Rightarrow \qquad \mathrm{Tr}\{\hat{\rho}^2\} \leq 1$$

□

Note 5.2. This is an important distinguishing feature of mixed ensembles. Given a density matrix, we can determine if it corresponds to pure ensemble by calculating $\mathrm{Tr}\{\hat{\rho}^2\}$.

$$\text{Pure Ensembles:} \quad \mathrm{Tr}\{\hat{\rho}^2\} = 1$$

$$\text{Mixed Ensembles:} \quad \mathrm{Tr}\{\hat{\rho}^2\} < 1$$

Lecture 9 - Thursday, February 05

Example 5.2. Consider the density operator

$$\hat{\rho} = \frac{1}{2}|+\rangle\langle+| + \frac{1}{2}|-\rangle\langle-|.$$

Show that this density operator corresponds to a mixed ensemble. Show that the density operator corresponds to a *maximally* mixed ensemble.

Solution. For the first part, we have

$$\hat{\rho} = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix} + \frac{1}{2}\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix} = \frac{1}{2}\mathbb{1} \qquad \Rightarrow \qquad \hat{\rho}^2 = \frac{1}{4}\mathbb{1}$$

and hence

$$\mathrm{Tr}\{\hat{\rho}^2\} = \frac{1}{4} + \frac{1}{4} = \frac{1}{2} < 1$$

For the second part, we think of a maximally mixed ensemble as one in which there is no preferred polarization. Therefore, if we orient the S-G analyzer along any direction in space, we will always get a 50%/50%

distribution. To see if the ensemble described by $\hat{\rho}$ is fully mixed, we calculate the expectation value of the angular momentum operator in the $\hat{n}$–direction.

$$S_n = \frac{\hbar}{2}\begin{pmatrix} \cos\theta & \sin\theta\, e^{-i\phi} \\ \sin\theta\, e^{i\phi} & -\cos\theta \end{pmatrix}$$

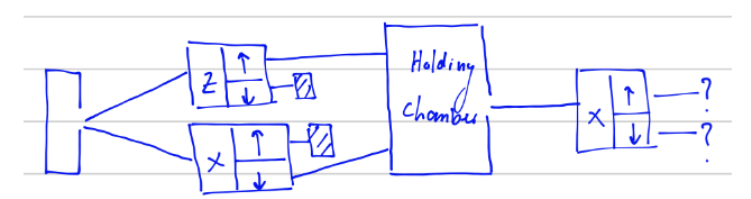
$$\langle S_n \rangle = \mathrm{Tr}\{S_n \hat{\rho}\} = \mathrm{Tr}\left\{ \frac{\hbar}{2}\begin{pmatrix} \cos\theta & \sin\theta\, e^{-i\phi} \\ \sin\theta\, e^{i\phi} & -\cos\theta \end{pmatrix} \frac{1}{2}\mathbb{1} \right\} = 0$$

We see that $\langle S_n \rangle = 0$ for any direction, therefore the spin state is completely unpolarized, or maximally mixed. □

Example 5.3. Consider the density operator

$$\hat{\rho} = \frac{1}{2}\,|+\rangle\langle +| + \frac{1}{2}\,|-\rangle_{xx}\langle -|\,.$$

Conceptually, we can think of composing an ensemble of spins that corresponds to $\hat{\rho}$ by constructing a holding chamber that collects the output of two S-G analyzers, as shown in the figure below.



The holding chamber creates an equal mix of particles in the $|+\rangle$ and $|-\rangle_x$ states, i.e., if you reach into the holding chamber and grab a particle, you are equally likely to get a spin in the $|+\rangle$ or $|-\rangle_x$ state.
Show that this density operator corresponds to a mixed ensemble.

Proof. We know that

$$\hat{\rho} = \begin{pmatrix} \frac{3}{4} & -\frac{1}{4} \\ -\frac{1}{4} & \frac{1}{4} \end{pmatrix}$$

Note that $\mathrm{Tr}\{\hat{\rho}\} = 1$. We wish to show that $\mathrm{Tr}\{\hat{\rho}^2\} < 1$.

$$\hat{\rho}^2 = \frac{1}{16}\begin{pmatrix} 3 & -1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} 3 & -1 \\ -1 & 1 \end{pmatrix} = \frac{1}{8}\begin{pmatrix} 5 & -2 \\ -2 & 1 \end{pmatrix}$$

so clearly $\mathrm{Tr}\{\hat{\rho}^2\} = \frac{3}{4} < 1$. In addition, we calculate $\langle S_x \rangle$:

$$\langle S_x \rangle = \mathrm{Tr}\{S_x \hat{\rho}\} = \mathrm{Tr}\left\{ \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{1}{4}\begin{pmatrix} 3 & -1 \\ -1 & 1 \end{pmatrix} \right\} = -\frac{\hbar}{4}$$

□

Note 5.3. The expectation value $\langle S_x \rangle$ for the state $\hat{\rho}$ can be thought of as

$$\langle S_x \rangle = \underbrace{\text{Prob.}(|+\rangle)}_{\frac{1}{2}} \underbrace{\langle + | S_x | + \rangle}_{0} + \underbrace{\text{Prob.}(|-\rangle_x)}_{\frac{1}{2}} \underbrace{\langle - _x | S_x | - _x \rangle}_{-\frac{\hbar}{2}}$$

Therefore $\langle S_x \rangle = -\frac{\hbar}{4}$.

Exercise 5.2. If a measurement of S_x is performed, what is the probability of obtaining $\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$?

6 Midterm Review

Exercise 6.1. Consider a quantum system described by a basis $|a_1\rangle$, $|a_2\rangle$, and $|a_3\rangle$. The system is initially in the state

$$|\psi_i\rangle = \frac{i}{\sqrt{3}}|a_1\rangle + \sqrt{\frac{2}{3}}|a_2\rangle$$

Find the probability that the system is measured to be in the final state

$$|\psi_f\rangle = \frac{1+i}{\sqrt{3}}|a_1\rangle + \frac{1}{\sqrt{6}}|a_2\rangle + \frac{1}{\sqrt{6}}|a_3\rangle$$

Proof. The probability is given by

$$\begin{aligned}\text{Prob} &= |\langle\psi_i|\psi_f\rangle|^2 \\ &= \left|\begin{pmatrix} -\frac{i}{\sqrt{3}} & \sqrt{\frac{2}{3}} & 0 \end{pmatrix}\begin{pmatrix} \frac{1+i}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \end{pmatrix}\right|^2 \\ &= \frac{5}{9}\end{aligned}$$

as desired. □

Exercise 6.2. Consider a 3 dimensional ket space. In the basis defined by the orthonormal kets $|1\rangle$, $|2\rangle$, $|3\rangle$ the operators $\hat{A}$ and $\hat{B}$ are represented by

$$\hat{A} = \begin{pmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & a_3 \end{pmatrix} \qquad \hat{B} = \begin{pmatrix} b_1 & 0 & 0 \\ 0 & 0 & b_2 \\ 0 & b_2 & 0 \end{pmatrix}$$

Find the eigenvalues and the corresponding eigenvectors of the operators.

Proof. Standard computation. □

Lecture 10 - Tuesday, February 10

Exercise 6.3. The probability of obtaining $S_z = \frac{\hbar}{2}$ is 90% and the probability of obtaining $S_y = \frac{\hbar}{2}$ is 20%. Using this information, determine the state of the particle up to an overall phase factor.

Solution. We know that

$$|\langle +|\psi\rangle|^2 = 0.9$$

and hence we can take (by convention) $a = \sqrt{0.9}$. Recall that our state, denoted as $|\psi\rangle = a|+\rangle + b|-\rangle$, has to be normalized, so we must have $|b|^2 = 0.1$. This tells us that $b = |b|e^{i\theta}$. From the second information, we know that

$$\left|\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix}\right|^2 = 0.2 \quad \Rightarrow \quad i\sqrt{0.09}\underbrace{(e^{-i\theta} - e^{i\theta})}_{=2i\sin\theta} = -0.6$$

Solving for θ we get $\theta = -\pi/2$, and hence

$$|\psi\rangle = \sqrt{0.9}\,|+\rangle - i\sqrt{0.1}\,|-\rangle$$

as desired. □

Exercise 6.4. Determine the matrix representations of S_x and S_y using the eigenstates of S_y.

Proof. What are somethings that we know? In the basis of S_z, we know

$$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

In S_y basis, we would have

$$S_y = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and this can be easily verified via the change of basis method. Similarly, we can also compute S_x this way.

$$S_x = \begin{pmatrix} {}_y\langle +|\, S_x\, |+\rangle_y & {}_y\langle +|\, S_x\, |-\rangle_y \\ {}_y\langle -|\, S_x\, |+\rangle_y & {}_y\langle -|\, S_x\, |-\rangle_y \end{pmatrix}$$

Now compute these inner products in the z-basis to get S_x in terms of the y-basis. It is possible to convert the $|\pm\rangle_y$ in terms of the x basis to make the computations easier. Another way to do it is to let:

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}$$

The matrix with $|\pm\rangle_y$ as its columns, then what we want is $U^{-1}S_xU$ and $U^{-1}S_yU$. Note $U^{-1} = U^\dagger$. □

Lecture 11 - Thursday, February 12

In class midterm today

7 Time Evolution of Quantum States

Lecture 12 - Tuesday, February 24

So far we have not discussed systems that change in time. We will now develop a theory for how kets evolve in time, similar to Newton's laws of motion.

We know classical systems subject to external forces evolve according to Newton's law $\vec{\mathbf{F}} = m\vec{\mathbf{a}}$. In QM, the Schrödinger equation plays the the equivalent role to $\vec{\mathbf{F}} = m\vec{\mathbf{a}}$ in describing the time evolution of the quantum state $|\psi\rangle$.

Comment 7.1. The first important point to keep in mind is that time is treated as a continuous parameter in QM. There is no operator that corresponds to time.

How does a ket change in time? We need an operator that transforms a ket at one time to a ket at a different time. Let's use the approach we developed for rotations to construct an unitary operator that translates a state by an infinitesimal amount of time. Let's first review the properties of the infinitesimal translation operator.

7.1 Infinitesimal Transformations

Operators corresponding to observables, such as angular momentum, linear momentum, position and energy all generate transformations of states in Hilbert space. Angular momentum, for example rotates kets. We will see later that the linear momentum operator will produce translations, and the energy operator will produce a translation of states in time. We can build continuous transformations by applying a series of infinitesimal transformations.

The infinitesimal transformation operator has the basic form

$$U(\varepsilon) = \mathbb{1} - i\varepsilon\hat{G}$$

where $\hat{G}$ is a Hermitian operator corresponding to the particular observable in question, e.g., angular momentum, and ε is the infinitesimal quantity, e.g., $\mathrm{d}\phi$ for the case of rotations.

There are two reasons for choosing $U(\varepsilon)$ to have this mathematical form.

- First, we require that $\lim_{\varepsilon\to 0} U(\varepsilon) = 1$.
- Second, $U(\varepsilon)$ should be unitary, that is, it should transform a state without changing its norm. Another way of saying this is that it should conserve probability. We therefore require that $UU^\dagger = 1$:

$$\begin{aligned} UU^\dagger &= (1 - i\epsilon G)(1 + i\epsilon G^\dagger) \\ &= 1 + i\epsilon G - i\epsilon G + \epsilon^2 G^2 \end{aligned}$$

We see that terms of $\mathcal{O}(\epsilon)$ cancel. Neglecting terms of order $\mathcal{O}(\epsilon^2)$, $UU^\dagger = 1$, as required.

7.2 The Hamiltonian

Let the state of the system at time t be $|\psi(t)\rangle$. We define a unitary operator $U(t+\delta t, t)$, which translates the state $|\psi(t)\rangle$ in time to $|\psi(t+\delta t)\rangle$.

$$U(t+dt, t) = 1 - i\Omega\, dt \tag{1}$$

where $\Omega = \Omega^\dagger$ is a Hermitian operator.

We need to identify the physical observable that corresponds to the operator Ω.

Discovery 7.1. We note that Ω has units of frequency. We recall from the Planck-Einstein relationship in quantum theory that energy and frequency are related $E = \hbar\omega$. From classical mechanics, we also know that the Hamiltonian $\mathcal{H}$ generates evolution in time. $\mathcal{H}$ is equal to the total energy of the system. It is therefore natural to associate Ω with the total energy of the system.

$$\Omega = \frac{\mathcal{H}}{\hbar} \tag{2}$$

We rewrite eq.(1) as

$$U(t+\delta t, t) = 1 - \frac{i\mathcal{H}\delta t}{\hbar} \tag{3}$$

Note 7.1. It is important to note that $\mathcal{H}$ can be time dependent. In eq.(3) we are considering $\mathcal{H}(t)$, i.e., the Hamiltonian at time t.

Applying the $U(t+\delta t, t)$ to $|\psi(t)\rangle$ we obtain

$$\begin{aligned} U(t+\delta t, t)\,|\psi(t)\rangle &= |\psi(t+\delta t)\rangle \\ \left(1 - \frac{i\mathcal{H}\delta t}{\hbar}\right)|\psi(t)\rangle &= |\psi(t+\delta t)\rangle \\ &= |\psi(t)\rangle + \frac{d}{dt}|\psi(t)\rangle\ \delta t + \mathcal{O}(\delta t^2) \end{aligned}$$

$$\boxed{\mathcal{H}\ |\psi(t)\rangle = i\hbar \frac{d}{dt}|\psi(t)\rangle} \tag{4}$$

7.2.1 Postulate 6

Theorem 7.1. Postulate 6

The time evolution of a quantum system is determined by the Hamiltonian or total energy operator $\mathcal{H}(t)$ through the Schrödinger equation

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \mathcal{H}(t)\ |\psi(t)\rangle \tag{5}$$

The spectrum of allowed energies of a quantum system corresponds to the eigenvalues of the Hamiltonian $\{E\}$. The corresponding eigenvectors $\{|E\rangle\}$ are referred to as **energy eigenkets**. We will begin our

study of the Schrödinger equation first considering a time-independent Hamiltonian.

$$\mathcal{H}(|E_n\rangle) = E_n\,|E_n\rangle$$

The Hamiltonian is a Hermitian operator, therefore the basis eigenkets form a complete and orthonormal basis.

In the energy basis, the operator $\mathcal{H}$ is diagonal

$$\mathcal{H} = \begin{pmatrix} E_1 & 0 & 0 & \cdots \\ 0 & E_2 & 0 & \cdots \\ 0 & 0 & E_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

We can represent any time-dependent state $|\psi(t)\rangle$ in terms of the energy eigenvectors.

$$|\psi(t)\rangle = \sum_n c_n(t)\,|E_n\rangle$$

Note 7.2. **Important:** For a time independent Hamiltonian, the basis vectors are time independent. The time dependence of $|\psi(t)\rangle$ enters through the the coefficients $c(t)$.

Solve for the time dependence of a particular $c_n(t)$.

$$\begin{aligned}
i\hbar \frac{d}{dt} \sum_n c_n(t)\,|E_n\rangle &= \mathcal{H} \sum_m c_m(t)\,|E_m\rangle \\
i\hbar \sum_n \frac{dc_n}{dt}\,|E_n\rangle &= \sum_m c_m E_m\,|E_m\rangle \\
i\hbar \sum_n \frac{dc_n}{dt}\,\underbrace{\langle E_k|E_n\rangle}_{\delta_{kn}} &= \sum_m c_m E_m\,\underbrace{\langle E_k|E_m\rangle}_{\delta_{km}} \\
i\hbar \frac{dc_k}{dt} &= c_k E_k \\
\frac{dc_k}{c_k} &= \frac{E_k}{i\hbar}\,dt \\
\ln c_k &= -\frac{iE_k}{\hbar}\,t + \text{const.} \\
c_k(t) &= c_k(t=0)\exp\{-iE_k t/\hbar\}
\end{aligned}$$

$$\boxed{|\psi(t)\rangle = \sum_n c_n(0)\exp\{-iE_n t/\hbar\}\,|E_n\rangle}$$

Proposition 7.1. For a time-independent Hamiltonian, the time dependence of of $|\psi(t)\rangle$ is equal to the sum of energy eigenkets multiplied by a time-dependent phase factor.

Example 7.1. Suppose we start from an energy eigenstate of the Hamiltonian $|\psi(0)\rangle = |E_m\rangle$. Calculate $|\psi(t)\rangle$, and the probability $|\langle\psi(0)|\psi(t)\rangle|^2$ that the system remains in the original state $|\psi(0)\rangle$.

$$\begin{aligned} |\psi(t)\rangle &= c_m(0)\exp\{-iE_mt/\hbar\}\,|E_m\rangle \\ |\langle\psi(0)\,|\psi(0)\rangle\,|^2 &= 1 \\ |c_m(0)|^2 &= 1 \quad \Rightarrow \quad c_m(0) = 1 \\ |\langle\psi(0)|\psi(t)\rangle|^2 &= |\exp\{-iE_mt/\hbar\}\,\langle E_m|E_m\rangle|^2 = 1 \end{aligned}$$

We see that the time dependence of an energy eigenket is through the time-dependent phase factor $\exp\{-iE_mt/\hbar\}$. As we have noticed before, an overall phase factor does not affect the probability. We refer to an energy eignestate as a stationary state, because a system that starts out in an energy eignestate remains in that eigenstate. Let's consider a system that starts from a state that is not an energy eignestate.

$$|\psi(0)\rangle = c_1(0)\,|E_1\rangle + c_2(0)\,|E_2\rangle$$

In general, $|\psi(0)\rangle$ is not an eigenstate of $\mathcal{H}$.

$$\mathcal{H}\,|\psi(0)\rangle = E_1c_1(0)\,|E_1\rangle + E_2c_2(0)\,|E_2\rangle \neq \text{const.}\,|\psi(0)\rangle$$

From the time-dependent state eq.(7) we derived, we can immediately write the expression for the $|\psi(t)\rangle$. We define the angular frequency $\omega_n := \frac{E_n}{\hbar}$. Let $c_n := c_n(0)$.

$$|\psi(t)\rangle = c_1(0)e^{-i\omega_1 t}\,|E_1\rangle + c_2(0)e^{-i\omega_2 t}\,|E_2\rangle$$

Let's calculate the probability that the system remains in the initial state $|\psi(0)\rangle$.

$$\begin{aligned} |\langle\psi(0)|\psi(t)\rangle|^2 &= \left|\begin{pmatrix} c_1^* & c_2^* \end{pmatrix}\begin{pmatrix} c_1e^{-i\omega_1 t} \\ c_2e^{-i\omega_2 t}\end{pmatrix}\right|^2 \\ &= \left||c_1|^2e^{-i\omega_1 t} + |c_2|^2e^{-i\omega_2 t}\right|^2 \\ &= |c_1|^4 + |c_2|^4 + |c_1|^2|c_2|^2\left(e^{i(\omega_2-\omega_1)t} + e^{-i(\omega_2-\omega_1)t}\right) \\ &= |c_1|^4 + |c_2|^4 + 2|c_1|^2|c_2|^2\cos\big[(\omega_2-\omega_1)t\big]. \end{aligned}$$

Suppose we start from a normalized state where $|c_1|^2 + |c_2|^2 = 1$, and let $|c_1|^2 = |c_2|^2 = \frac{1}{2}$.

$$|\langle\psi(0)|\psi(t)\rangle|^2 = \frac{1}{2}\Big[1 + \cos\big[(\omega_2-\omega_1)t\big]\Big]$$

If the system does not start from an eigenstate, the probability evolves in time. What is the expectation value of the Hamiltonian?

$$\begin{aligned} \langle\psi(t)|\mathcal{H}|\psi(t)\rangle &= \begin{pmatrix} c_1^*e^{i\omega_1 t} & c_2^*e^{i\omega_2 t}\end{pmatrix}\begin{pmatrix} c_1E_1e^{-i\omega_1 t} \\ c_2E_2e^{-i\omega_2 t}\end{pmatrix} \\ &= E_1|c_1|^2 + E_2|c_2|^2 \\ &= P(E_1)E_1 + P(E_2)E_2 \end{aligned}$$

where $P(E_n)$ is the probability to measure energy E_n.

Note 7.3. We note that the expectation value of the Hamiltonian is time independent, as it must. We see that, while the superposition evolves in time, the probability that the system is in states $|E_1\rangle$ or $|E_2\rangle$ is stationary.

7.3 Spin Precession

In this lecture, we will treat the dynamics of a spin in a static magnetic field using the quantum mechanical formalism.

Before we delve into the quantum problem, it is instructive to consider the dynamics of a classical magnetic moment $\vec{\mu}$ in the presence of a uniform external field $\vec{\mathbf{B}}$ to help build our intuition. Recall the relationship from classical mechanics between angular momentum $\vec{\mathbf{L}}$ of a rotating body and the sum of all the torques $\vec{\tau}$ acting on the body.

$$\frac{\mathrm{d}\vec{\mathbf{L}}}{\mathrm{d}t} = \sum \vec{\tau}$$

Discovery 7.2. This relationship is analogous to the relationship

$$\frac{d\vec{p}}{dt} = \sum \vec{F}$$

for linear motion.

Recall that a uniform magnetic field produces a torque

$$\vec{\tau} = \vec{\mu} \times \vec{B}.$$

Also recall that $\vec{\mu}$ and is related to the spin angular momentum $\vec{S}$

$$\vec{\mu} = g\left(\frac{q}{2m}\right)\vec{S}$$

The Landé g-factor is a dimensionless number. For an electron spin $g \approx 2$. q is the charge of the particle, and m is the particle mass.

We can use the relationship between $\vec{\mu}$ and $\vec{S}$ to express the torque equation only in terms of a single physical observable

$$\frac{d\vec{S}}{dt} = \vec{\tau} = \vec{\mu} \times \vec{B} = g\underbrace{\left(\frac{q}{2m}\right)}_{\gamma}\vec{S} \times \vec{B}$$

where γ is called the **gyromagnetic ratio**. For an electron spin,

$$\gamma_e \approx 2\left(\frac{-1.6 \times 10^{-19}\ \mathrm{C}}{2 \cdot 9.11 \times 10^{-31}\ \mathrm{kg}}\right) = 1.76 \times 10^{11}\ (\mathrm{s{\cdot}T})^{-1}$$
$$\frac{\gamma_e}{2\pi} \approx -28\ \mathrm{GHz/T}$$

The classical torque equations are

$$\boxed{\begin{aligned}\frac{d\vec{S}}{dt} &= \gamma\,(\vec{S}\times\vec{B})\\ \frac{d\vec{\mu}}{dt} &= \gamma\,(\vec{\mu}\times\vec{B})\end{aligned}}$$

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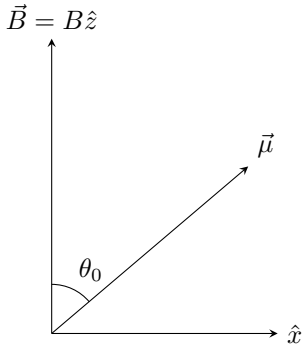
To see the dynamics generated by the magnetic torque, consider a magnetic moment $\vec{\mu}$ that is initially canted by an angle θ_0 with respect to $\vec{B}$.



- Initial state at $t = 0$:

$$\vec{\mu}(t=0) = \mu\big[\sin\theta_0\,\hat{x} + \cos\theta_0\,\hat{z}\big]$$

- For $t > 0$:

$$\vec{\mu}(t) = \mu\big[\sin\theta(t)\cos\varphi(t)\,\hat{x} + \sin\theta(t)\sin\varphi(t)\,\hat{y} + \cos\theta(t)\,\hat{z}\big]$$

  where, in principle, $\theta(t)$ and $\varphi(t)$ can be time dependent.

$$\frac{d\vec{\mu}}{dt} = \gamma\left(\vec{\mu}\times\vec{B}\right) = \begin{vmatrix}\hat{x} & \hat{y} & \hat{z}\\ \mu_x & \mu_y & \mu_z\\ 0 & 0 & B\end{vmatrix}$$

$$\begin{pmatrix}\dot{\mu}_x\\ \dot{\mu}_y\\ \dot{\mu}_z\end{pmatrix} = \begin{pmatrix}\gamma B\,\mu_y\\ -\gamma B\,\mu_x\\ 0\end{pmatrix}$$

We have three (coupled) first order linear differential equations.

> **Note 7.4.** Note that we have used the compact dot notation
>
> $$\dot{f}(t) := \frac{df}{dt}$$
>
> to indicate the time derivative.

If we first consider the equation for μ_z,

$$\dot{\mu}_z = 0 \qquad \Rightarrow \qquad \dot{\theta}\sin\theta = 0$$

We must have $\dot{\theta} = 0$, therefore $\theta(t) = \text{const.} = \theta_0$.

Discovery 7.3. The only time dependence is therefore through $\varphi(t)$.

Next, let's consider the equation for μ_x:

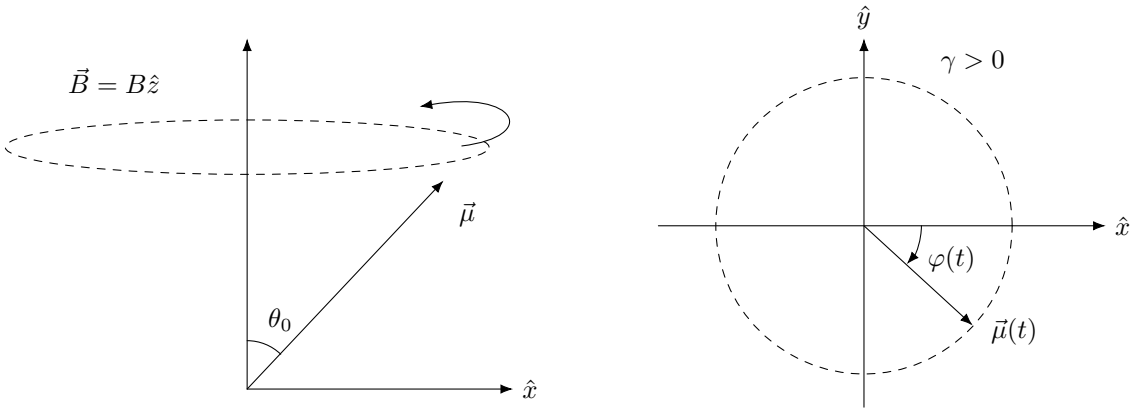
$$\begin{aligned} \dot{\mu}_x &= \gamma B\, \mu_y(t) \\ -\dot{\varphi}\, \mu \sin\theta_0 \sin\varphi(t) &= \gamma B\, \mu \sin\theta_0 \sin\varphi(t) \qquad \Rightarrow \\ \dot{\varphi} &= -\gamma B \\ \varphi(t) &= -\underbrace{\gamma B}_{\omega_0}\, t + \varphi(t=0) \end{aligned}$$

Definition 7.1. **[Larmor Frequency]**

$\omega_0 = \gamma B$ is the **Larmor frequency**.

With $\varphi(t=0) = 0$, we express the time dependent $\vec{\mu}(t)$.

$$\boxed{\vec{\mu}(t) = \mu\Big[\sin\theta_0 \cos(\omega_0 t)\, \hat{x} - \sin\theta_0 \sin(\omega_0 t)\, \hat{y} + \cos\theta_0\, \hat{z}\Big]}$$



A classical spin precesses around the static external field at the Larmor frequency. Note that γ can be positive or negative depending on the sign of the charge of the spin.

Comment 7.2. For positively charged spins, like protons, which are also spin-1/2, $\gamma > 0$ and the precession is clockwise. For electrons, that carry negative charge, the precession is counterclockwise.

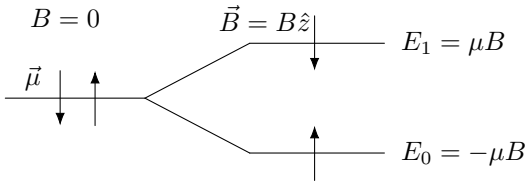
7.4 Quantum Mechanical Spin Precession

We start by considering the Hamiltonian of a spin-1/2 particle in a uniform magnetic field.

$$\mathcal{H} = -\vec{\mu} \cdot \vec{B} = -\left(\frac{gq}{2m}\right) \vec{S} \cdot \vec{B} = -\gamma\, \vec{S} \cdot \vec{B}$$

We know that there are only two projections of $\vec{S}\cdot\hat{n}$, $\left(\pm\frac{\hbar}{2}\right)$, that can be observed for any direction $\hat{n}$ in space. Therefore, there are only two values of energy, corresponding to the two spin projections in the direction of the applied magnetic field $\vec{B} = B\hat{n}$.

$$E_0 = -\frac{\hbar\omega_0}{2}, \qquad E_1 = \frac{\hbar\omega_0}{2} \tag{20}$$



The energy difference between the two states is

$$\Delta E = E_1 - E_0 = \left(\frac{gqB}{2m}\right)\hbar = 2\mu B = \omega_0\hbar$$
$$\mu = \frac{gq\hbar}{4m} = \frac{\gamma\hbar}{2}$$

Let's consider the situation of a time-independent, or static, external field $\vec{B} = B\hat{z}$ applied in the z-direction.The Hamiltonian for this problem is

$$\mathcal{H} = -\omega_0 S_z$$

Note that the energy basis is the same as the S_z basis since the Hamiltonian is just proportional to S_z.

$$\mathcal{H} = -\frac{\hbar\omega_0}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$
$$\mathcal{H}\left|+\right\rangle = E_0\left|+\right\rangle$$
$$\mathcal{H}\left|-\right\rangle = E_1\left|-\right\rangle$$

We can express any state that is a linear superposition of the energy eigenkets $|\pm\rangle$ as

$$\begin{aligned}|\psi(t)\rangle &= c_1\exp\{-iE_0t/\hbar\}\left|+\right\rangle + c_2\exp\{-iE_1t/\hbar\}\left|-\right\rangle\\ &= c_1e^{i\omega_0t/2}\left|+\right\rangle + c_2e^{-i\omega_0t/2}\left|-\right\rangle\end{aligned}$$

Let's determine the dynamics of a spin in a uniform external field. We do so by calculating expectation values of $\vec{S}$ for an arbitrary superposition $|\psi(t)\rangle$.

$$|\psi(t)\rangle = \begin{pmatrix}c_1e^{i\omega_0t/2}\\ c_2e^{-i\omega_0t/2}\end{pmatrix} := \begin{pmatrix}a\\ b\end{pmatrix}$$

Expectation value $\langle S_z \rangle$:

$$\begin{aligned}
\langle \psi(t)|S_z|\psi(t)\rangle &= (a^* \;\; b^*)\,\frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix}\\
&= \frac{\hbar}{2}(a^* \;\; b^*)\begin{pmatrix}a\\ -b\end{pmatrix}\\
&= \frac{\hbar}{2}\big(|a|^2 - |b|^2\big)\\
&= \boxed{\frac{\hbar}{2}\big(|c_1|^2 - |c_2|^2\big)}
\end{aligned} \tag{2}$$

Note 7.5. Because the energy is conserved ($\mathcal{H}$ is time independent), the average energy, i.e., $\langle \mathcal{H} \rangle$ is time independent (conserved).
Because $[S_z, \mathcal{H}] = 0$, it means that $\langle S_z \rangle$ must also be conserved.

Expectation value $\langle S_x \rangle$:

$$\begin{aligned}
\langle \psi(t)|S_x|\psi(t)\rangle &= (a^* \quad b^*)\,\frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix} = \frac{\hbar}{2}\,(a^* \quad b^*)\begin{pmatrix}b\\ a\end{pmatrix}\\
&= \frac{\hbar}{2}(a^*b + b^*a)\\
&= \hbar\,\mathrm{Re}\{a^*b\}\\
&= \hbar\,\mathrm{Re}\Big\{c_1^* e^{-i\omega_0 t/2}\, c_2 e^{-i\omega_0 t/2}\Big\}\\
&= \boxed{\hbar\,\mathrm{Re}\big\{c_1^* c_2 e^{-i\omega_0 t}\big\}}
\end{aligned}$$

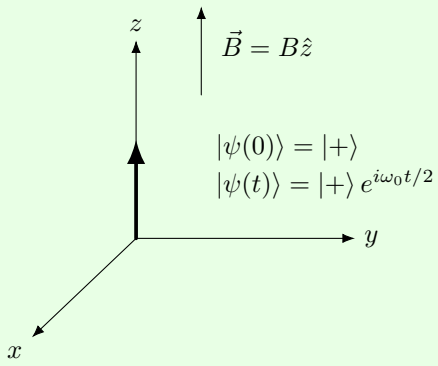
Expectation value $\langle S_y \rangle$:

$$\begin{aligned}
\langle \psi(t)|S_y|\psi(t)\rangle &= (a^* \quad b^*)\,\frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix} = \frac{i\hbar}{2}\,(a^* \quad b^*)\begin{pmatrix}-b\\ a\end{pmatrix}\\
&= \frac{i\hbar}{2}(-a^*b + b^*a)\\
&= \hbar\,\mathrm{Im}\{a^*b\}\\
&= \hbar\,\mathrm{Im}\Big\{c_1^* e^{-i\omega_0 t/2}\, c_2 e^{-i\omega_0 t/2}\Big\}\\
&= \boxed{\hbar\,\mathrm{Im}\big\{c_1^* c_2 e^{-i\omega_0 t}\big\}}
\end{aligned}$$

Example 7.2. Consider a spin initially polarized in the z-direction: $(c_1 = 1,\ c_2 = 0)$.

$$|\psi(0)\rangle = |+\rangle$$

$$|\psi(t)\rangle = e^{i\omega_0 t/2}\,|+\rangle$$



Since $|\psi(0)\rangle$ is an eigenstate of the Hamiltonian, it corresponds to a stationary state.

$$\text{eqns. (2), (3), (4)} \qquad \boxed{\langle S_z\rangle = \frac{\hbar}{2}, \quad \langle S_x\rangle = \langle S_y\rangle = 0}$$

7.4.1 Ehrenfest's Theorem

Theorem 7.2. Ehrenfest's Theorem

The expectation value of quantum observables obey classical laws.

Note 7.6. The dynamics that the expectation value of $\vec{\mathbf{S}}$ exhibits is the same as that of a classical magnetic moment precessing around a uniform magnetic field.

7.5 Magnetic Resonance

7.5.1 Time-Dependent Hamiltonian for Magnetic Resonance

In this lecture, we will consider the dynamics of a spin-1/2 particle in the presence of a time-dependent magnetic field $\vec{B}_1(t)$ applied perpendicular to the static external field

$$\vec{B} = B_0\hat{z} + \vec{B}_1(t).$$

$$\vec{B}_1(t) = B_1\big(\cos(\omega t)\hat{x} - \sin(\omega t)\hat{y}\big) \tag{21}$$

$\vec{B}_1(t)$ represents a circularly polarized magnetic field that rotates in the clockwise sense. The spin Hamilto-

nian is now time dependent

$$\begin{aligned}\mathcal{H}(t) &= -\vec{\mu}\cdot\vec{B} = -\frac{gq}{2m}\,\vec{S}\cdot\vec{B} = -\gamma\,\vec{S}\cdot\vec{B} \\ &= -\omega_0 S_z - \omega_1\big[\cos(\omega t)S_x - \sin(\omega t)S_y\big]\end{aligned}$$

where $\omega_0 = \gamma B_0$ and $\omega_1 = \gamma B_1$ and $\gamma = \dfrac{gq}{2m}$.

$$\mathcal{H}(t) = -\frac{\hbar\omega_0}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} - \frac{\hbar\omega_1}{2}\cos(\omega t)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} + \frac{\hbar\omega_1}{2}\sin(\omega t)\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$$

$$\boxed{\mathcal{H}(t) = -\frac{\hbar}{2}\begin{pmatrix}\omega_0 & \omega_1 e^{i\omega t}\\ \omega_1 e^{-i\omega t} & -\omega_0\end{pmatrix}} \tag{22}$$

We can calculate the time dependence of state $|\psi(t)\rangle$ by solving the time-dependent Schrödinger equation (SE).

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \mathcal{H}(t)|\psi(t)\rangle \tag{23}$$

To do so, we express $|\psi(t)\rangle$ in terms of time-dependent coefficients and substitute into the SE.

$$|\psi(t)\rangle = \begin{pmatrix}c_1(t)\\ c_2(t)\end{pmatrix}$$

$$i\hbar\begin{pmatrix}\dot{c}_1\\ \dot{c}_2\end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix}\omega_0 & \omega_1 e^{i\omega t}\\ \omega_1 e^{-i\omega t} & -\omega_0\end{pmatrix}\begin{pmatrix}c_1\\ c_2\end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix}\omega_0 c_1 + \omega_1 e^{i\omega t}c_2\\ \omega_1 e^{-i\omega t}c_1 - \omega_0 c_2\end{pmatrix}$$

We need to solve two coupled differential equations

$$\frac{dc_1}{dt} = \frac{i}{2}\big(\omega_0 c_1 + \omega_1 e^{i\omega t}c_2\big)$$

$$\frac{dc_2}{dt} = \frac{i}{2}\big(\omega_1 e^{-i\omega t}c_1 - \omega_0 c_2\big)$$

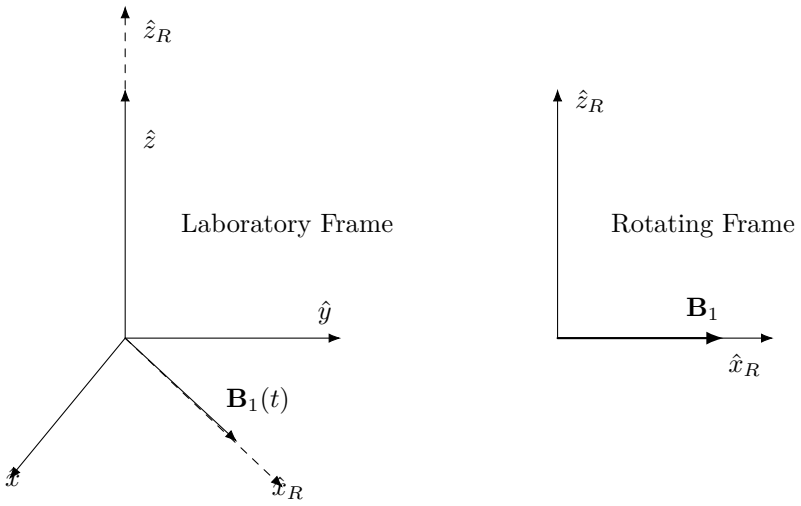
We can proceed to solve these equations directly, however the math involves a lot of algebra and is not very illuminating. The direct solution to the problem is also worked out in McIntyre.

Instead, I will outline another approach which is a bit more sophisticated, but far more widely used and informative.

7.5.2 Rotating Frame Transformation

Through a suitable reference frame transformation, we can transform the time dependent Hamiltonian into a time-independent one. We can then solve the eigenvalue problem for the time-independent Hamiltonian, and immediately write down the time-dependent solutions for arbitrary superposition of energy eigenkets.

The key thing to notice about this problem is that if we transform into a reference frame that is rotating at frequency ω (the frequency of the time-dependent magnetic field) about the z-axis, then the applied field appears stationary.



This transformation is referred to as the Rotating Frame Transformation, and is widely used in atomic physics and magnetic resonance to transform the time dependent problem to one that is time independent. We will refer to the stationary reference frame as the lab frame. This is the frame in which the applied field is rotating at frequency ω. We will refer to the reference frame that is rotating about the z-axis at frequency ω as the rotating frame. We will transform between these two frames via a unitary transformation of coordinates.

Let $|\psi_L\rangle$ be the state in the laboratory frame, and let $|\psi_R\rangle$ be the state in the rotating frame. We can relate these two states to each other through a unitary transformation U, with $UU^\dagger = 1$.

$$|\psi_L\rangle = U\,|\psi_R\rangle \tag{6}$$

$$|\psi_R\rangle = U^\dagger|\psi_L\rangle \tag{7}$$

We seek to find a unitary U that transforms $\mathcal{H}(t)$ into a time-independent Hamiltonian.

$$i\hbar\frac{d}{dt}\Big[\underbrace{UU^\dagger}_{1}|\psi_L\rangle\Big] = \mathcal{H}(t)\,\underbrace{UU^\dagger}_{1}|\psi_L\rangle$$

$$i\hbar\frac{d}{dt}\Big[U\,|\psi_R\rangle\Big] = \mathcal{H}(t)\,U\,|\psi_R\rangle$$

$$i\hbar\frac{dU}{dt}\,|\psi_R\rangle + i\hbar U\frac{d}{dt}\,|\psi_R\rangle = \mathcal{H}(t)\,U\,|\psi_R\rangle$$

Multiply both sides of the previous equation by $U^\dagger$.

$$i\hbar U^\dagger\frac{dU}{dt}\,|\psi_R\rangle + i\hbar U^\dagger\underbrace{U}_{1}\frac{d}{dt}\,|\psi_R\rangle = U^\dagger\mathcal{H}(t)U\,|\psi_R\rangle$$

$$i\hbar\frac{d}{dt}\,|\psi_R\rangle = \underbrace{\left\{U^\dagger\mathcal{H}(t)U - i\hbar U^\dagger\frac{dU}{dt}\right\}}_{\mathcal{H}_R}|\psi_R\rangle$$

We define the Hamiltonian in the rotating frame

$$\mathcal{H}_R := U^\dagger \mathcal{H}(t) U - i\hbar U^\dagger \frac{dU}{dt} \tag{8}$$

$$i\hbar \frac{d}{dt} |\psi_R\rangle = \mathcal{H}_R |\psi_R\rangle \tag{9}$$

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We seek to find a U that makes $\mathcal{H}_R$ time independent.

In the rotating frame, the time-dependent field should be static. Therefore, we wish to transform into a frame that is rotating clockwise about the z-axis at the same frequency as the time-dependent magnetic field $\vec{B}_1(t)$.

Recall from our discussion of continuous rotations that a counterclockwise rotation around the z-axis by angle ϕ_0 was given by

$$U(\phi_0) = e^{-i\phi_0 S_z/\hbar} = e^{-i\phi_0 \sigma_z/2} \tag{10}$$

with $\sigma_z := \frac{2}{\hbar} S_z$.

To find a matrix representation of eq. (10), we use the result: (A proof is provided in the lecture on continuous rotations)

$$\begin{aligned} e^{-i\phi_0\sigma_z/2} &= \mathbb{1}\cos\left(\frac{\phi_0}{2}\right) - i\sigma_z \sin\left(\frac{\phi_0}{2}\right) \\ &= \begin{pmatrix} \cos\left(\frac{\phi_0}{2}\right) - i\sin\left(\frac{\phi_0}{2}\right) & 0 \\ 0 & \cos\left(\frac{\phi_0}{2}\right) + i\sin\left(\frac{\phi_0}{2}\right) \end{pmatrix} = \begin{pmatrix} e^{-i\phi_0/2} & 0 \\ 0 & e^{i\phi_0/2} \end{pmatrix} \end{aligned} \tag{11}$$

Let $\phi_0 = -wt$ (clockwise rotation):

$$\boxed{U(Wt) = \begin{pmatrix} e^{i\frac{wt}{2}} & 0 \\ 0 & e^{i\frac{-wt}{2}} \end{pmatrix}} \tag{12}$$

Let's see how this unitary transformation works. We started out with an initial state $|+\rangle_x$, and found that in the presence of a static magnetic field $B_0\hat{\mathbf{z}}$, the state precesses in time.

$$|\psi_L(t)\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle + e^{-i\omega_0 t}|-\rangle\right)$$

We can view this state as precessing clockwise around the z-axis.

In the frame that rotates clockwise around the z-axis at frequency ω_0, this state should appear stationary.

$$U(\omega_0 t) = \begin{pmatrix} e^{i\omega_0 t/2} & 0 \\ 0 & e^{-i\omega_0 t/2} \end{pmatrix}$$

We use eq. (7) to transform the lab frame state $|\psi_L(t)\rangle$ to the rotating frame.

$$\begin{aligned}
|\psi_R\rangle &= U^\dagger |\psi_L\rangle \\
&= \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\omega_0 t/2} & 0 \\ 0 & e^{i\omega_0 t/2} \end{pmatrix} \begin{pmatrix} 1 \\ e^{-i\omega_0 t} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\omega_0 t/2} \\ e^{-i\omega_0 t/2} \end{pmatrix} \\
&= \frac{e^{-i\omega_0 t/2}}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = e^{-i\omega_0 t/2} |+\rangle_x
\end{aligned}$$

We see that, up to an overall phase factor $e^{-i\omega_0 t/2}$, which does not affect measurable probabilities, the state $|\psi_R\rangle = |+\rangle_x$.

We can likewise use eq. (6) to transform from the rotating frame back to the lab frame.

$$\begin{aligned}
|\psi_L(t)\rangle &= U |\psi_R\rangle \\
&= \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\omega_0 t/2} & 0 \\ 0 & e^{-i\omega_0 t/2} \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\omega_0 t/2} \\ e^{-i\omega_0 t/2} \end{pmatrix} \\
&= \frac{e^{i\omega_0 t/2}}{\sqrt{2}} \left(|+\rangle + e^{-i\omega_0 t} |-\rangle \right)
\end{aligned}$$

We will now use eq. (12) to evaluate the rotating frame Hamiltonian given by eq. (8).

$$\begin{aligned}
U^\dagger \mathcal{H}(t) U &= \frac{\hbar}{2} \begin{pmatrix} e^{-i\omega t/2} & 0 \\ 0 & e^{i\omega t/2} \end{pmatrix} \underbrace{\begin{pmatrix} \omega_0 & \omega_1 e^{i\omega t} \\ \omega_1 e^{-i\omega t} & -\omega_0 \end{pmatrix} \begin{pmatrix} e^{i\omega t/2} & 0 \\ 0 & e^{-i\omega t/2} \end{pmatrix}}_{\begin{pmatrix} \omega_0 e^{i\omega t/2} & \omega_1 e^{i\omega t/2} \\ \omega_1 e^{-i\omega t/2} & -\omega_0 e^{-i\omega t/2} \end{pmatrix}} \\
&= -\frac{\hbar}{2} \begin{pmatrix} \omega_0 & \omega_1 \\ \omega_1 & -\omega_0 \end{pmatrix} \\
i\hbar U^\dagger \frac{dU}{dt} &= i\hbar \begin{pmatrix} e^{-i\omega t/2} & 0 \\ 0 & e^{i\omega t/2} \end{pmatrix} \frac{i\omega}{2} \begin{pmatrix} e^{i\omega t/2} & 0 \\ 0 & -e^{-i\omega t/2} \end{pmatrix} \\
&= -\frac{\hbar\omega}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\end{aligned}$$

Eq. (8) becomes

$$\begin{aligned}
\mathcal{H}_R &= -\frac{\hbar}{2} \begin{pmatrix} \omega_0 & \omega_1 \\ \omega_1 & -\omega_0 \end{pmatrix} + \frac{\hbar\omega}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\
&= -\frac{\hbar}{2} \begin{pmatrix} \omega_0 - \omega & \omega_1 \\ \omega_1 & -(\omega_0 - \omega) \end{pmatrix}
\end{aligned} \tag{13}$$

We introduce the detuning parameter $\Delta := \omega_0 - \omega$, and express the Schrödinger equation in the rotating frame.

$$i\hbar \frac{d}{dt} |\psi_R\rangle = -\frac{\hbar}{2} \begin{pmatrix} \Delta & \omega_1 \\ \omega_1 & -\Delta \end{pmatrix} |\psi_R\rangle \tag{14}$$

$$\mathcal{H}_R = -\frac{\hbar\Delta}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} - \frac{\hbar\omega_1}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

$$\boxed{\mathcal{H}_R = -\Delta S_z - \omega_1 S_x} \tag{15}$$

The Hamiltonian in the rotating frame corresponds to a magnetic moment in the presence of an effective magnetic field that is stationary in the rotating frame.

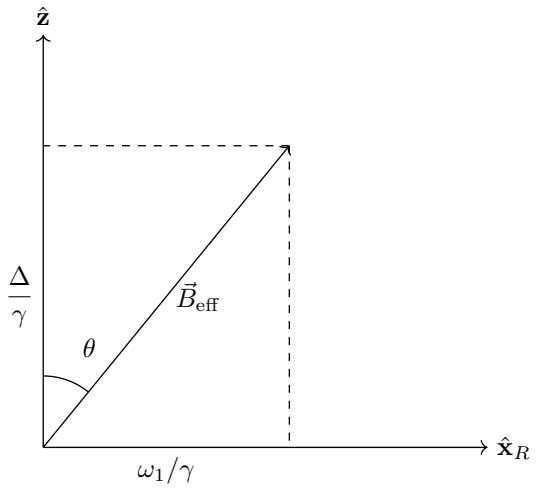
$$\vec{B}_{\text{eff}} = \frac{\Delta}{\gamma}\,\hat{\mathbf{z}} + \frac{\omega_1}{\gamma}\,\hat{\mathbf{x}} \tag{16}$$

$$\mathcal{H}_R = -\gamma \vec{B}_{\text{eff}} \cdot \vec{S} \tag{17}$$

$$\mathcal{H}_R = -\gamma \left\|\vec{B}_{\text{eff}}\right\| S_n \tag{18}$$

In eq. (18) the operator S_n is the spin-1/2 operator in the $\hat{\mathbf{n}}$-direction, where $\hat{\mathbf{n}}$ refers to the direction of the effective field.

$$\hat{\mathbf{n}} = \frac{\vec{B}_{\text{eff}}}{\left\|\vec{B}_{\text{eff}}\right\|}, \qquad B_{\text{eff}} := \left\|\vec{B}_{\text{eff}}\right\| = \frac{1}{\gamma}\sqrt{\Delta^2 + \omega_1^2}$$



In the rotating frame, the field in the z-direction is proportional to the detuning parameter $\Delta = \omega_0 - \omega$ rather than ω_0. On resonance ($\omega = \omega_0$), the field in z-direction vanishes.

We can express the rotating frame Hamiltonian $\mathcal{H}_R$ in terms of the eigenkets of the operator S_n. The $|\pm\rangle_n$ basis is the energy basis in the rotating frame.

$$|+\rangle_n = \cos\left(\frac{\theta}{2}\right)|+\rangle + \sin\left(\frac{\theta}{2}\right)|-\rangle \tag{19}$$

$$|-\rangle_n = \sin\left(\frac{\theta}{2}\right)|+\rangle - \cos\left(\frac{\theta}{2}\right)|-\rangle \tag{20}$$

In the $|\pm\rangle_n$ basis, $\mathcal{H}_R$ has the same representation as the operator S_z in the $|\pm\rangle$ basis.

$$\mathcal{H}_R = -\frac{\hbar}{2}\sqrt{\Delta^2+\omega_1^2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \tag{21}$$

$$\begin{aligned}\mathcal{H}_R|+\rangle_n &= -\frac{\hbar}{2}\sqrt{\Delta^2+\omega_1^2}\,|+\rangle_n := -\frac{\hbar\omega_e}{2}|+\rangle_n\\ \mathcal{H}_R|-\rangle_n &= \frac{\hbar}{2}\sqrt{\Delta^2+\omega_1^2}\,|-\rangle_n := \frac{\hbar\omega_e}{2}|-\rangle_n\end{aligned} \tag{22}$$

We can express the Schrödinger equation in the rotating frame in the diagonal basis $|\pm\rangle_n$.

$$i\hbar\frac{d}{dt}|\psi_R\rangle = -\frac{\hbar\omega_e}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}|\psi_R\rangle \tag{23}$$

A general time-dependent superposition is thus

$$|\psi_R(t)\rangle = c_1 e^{i\omega_e t/2}|+\rangle_n + c_2 e^{-i\omega_e t/2}|-\rangle_n \tag{24}$$

In the next lecture, we will use this result to study the spin dynamics.

7.5.3 Transition Between Two States

Question 7.1.

Suppose initially that there is only a static external field $B_0\hat{\mathbf{z}}$, and the initial state is $|\psi(0)\rangle = |-\rangle$. If we turn on a time-dependent field

$$\vec{\mathbf{B}}_1(t) = B_1\big(\cos(\omega t)\hat{\mathbf{x}} - \sin(\omega t)\hat{\mathbf{y}}\big)$$

What is the probability of making a transition from $|-\rangle \to |+\rangle$?

To answer this question, we need to first express the initial state in the energy basis $|\pm\rangle_n$.

$$|\psi(0)\rangle = \big(|+_n\rangle\langle+_n| + |-_n\rangle\langle-_n|\big)\,|\psi(0)\rangle$$

$$c_1 = \langle+_n|-\rangle, \qquad c_2 = \langle-_n|-\rangle$$

$$c_1 = \sin\left(\frac{\theta}{2}\right), \qquad c_2 = -\cos\left(\frac{\theta}{2}\right)$$

$$\boxed{|\psi_R(t)\rangle = \sin\left(\frac{\theta}{2}\right)e^{i\omega_e t/2}|+\rangle_n - \cos\left(\frac{\theta}{2}\right)e^{-i\omega_e t/2}|-\rangle_n} \tag{25}$$

The probability to be in the state $|+\rangle$ is

$$\begin{aligned} P_+ &= |\langle +|\psi_R(t)\rangle|^2 \\ &= \left|\sin\left(\frac{\theta}{2}\right) e^{i\omega_e t/2}\langle +|+\rangle_n - \cos\left(\frac{\theta}{2}\right) e^{-i\omega_e t/2}\langle +|-\rangle_n\right|^2 \\ &= \left|\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right) e^{i\omega_e t/2} - \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right) e^{-i\omega_e t/2}\right|^2 \\ &= \sin^2\theta\,\sin^2\left(\frac{\omega_e t}{2}\right) \end{aligned}$$

We can express $\sin^2\theta$ in terms of the components of the effective magnetic field.

$$\sin^2\theta = \frac{\omega_1^2}{\Delta^2+\omega_1^2}$$

Hence we have

$$\begin{aligned} P(-\to +) &= \left[\frac{\omega_1^2}{\Delta^2+\omega_1^2}\right]\sin^2\left(\frac{\omega_e t}{2}\right) \\ &= \frac{1}{2}\left[\frac{\omega_1^2}{\Delta^2+\omega_1^2}\right](1-\cos(\omega_e t)) \end{aligned}$$

We see that we can make a transition from the $|-\rangle$ to the $|+\rangle$ state with probability $P(-\to +) = 1$ provided that $\Delta = 0$. The time that it takes to make the transition between the two states is determined by the Rabi

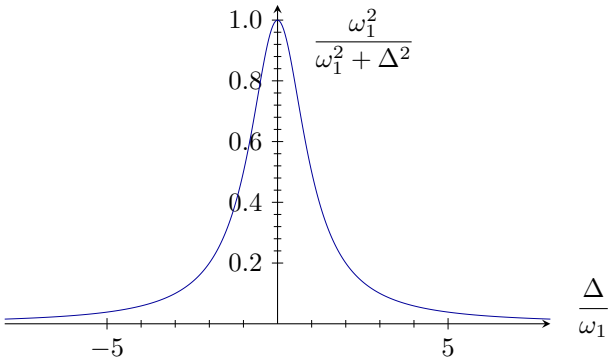


Figure 5: Resonance lineshape

frequency. We define the Rabi frequency for $\Delta = 0$, $\omega_e = \omega_1$. For $\Delta = 0$, if we apply a resonant pulse for a time

$$\tau_\pi = \frac{\pi}{\omega_1},$$

then the spin will make a transition between $|+\rangle$ and $|-\rangle$ states with $P = 1$. Such a pulse is referred to as a π-pulse.

7.5.4 Arbitrary Unitary Control

Let's evaluate the state of the spin in the rotating frame for the case of resonant rf excitation ($\Delta = 0$). For $\Delta = 0$, the angle that describes the effective field is $\theta = \pi/2$, and eq.(10) and eq.(11) become

$$|+\rangle_n = \frac{1}{\sqrt{2}}\big(|+\rangle + |-\rangle\big) = |+\rangle_x \tag{26}$$

$$|-\rangle_n = \frac{1}{\sqrt{2}}\big(|+\rangle - |-\rangle\big) = |-\rangle_x \tag{27}$$

$$|\psi_R(t)\rangle = \frac{1}{\sqrt{2}}\left(e^{i\omega_1 t/2}|+\rangle_n - e^{-i\omega_1 t/2}|-\rangle_n\right) \tag{28}$$

Substituting eq.(26) and eq.(27) into eq.(28), we find, up to an overall phase factor,

$$\boxed{|\psi_R(t)\rangle = \sin\left(\frac{\omega_1 t}{2}\right)|+\rangle - i\cos\left(\frac{\omega_1 t}{2}\right)|-\rangle} \tag{29}$$

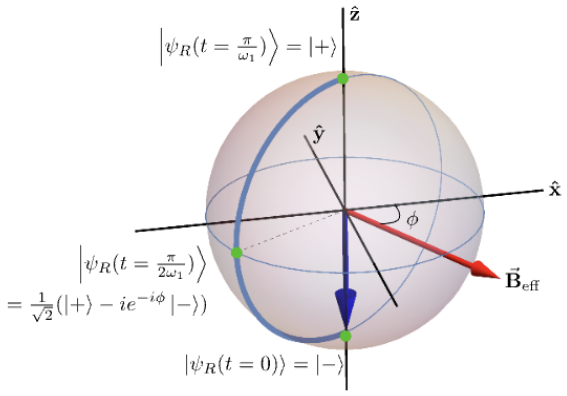


Figure 6: Bloch sphere representation of the state trajectory.

We see that in the rotating frame, the state precesses around $\vec{B}_{\text{eff}}$.

By changing the length of the rf-pulse, we can rotate the state vector from the $|-\rangle$ state to any point along the longitudinal line. For example, by applying the rf pulse for a time

$$\tau_{\pi/2} = \frac{\pi}{2\omega_1},$$

we rotate the state from $|-\rangle$ to the state $|-\rangle_y$.

Such a pulse is called a $\pi/2$ pulse, which creates a particular coherent superposition of states $|-\rangle$ and $|+\rangle$ corresponding to the state $|-\rangle_y$.

We can create arbitrary trajectories on the Bloch sphere, by controlling the direction of $\vec{B}_{\text{eff}}$. One way to do this is to vary θ, which we can do by changing the resonance offset Δ. A second way is to add a phase offset ϕ to the applied rf field.

$$\vec{B}_1(t) = B_1\big(\cos(\omega t + \phi)\hat{x} - \sin(\omega t + \phi)\hat{y}\big) \tag{30}$$

The state vector that corresponds to the rotated $\vec{B}_1(t)$ is

$$\boxed{|\psi_R(t)\rangle = \sin\left(\frac{\omega_1 t}{2}\right)|+\rangle - ie^{-i\phi}\cos\left(\frac{\omega_1 t}{2}\right)|-\rangle} \tag{18}$$

Discovery 7.4. Thus, by changing both the resonance offset and the phase of the applied rf field, the state vector can be controlled over the entire Bloch sphere.

8 Quantum Mechanics in the Position Basis

Lecture 15 - Thursday, March 05

We will now develop a quantum mechanical description of the motion of a particle subject to an external force. We would like the quantum mechanical version of Newton's Law

$$\vec{F} = m\vec{a},$$

which describes the classical trajectory $\vec{r}(t)$ of a particle of mass m subject to an external force $\vec{F}$.

In the classical description, we often start by considering a conservative force

$$\vec{F} = -\nabla V(\vec{r}),$$

where $V(\vec{r})$ is the potential energy. In one dimension, we express the total energy E of a classical particle moving in a time-independent potential $V(x)$ by

$$E = \frac{p^2}{2m} + V(x)$$

where $p = m\dot{x}$. The condition that $E = \text{const.}$ leads to Newton's Law of motion for a conservative force.

$$\begin{aligned}
\dot{E} &= \frac{2p}{2m}\dot{p} + \frac{dV}{dx}\dot{x} = 0 \\
&= p\dot{p} + \frac{dV}{dx}\underbrace{m\dot{x}}_{p} = 0 \\
&= p\left(\dot{p} + \frac{dV}{dx}\right) = 0
\end{aligned}$$

$$\boxed{F = \dot{p} = -\frac{dV}{dx}}$$

Comment 8.1. Just as Newton's Law allows us to calculate the trajectory of a particle or a system of particles, we will see that the Schrödinger equation will allow us to calculate the evolution of a quantum state in space and time.

8.1 Position Representation

So far, we have dealt with a finite Hilbert space, in which there are a finite number of possible measurement outcomes, such as $\pm\hbar/2$ for the spin-1/2 system. We would like to extend our formalism to an infinite dimensional Hilbert space.

In particular, we would like to treat position as an operator, whose eigenvalue corresponds to the position of a particle.

$$\hat{x}|x\rangle = x|x\rangle \tag{1}$$

where

$$\begin{aligned} \hat{x} &:= \text{position operator} \\ |x\rangle &:= \text{position eigenvector} \\ x &:= \text{position eigenvalue} \end{aligned}$$

Here, the position eigenvalue $x \in (-\infty, \infty)$ runs over all one-dimensional space.

8.1.1 Normalization in the Position Basis

Unlike systems that have a discrete spectrum of eigenvalues, the position operator has an infinite number of eigenvalues. This distinction has important consequences, especially when it comes to normalization. Consider an arbitrary superposition

$$|\psi\rangle = \sum_i \langle x_i|\psi\rangle |x_i\rangle \tag{2}$$

Let's normalize $|\psi\rangle$:

$$\begin{aligned} \langle\psi|\psi\rangle &= \sum_i \langle\psi|x_i\rangle\langle x_i|\psi\rangle \\ &= \sum_i |\langle x_i|\psi\rangle|^2 \end{aligned}$$

There is a problem with this approach. In a finite range $x \in [x', x' + \Delta x]$, there are an infinite number of states, and an infinite number of terms in the sum:

$$\langle\psi|\psi\rangle = |\langle x'|\psi\rangle|^2 + |\langle x' + dx|\psi\rangle|^2 + \cdots + |\langle x' + \Delta x|\psi\rangle|^2$$

If the probabilities $|\langle x|\psi\rangle|^2$ are non-zero, then even if they are small but finite, the sum over an infinite number of terms means that $\langle\psi|\psi\rangle$ diverges.

We can fix this issue by carrying out the sum such that the probability to occupy a finite range in x remains finite, while the probability to be in any particular position eigenstate is zero.

Lemma 8.1. The key point is to redefine the completeness criterion for an infinite dimensional Hilbert space.

$$\sum_n |n\rangle\langle n| = 1 \qquad \longrightarrow \qquad \int_{-\infty}^{\infty} |x\rangle\langle x|\, dx = 1$$

Expand $\langle\psi|\psi\rangle$ in the position basis.

$$\langle\psi|\psi\rangle = \langle\psi| \left[\int_{-\infty}^{\infty} |x\rangle\langle x|\, dx\right] |\psi\rangle \tag{3}$$

$$\langle\psi|\psi\rangle = \int_{-\infty}^{\infty} |\langle x|\psi\rangle|^2\, dx \tag{4}$$

We interpret $|\langle x|\psi\rangle|^2\, dx$ as the probability for a particle to be in the region $x \in (x', x' + dx)$.

Note 8.1. The quantity $|\langle x|\psi\rangle|^2$ is therefore a *probability density*, and has the units of inverse length (m^{-1}).

Notice that the probability of finding the particle at a particular position vanishes, provided that the probability density at that position remains finite.

$$\text{Probability of being at position } x:$$
$$\lim_{dx\to 0} |\langle x|\psi\rangle|^2\, dx \to 0$$

By introducing the probability density, we overcome the divergence problem we encountered earlier for a discrete basis.

Definition 8.1. **[Wavefunction]**

We introduce the **wavefunction**:

$$\psi(x) := \langle x|\psi\rangle \tag{5}$$

$\psi(x)$ is a complex function of x.

In order for the state $|\psi\rangle$ to be normalizable, we require that

$$\begin{aligned}\langle\psi|\psi\rangle &= \int_{-\infty}^{\infty} |\langle x|\psi\rangle|^2\, dx \\ &= \int_{-\infty}^{\infty} |\psi(x)|^2\, dx = 1\end{aligned} \tag{6}$$

Physically, the normalization condition states that the probability of finding the particle over all space is 1.

Proposition 8.1. The probability of finding the particle in a particular region $x \in [x_1, x_2]$ is

$$P(x_1, x_2) = \int_{x_1}^{x_2} |\psi(x)|^2\, dx$$

Example 8.1. Normalization

In the following example, we consider the wavefunction

$$\psi(x) = \begin{cases} 0, & x < 0 \\ A\sin\left(\dfrac{2\pi x}{L}\right), & 0 \le x \le L \\ 0, & x > L \end{cases}$$

To normalize the state we require

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = A^2 \int_0^L \sin^2\left(\frac{2\pi x}{L}\right) dx = 1$$

Using

$$\int_0^L \sin^2\left(\frac{2\pi x}{L}\right) dx = \frac{L}{2},$$

we obtain

$$A^2\left(\frac{L}{2}\right) = 1 \quad \Rightarrow \quad A = \sqrt{\frac{2}{L}}.$$

Thus the normalized wavefunction is

$$\psi(x) = \begin{cases} 0, & x < 0 \\ \sqrt{\dfrac{2}{L}}\sin\left(\dfrac{2\pi x}{L}\right), & 0 \le x \le L \\ 0, & x > L \end{cases}$$

8.1.2 Inner Product

Lemma 8.2. We can use the completeness relationship to calculate the inner product of two state vectors $|\psi\rangle$ and $|\phi\rangle$ in the position basis.

$$\langle\phi|\psi\rangle = \langle\phi| \left[\int_{-\infty}^{\infty} |x\rangle\langle x| \, dx\right] |\psi\rangle \tag{7}$$

$$= \int_{-\infty}^{\infty} \langle\phi|x\rangle\langle x|\psi\rangle \, dx \tag{8}$$

$$= \int_{-\infty}^{\infty} \phi^*(x)\psi(x) \, dx \tag{9}$$

8.1.3 The Dirac-Delta Function

Let's use the completeness relationship to express a position eigenket $|x'\rangle$ in the position basis.

$$\mathbf{1}\,|x'\rangle = \int_{-\infty}^{\infty} \langle x|x'\rangle\,|x\rangle \, dx$$

The function $\langle x|x'\rangle$ has the property that if we integrate over all x, it is zero for all values except x'. This function is called the Dirac-delta function

$$\delta(x - x') := \langle x|x'\rangle.$$

Comment 8.2. The Dirac-delta function is analogous to the Kronecker-Delta function we used to express the orthogonality of basis kets in finite dimensions.

Proposition 8.2. The Dirac-delta function has the following properties:

$$\int_{-\infty}^{\infty} \delta(x - x')\, dx = 1 \tag{10}$$

$$\int_{-\infty}^{\infty} \delta(x - x')\, f(x)\, dx = f(x') \tag{11}$$

8.2 Operators of Position

Consider the action of the position operator on an arbitrary state.

$$\hat{x}|\psi\rangle = \hat{x} \int_{-\infty}^{\infty} dx\, |x\rangle\langle x|\psi\rangle \tag{12}$$

$$= \int_{-\infty}^{\infty} dx\, \langle x|\psi\rangle\, \hat{x}|x\rangle \tag{13}$$

$$= \int_{-\infty}^{\infty} dx\, \langle x|\psi\rangle\, x|x\rangle \tag{14}$$

We see that we can replace the operator $\hat{x}$ with the eigenvalue x if we expand $|\psi\rangle$ in the position basis.

In fact we can replace any operator that can be represented as a power series of $\hat{x}$, as a function of x by expanding $|\psi\rangle$ in the position basis.

$$\hat{A} = \sum_n a_n \hat{x}^n$$

and then we have

$$\hat{A}|\psi\rangle = \int_{-\infty}^{\infty} dx\, \langle x|\psi\rangle \sum_n a_n \hat{x}^n |x\rangle$$

$$= \int_{-\infty}^{\infty} dx\, \langle x|\psi\rangle \sum_n a_n x^n |x\rangle$$

As a result,

$$\boxed{\hat{A} \longrightarrow A(x)}$$

$$\langle x'|\hat{A}|\psi\rangle = \int_{-\infty}^{\infty} dx\, \langle x|\psi\rangle\, A(x)\, \langle x'|x\rangle$$

$$\langle x'|\hat{A}|\psi\rangle = A(x')\psi(x')$$

8.3 The Momentum Operator

Here are some key results in this section:

$$\hat{p} \longmapsto -i\hbar\frac{d}{dx}$$

$$\hat{p}|\psi\rangle = \int dx\, |x\rangle \left[-i\hbar\frac{d}{dx}\langle x|\psi\rangle\right]$$

$$\langle x|\hat{p}^{\,n}|\psi\rangle = (-i\hbar)^n \frac{d^n\psi(x)}{dx^n}$$

$$\langle \phi|\hat{p}^{\,n}|\psi\rangle = (-i\hbar)^n \int dx\, \phi^*(x)\frac{d^n\psi}{dx^n}$$

$$\langle x|\hat{p}|x'\rangle = -i\hbar\frac{d}{dx}\,\delta(x-x')$$

8.3.1 Infinitesimal Translation Operator

The goal of this lecture is to derive a representation of the momentum operator in the position representation. Let's start by considering the operator of infinitesimal translation.

The operator $\hat{T}(\Delta x)$ translates the position eigenstate $|x\rangle$ by Δx to $|x+\Delta x\rangle$.

$$\hat{T}(\Delta x)\,|x\rangle := |x+\Delta x\rangle \tag{1}$$

Let's compute the effect of $\hat{T}(\Delta x)$ on an arbitrary state $|\psi\rangle$.

$$\begin{aligned}
|\psi'\rangle &= \hat{T}(\Delta x)|\psi\rangle \\
&= \hat{T}(\Delta x)\int dx'\, |x'\rangle\langle x'|\psi\rangle \\
&= \int dx'\, |x'+\Delta x\rangle\langle x'|\psi\rangle \\
\text{Redefine: } x'\to x'-\Delta x &= \int dx'\, |x'\rangle\langle x'-\Delta x|\psi\rangle
\end{aligned}$$

Hence we have

$$\begin{aligned}
\langle x|\psi'\rangle &= \int dx'\, \langle x|x'\rangle\langle x'-\Delta x|\psi\rangle \\
&= \int dx'\, \delta(x-x')\langle x'-\Delta x|\psi\rangle \\
&= \langle x-\Delta x|\psi\rangle
\end{aligned}$$

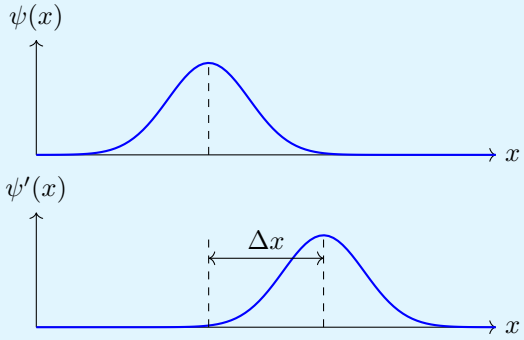
As a result, we derived that

$$\boxed{\psi'(x) = \psi(x - \Delta x)} \tag{2}$$

Note 8.2. Note, $\delta(x)$ is an even function: $\delta(x) = \delta(-x)$.

$$\therefore \quad \int dx'\, \delta(x - x')\, f(x') = f(x)$$
$$\int dx'\, \delta(x' - x)\, f(x') = f(x)$$

Discovery 8.1. $\hat{T}(\Delta x)$ translates the state $|\psi\rangle$ by Δx, where $|\psi'\rangle$ is the translated state.



Thus, we must have

$$\begin{aligned} \langle\psi|\psi\rangle &= \langle\psi'|\psi'\rangle \\ &= \langle\psi|\hat{T}^\dagger(\Delta x)\hat{T}(\Delta x)|\psi\rangle \\ \Rightarrow \quad \hat{T}^\dagger(\Delta x)\hat{T}(\Delta x) &= 1 \end{aligned}$$

Proposition 8.3. We have the following properties:

1. $\hat{T}(\Delta x)$ is unitary.
2. $\hat{T}(\Delta x)$ must also satisfy
$$\lim_{\Delta x \to 0} \hat{T}(\Delta x) \to 1.$$

As we've discussed before, we can satisfy these two requirements by constructing the infinitesimal translation operator to have the following form

$$\hat{T} = 1 - i\hat{K}\Delta x \tag{3}$$

where $\hat{K}$ is a Hermitian operator. Applying the unitarity requirement to eq. (3), we find

$$\begin{aligned}\hat{T}^\dagger(\Delta x)\hat{T}(\Delta x) &= 1 \\ &= [1 + i\hat{K}^\dagger \Delta x][1 - i\hat{K}\Delta x] \\ &= 1 + i\Delta x(\hat{K}^\dagger - \hat{K}) + \mathcal{O}\big((\Delta x)^2\big).\end{aligned}$$

The term of order $\mathcal{O}(\Delta x)$ is zero since $\hat{K}^\dagger = \hat{K}$. Considering Δx to be an infinitesimal quantity, in the limit $\Delta x \to 0$, we can neglect terms $\mathcal{O}((\Delta x)^2)$.

$$\therefore \quad \hat{T}^\dagger(\Delta x)\hat{T}(\Delta x) = 1.$$

Proposition 8.4. $\hat{T}$ has the property

$$\hat{T}(\Delta x_1)\hat{T}(\Delta x_2) = \hat{T}(\Delta x_1 + \Delta x_2)$$

Proof. We have:

$$\begin{aligned}\Rightarrow \quad \hat{T}(\Delta x_1)\hat{T}(\Delta x_2) &= [1 - i\hat{K}\Delta x_1][1 - i\hat{K}\Delta x_2] \\ &= 1 - i\hat{K}(\Delta x_1 + \Delta x_2) + \mathcal{O}\big((\Delta x)^2\big) \\ &\approx 1 - i\hat{K}(\Delta x_1 + \Delta x_2) \\ &= \hat{T}(\Delta x_1 + \Delta x_2).\end{aligned}$$

as desired. □

We know from classical mechanics that momentum $\vec{p}$ is the generator of translation. Therefore, it is reasonable to associate $\hat{K}$ with the momentum operator $\hat{p}$. However, we know that $\hat{K}$ must have units of (m^{-1}), because $\hat{K}\Delta x$ is dimensionless. The constant of proportionality between $\hat{K}$ and $\hat{p}$ turns out to be $\hbar$.

$$\hat{K} = \frac{\hat{p}}{\hbar}$$

$$\hat{T}(\Delta x) = 1 - \frac{i\hat{p}\,\Delta x}{\hbar} \tag{4}$$

We are now ready to calculate the representation of $\hat{p}$ in the $\hat{x}$–basis.

We start by expanding $|\psi\rangle$ in the $\hat{x}$–basis using the completeness relationship. We then use the relationship $\hat{T}(\Delta x)|x\rangle = |x + \Delta x\rangle$.

$$\begin{aligned}\hat{T}(\Delta x)|\psi\rangle &= \hat{T}(\Delta x)\int dx\,|x\rangle\langle x|\psi\rangle \\ &= \int dx\,|x + \Delta x\rangle\langle x|\psi\rangle \\ &= \int dx\,|x\rangle\langle x - \Delta x|\psi\rangle\end{aligned}$$

Taylor series expansion of $\langle x - \Delta x|\psi\rangle$ around the point x:

$$\begin{aligned}\langle x - \Delta x|\psi\rangle &= \langle x|\psi\rangle - \Delta x\frac{d}{dx}\langle x|\psi\rangle + \mathcal{O}((\Delta x)^2) + \cdots \\ &\approx \langle x|\psi\rangle - \Delta x\frac{d}{dx}\langle x|\psi\rangle\end{aligned}$$

$$\boxed{\hat{T}(\Delta x)|\psi\rangle = \int dx\,|x\rangle\left[\langle x|\psi\rangle - \Delta x\frac{d}{dx}\langle x|\psi\rangle\right]} \tag{5}$$

8.3.2 Representation of the Momentum Operator in the Position Basis

Next, we once again calculate $\hat{T}(\Delta x)|\psi\rangle$, this time using eq. (4) to relate $\hat{T}$ to the momentum operator $\hat{p}$. By equating this result with the previous result (eq. (5)), we determine a representation of $\hat{p}$ in the $\hat{x}$–basis.

$$\begin{aligned}\hat{T}(\Delta x)|\psi\rangle &= \left[1 - \frac{i\hat{p}\,\Delta x}{\hbar}\right]|\psi\rangle \\ &= \int dx\,|x\rangle\left[\langle x|\psi\rangle - \Delta x\frac{d}{dx}\langle x|\psi\rangle\right] \\ &= |\psi\rangle - \Delta x\int dx\,|x\rangle\frac{d}{dx}\langle x|\psi\rangle.\end{aligned}$$

Simplifying the statement above, we find

$$\boxed{\hat{p}|\psi\rangle = \int dx\,|x\rangle\left[-i\hbar\frac{d}{dx}\langle x|\psi\rangle\right]} \tag{6}$$

$$\boxed{\langle x|\hat{p}|\psi\rangle = -i\hbar\frac{d}{dx}\langle x|\psi\rangle = -i\hbar\frac{d\psi(x)}{dx}} \tag{7}$$

Eq. (7) is a key result: it states that the position space representation of the state $\hat{p}|\psi\rangle$ is equivalent to the differential operator $-i\hbar\frac{d}{dx}$ acting on the wavefunction $\psi(x)$.

We can therefore associate the operator $\hat{p}$ acting on states in the x–basis with the differential operator $-i\hbar\frac{d}{dx}$ acting on functions of x.

$$\boxed{\hat{p} \mapsto -i\hbar\frac{d}{dx}} \tag{8}$$

We can use eq. (6) and eq. (7) to derive several key results:

1. The matrix element of $\hat{p}$ for two arbitrary states $|\phi\rangle$ and $|\psi\rangle$. From eq. (6):

$$\langle\phi|\hat{p}|\psi\rangle = \left\langle \phi\left|\int dx\,|x\rangle\left(-i\hbar\frac{d}{dx}\right)\langle x|\psi\rangle\right.\right\rangle \tag{9}$$

$$= \int dx\,\langle\phi|x\rangle\left(-i\hbar\frac{d}{dx}\right)\langle x|\psi\rangle \tag{10}$$

$$= -i\hbar\int dx\,\phi^*(x)\frac{d\psi}{dx}. \tag{11}$$

2. From eq. (7):

$$\langle x|\hat{p}^{\,n}|\psi\rangle = (-i\hbar)^n\frac{d^n\psi}{dx^n}. \tag{12}$$

3. From eq. (11):

$$\langle\phi|\hat{p}^n|\psi\rangle = (-i\hbar)^n \int dx\, \phi^*(x) \frac{d^n\psi}{dx^n}. \tag{13}$$

4. The matrix element of $\hat{p}$ for two position eigenstates $|x\rangle$ and $|x'\rangle$. From eq. (7):

$$\begin{aligned}\langle x|\hat{p}|x'\rangle &= -i\hbar\frac{d}{dx}\langle x|x'\rangle \\ &= -i\hbar\frac{d}{dx}\delta(x-x').\end{aligned} \tag{14}$$

8.3.3 Position and Momentum Commutation Relationship

We know that $\hat{T}(\Delta x)$ does not commute with $\hat{x}$ because $|x\rangle$ is not an eigenstate of $\hat{T}(\Delta x)$.

$$\hat{T}(\Delta x)|x\rangle = |x+\Delta x\rangle$$

Question 8.1.

What is the commutator $[\hat{x}, \hat{T}(\Delta x)]$?

Solution. We have

$$\begin{aligned}[\hat{x}, \hat{T}(\Delta x)]|\psi\rangle &= \hat{x}\hat{T}(\Delta x)|\psi\rangle - \hat{T}(\Delta x)\hat{x}|\psi\rangle \\ &= \hat{x}\hat{T}(\Delta x)\int dx\,|x\rangle\langle x|\psi\rangle - \hat{T}(\Delta x)\hat{x}\int dx\,|x\rangle\langle x|\psi\rangle \\ &= \int dx\,(x+\Delta x)|x+\Delta x\rangle\langle x|\psi\rangle - \int dx\,x|x+\Delta x\rangle\langle x|\psi\rangle \\ &= \int dx\,x|x\rangle\langle x-\Delta x|\psi\rangle - \int dx\,(x-\Delta x)|x\rangle\langle x-\Delta x|\psi\rangle \\ &= \Delta x\int dx\,|x\rangle\langle x-\Delta x|\psi\rangle.\end{aligned}$$

Taylor expansion:

$$\langle x-\Delta x|\psi\rangle \approx \langle x|\psi\rangle - \Delta x\frac{d}{dx}\langle x|\psi\rangle.$$

Hence

$$\begin{aligned}[\hat{x}, \hat{T}(\Delta x)]|\psi\rangle &\approx \Delta x\int dx\,|x\rangle\left[\langle x|\psi\rangle - \Delta x\frac{d}{dx}\langle x|\psi\rangle\right] \\ &= \Delta x\int dx\,|x\rangle\langle x|\psi\rangle - \mathcal{O}((\Delta x)^2)\int dx\,|x\rangle\frac{d}{dx}\langle x|\psi\rangle.\end{aligned}$$

Neglecting terms of order $\mathcal{O}((\Delta x)^2)$,

$$[\hat{x}, \hat{T}(\Delta x)]|\psi\rangle = \Delta x\int dx\,|x\rangle\langle x|\psi\rangle = \Delta x|\psi\rangle.$$

Therefore,

$$\boxed{[\hat{x}, \hat{T}(\Delta x)] = \Delta x} \tag{15}$$

as desired. □

Furthermore, we can find that

$$[\hat{x}, (1 - i\hat{K}\Delta x)] = \Delta x$$
$$[\hat{x}, 1] - i\Delta x[\hat{x}, \hat{K}] = \Delta x$$

Since $[\hat{x}, 1] = 0$, we find that

$$-i\Delta x[\hat{x}, \hat{K}] = \Delta x$$

and

$$[\hat{x}, \hat{K}] = i$$

Using $\hat{K} = \frac{\hat{p}}{\hbar}$,

$$\boxed{[\hat{x}, \hat{p}] = i\hbar} \tag{16}$$

Note 8.3. We see that $\hat{x}$ and $\hat{p}$ do not commute. This has many important implications, as we will discover.

8.4 Infinite Square Well Potential

Lecture 16 - Tuesday, March 10

8.4.1 Hamiltonian in the Position Basis

Now that we have developed a theoretical framework of the Hilbert space in the position basis, we will now introduce the representation of the Hamiltonian operator in the position basis.

Recall that the Hamiltonian corresponds to the total energy of a particle. We express the total energy of a classical particle as the sum of the kinetic and potential energy

$$E = \frac{p^2}{2m} + V(x) \tag{1}$$

where, m is the particle mass, ρ is the particle momentum, and $V(x)$ is the potential energy as a function of position.

Note 8.4. This expression is valid provided that the particle is moving substantially slower than the speed of light.

To express the energy of a quantum particle, we simply replace the physical observables in the expression of energy with the corresponding quantum mechanical operators.

The Hamiltonian that corresponds to the total energy is

$$\mathcal{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \tag{2}$$

Taking the position representation, we compute

$$\langle x|\mathcal{H}|\psi\rangle = \frac{1}{2m}\langle x|\hat{p}^2|\psi\rangle + \langle x|V(\hat{x})|\psi\rangle$$

Using the position representation of the momentum operator

$$\hat{p} = -i\hbar \frac{d}{dx},$$

we obtain

$$= -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \langle x| \int dx'\, V(\hat{x})|x'\rangle\langle x'|\psi\rangle$$

Since $V(\hat{x})|x'\rangle = V(x')|x'\rangle$, this becomes

$$= -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \int dx'\, V(x')\langle x|x'\rangle\langle x'|\psi\rangle$$

Using the orthogonality relation

$$\langle x|x'\rangle = \delta(x - x'),$$

the integral simplifies to

$$\boxed{\mathcal{H}\psi(x) := \langle x|\mathcal{H}|\psi\rangle = -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x)} \tag{3}$$

Given a time-independent potential $V(x)$, eq.(3) let's us calculate the wavefunction $\psi(x)$ that corresponds to a fixed energy E. Said more precisely, we can use eq.(3) to calculate the eigenfucntion $\psi(x)$ of $\mathcal{H}$ that corresponds to a total energy E.

$$\mathcal{H}\psi(x) = E\psi(x) \tag{4}$$

Eq.(3) is extremely powerful. Given a potential energy, such as the electrostatic potential that an electron experiences from the nucleus of an atom, we can calculate the wavefunction of the particle experiencing that potential.

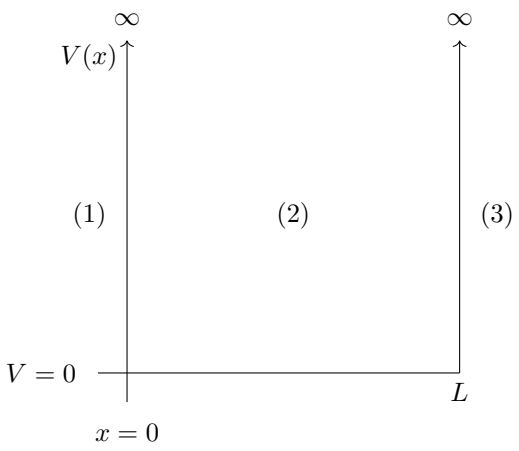
> **Comment 8.3.** The square of the wavefunction gives us the probability density, i.e., the portability of finding the particle in some region of space.

For the case of an electron around the nucleus, eq.(3) let's us compute the orbitals corresponding to discrete energy states. Our knowledge of material science, condensed matter physics and chemistry, all start from a microscopic understanding of how electrons behave in the presence of different atomic scale potentials.

8.4.2 Infinite Square-Well Potential

We will start our study of eq.(3) by considering one of the simplest forms of $V(x)$. Consider the infinite square-well potential, which consists of a region of space spanning $0 < x < L$ where $V = 0$, and an infinite potential outside this region.

$$V(x) = \begin{cases} \infty & x < 0 \\ 0 & 0 \leq x \leq L \\ \infty & x > L \end{cases} \tag{5}$$



The potential is defined piecewise into three regions. We will find the solution in the three regions separately, and connect the solutions using the continuity of the wavefunction across the two boundaries.

In each region, we seek a solution of the form

$$\mathcal{H}\,\phi_\alpha(x) = -\frac{\hbar^2}{2m}\frac{d^2\phi_\alpha}{dx^2} + V_\alpha\phi_\alpha(x) = E\phi_\alpha(x) \tag{6}$$

$$\frac{d^2\phi_\alpha}{dx^2} = -\frac{2m}{\hbar^2}[E - V_\alpha]\phi_\alpha(x)$$

$$\frac{d^2\phi_\alpha}{dx^2} = -k_\alpha^2\phi_\alpha, \qquad k_\alpha^2 := \frac{2m}{\hbar^2}[E - V_\alpha] \tag{7}$$

where $\alpha = (1, 2, 3)$ refers to the region, and k_α is the wavenumber ($k = \frac{2\pi}{\lambda}$) that describes the variation of the wavefunction, and V_α is the potential in region α.

The general solution to eq.(7) has the form

$$\phi_\alpha(x) = A_\alpha e^{ik_\alpha x} + B_\alpha e^{-ik_\alpha x}$$

where A_α and B_α are constants to be determined by boundary conditions.
By combining eq.(6) and eq.(7) we find a useful relationship.

$$\underbrace{\frac{\hbar^2 k_\alpha^2}{2m}}_{\text{K.E.}}\phi_\alpha(x) + \underbrace{V(x)}_{\text{P.E.}}\phi_\alpha(x) = E\phi_\alpha(x) \tag{9}$$

$$\text{K.E.} = \frac{p_\alpha^2}{2m} = \frac{\hbar^2 k_\alpha^2}{2m} \tag{10}$$

$$\boxed{p_\alpha = \hbar k_\alpha \quad = \text{particle momentum in region } \alpha} \tag{11}$$

The relationship between p and k is general. Namely, in regions of space where the particle momentum is large, the wavenumber is also large, which means that the wavefunction has a shorter wavelength and varies more rapidly in space.

Note 8.5. If the particle momentum is small, the wavefunction varies more slowly in space.

We will always assume that the energy E of the particle is finite. Therefore, in regions (1) and (3)

$$k^2_{(1,3)} = \frac{2m}{\hbar^2}[E - V_{(1,3)}] \to -\infty$$

In general, if $k^2 < 0$ ($E < V$), we can express k as

$$k = i|k|.$$

In this case, eq.(8) has the form

$$\phi_\alpha(x) = A_\alpha e^{-|k_\alpha|x} + B_\alpha e^{|k_\alpha|x} \tag{12}$$

In contrast to eq.(8) that describes oscillatory solutions, eq.(12) describes exponentially growing and decaying solutions.

When finding the values for the arbitrary constants A_α and B_α, we must keep in mind that the solution has to be physical.

A fundamental aspect of being physical must be that the wavefunction is normalizable, i.e.,

$$\int_{\mathcal{R}} |\phi_\alpha(x)|^2 \, dx \quad \text{is finite}$$

where $\mathcal{R}$ is the region of space that supports the solution $\phi_\alpha(x)$.

We see, for example, that in region (1) where $x < 0$, the term in eq.(12) proportional to $e^{-|k_1|x}$ diverges, and if $A_1 \neq 0$, then $\phi_1(x)$ cannot be normalized. Therefore, we must insist that $A_1 = 0$. Similarly, in region (3) where $x > L$, the term $e^{|k_3|x}$ diverges. Therefore, we must make $B_3 = 0$. The solutions in regions (1) and (3) are, therefore,

$$\phi_1(x) = B_1 e^{|k_1|x}, \qquad x < 0$$
$$\phi_3(x) = A_3 e^{-|k_3|x}, \qquad x > L$$

We note that in regions (1) and (3) $|k_{(1,3)}| \to \infty$. The fact that the exponent becomes infinite means that the wavefunctions in regions (1) and (3) become exponentially small for any value of x in that region.

$$\lim_{|\epsilon|\to 0} \phi_1(-|\epsilon|) \to 0 \tag{13}$$

$$\lim_{\epsilon\to 0} \phi_3(L + \epsilon) \to 0 \tag{14}$$

In region (2), $V = 0$, and the solution has the form

$$\phi_2(x) = A_2 e^{ik_2 x} + B_2 e^{-ik_2 x}, \qquad k_2 = \sqrt{\frac{2mE}{\hbar^2}}$$

To find A_2 and B_2, we must connect the solutions in the three regions by requiring that the wavefunction

be continuous.

$$\phi(x) = \begin{cases} 0, & x < 0 \\ A_2 e^{ik_2 x} + B_2 e^{-ik_2 x}, & 0 \le x \le L \\ 0, & x > L \end{cases}$$

Applying the boundary condition at $x = 0$,

$$\begin{aligned} \phi_1(0) &= \phi_2(0) \\ A_2 + B_2 &= 0 \end{aligned}$$

Therefore,

$$\begin{aligned} \phi_2(x) &= A_2 \left(e^{ik_2 x} - e^{-ik_2 x} \right) \\ &= 2iA_2 \sin(k_2 x) \end{aligned}$$

Thus the wavefunction becomes

$$\phi(x) = \begin{cases} 0, & x < 0 \\ A \sin(k_2 x), & 0 \le x \le L \\ 0, & x > L \end{cases}$$

Apply the boundary condition at $x = L$:

$$\begin{aligned} \phi_2(L) &= \phi_3(L) \\ A \sin(k_2 L) &= 0 \end{aligned}$$

Since $A = 0$ corresponds to the trivial solution $\phi(x) = 0$, we require

$$\sin(k_2 L) = 0$$

Therefore,

$$k_n := k_2 = \frac{n\pi}{L}, \qquad n = 1, 2, 3, \ldots$$

Finally, we determine the constant A by normalizing the energy eigenkets:

$$\int_{-\infty}^{\infty} |\phi_n(x)|^2 dx = 1$$

Since the wavefunction is nonzero only in $[0, L]$,

$$A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

which gives

$$A = \sqrt{\frac{2}{L}}$$

Discovery 8.2. Eigenfunctions:

$$\phi_n(x) = \begin{cases} 0, & x < 0 \\ \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), & 0 \le x \le L \\ 0, & x > L \end{cases} \tag{15}$$

Discovery 8.3. Eigenenergies:

$$E_n = \frac{p_n^2}{2m} = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2mL^2} \tag{16}$$

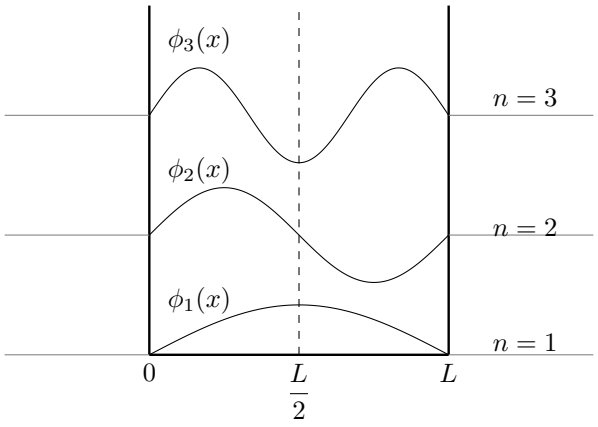


Figure 7: Eigenfunctions of the infinite one-dimensional square-well potential.

An important feature of the solutions is that they alternate between even and odd functions of x.

This is a general feature of any potential that has a an axis of symmetry. If an axis of symmetry exists, then the eigenfunctions alternate between even and odd functions, with respect to the symmetry axis.

Question 8.2.

The lowest energy state, referred to as the ground state, is always nodeless (does not cross zero). Can you think why?

Order of Magnitude Estimate of Ground State Energy of H Atom. Although the infinite square well potential is artificial and somewhat contrived, it still provides an order-of-magnitude estimate of the energy scale of the bound state of the electron in a hydrogen atom.

The ground-state energy of a particle of mass m confined to a region of space of size L is given by eq.(16)

$$E_1 = \frac{h^2}{8mL^2}$$

The typical length scale of a ground state atomic orbital is $\sim 2\,\mathrm{rA}$. The ground-state energy for an electron

is

$$E_1 = \frac{(6.63 \times 10^{-34}\,\text{J-s})^2}{8 \times 9.1 \times 10^{-31}\,\text{kg}\,(2 \times 10^{-10}\,\text{m})^2}$$

$$= 1.5 \times 10^{-18}\,\text{J} \times \frac{1\,\text{eV}}{1.6 \times 10^{-19}\,\text{J}} = 9.4\,\text{eV}$$

The binding energy of an electron to a proton in the hydrogen atom is 13.6 eV. □

An important aspect of the energy eigenfunctions is their orthogonality.

We have proved that the eigenkets of Hermitian operators are orthogonal. This fact also applies to the energy eigenfunctions of the Hamiltonian.

We express the inner product of wavefunctions in terms of the integral below. See eq. (7–9) in lecture 18 for details.

$$\langle \phi_n \mid \phi_m \rangle = \int_{-\infty}^{\infty} \phi_n^*(x)\, \phi_m(x)\, dx$$

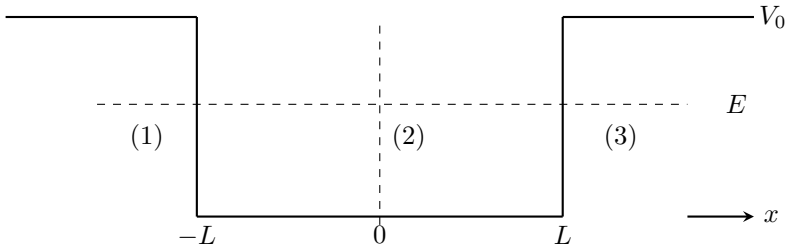
You can show two eigenfunctions of the infinite square-well potential for which $m \neq n$ is zero, and equal to 1 for $m = n$.

> **Comment 8.4.** In the next lecture, we will consider a square-well potential, where the potential outside the well is finite.
> We will compare the results with the case where the potential outside is infinite. This comparison will guide our intuition as to the interplay between the kinetic and potential terms in the Hamiltonian, and how they affect the shape of the wavefunction.

8.5 Finite Potential Square Well

Lecture 17 - Thursday, March 12

We want to once again consider the one-dimensional square well potential. This time, we want to calculate the problem for a finite potential V_0.



The square-well potential we consider is as follows

$$V(x) = \begin{cases} V_0, & x < -L, \\ 0, & -L \leq x \leq L, \\ V_0, & x > L. \end{cases} \tag{1}$$

You may notice that the well has a width $2L$ symmetrically placed around $x = 0$. I've set up the problem this way in anticipation of the solutions having even and odd parity with respect to the axis of symmetry of the well.

The Schrödinger equations in regions $\alpha = (1, 2, 3)$ is

$$\frac{d^2\psi_\alpha}{dx^2} = \frac{2m}{\hbar^2}(V_\alpha - E)\psi_\alpha(x) \tag{2}$$

We seek bound state solutions, where $E < V_0$. We define

$$\text{Regions 1 and 3:} \qquad \kappa = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)} \tag{3}$$

$$\text{Region 2:} \qquad k = \sqrt{\frac{2mE}{\hbar^2}} \tag{4}$$

The general form of the solutions in the three regions are

$$\phi(x) = \begin{cases} A_1 e^{\kappa x}, & x < -L, \\ A_2 \sin(kx) + B_2 \cos(kx), & -L \le x \le L, \\ B_3 e^{-\kappa x}, & x > L \end{cases} \tag{5}$$

Note 8.6. Note, I've written the exponentially-decaying solution in regions 1 and 3, and excluded the exponentially growing ones.

Comment 8.5. In region 2, I've used $\sin(kx)$ and $\cos(kx)$ solutions rather than the $e^{\pm ikx}$ solutions. I've done this because the real-valued functions are explicitly even and odd parity with respect to x.

We know the solutions will alternate between even and odd parity. Therefore, we can solve for one or the other parity by including only the function with the parity we wish to calculate.

Our approach for solving the problem will be to solve for each parity separately.

8.6 Boundary Conditions and Solution

To connect the solutions in the three regions, we need to apply two boundary conditions at $x = -L$ and $x = L$.

- The first boundary condition is the continuity of wavefunction. The wavefunction must be continuous in order to ensure that the probability density is defined at every point in space.

$$\begin{aligned} \phi_1(-L) &= \phi_2(-L) \\ A_1 e^{-\kappa L} &= -A_2 \sin(kL) + B_2 \cos(kL) \end{aligned} \tag{6}$$

$$\begin{aligned} \phi_2(L) &= \phi_3(L) \\ B_3 e^{-\kappa L} &= A_2 \sin(kL) + B_2 \cos(kL) \end{aligned} \tag{7}$$

- The second boundary condition requires the continuity of the derivative of the wavefunction.

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}[V(x) - E] \tag{8}$$

If the potential $V(x)$ is finite, then the Schrödinger equation requires that $\dfrac{d^2\psi}{dx^2}$ must also be finite. Therefore, the first derivative $\dfrac{d\psi}{dx}$ must be continuous.

$$\begin{aligned} \left.\frac{d\phi_1}{dx}\right|_{x=-L} &= \left.\frac{d\phi_2}{dx}\right|_{x=-L} \\ A_1\kappa e^{-\kappa L} &= k\big[A_2\cos(kL) + B_2\sin(kL)\big] \end{aligned} \tag{9}$$

$$\begin{aligned} \left.\frac{d\phi_2}{dx}\right|_{x=L} &= \left.\frac{d\phi_3}{dx}\right|_{x=L} \\ -B_3\kappa e^{-\kappa L} &= k\big[A_2\cos(kL) - B_2\sin(kL)\big] \end{aligned} \tag{10}$$

The solution to the problem involves 5 unknown quantities: A_1, A_2, B_2, B_3 and E. These quantities must be determined in a self-consistent manner from eqns. (6), (7), (9) and (10). We will solve for the even and odd parity solutions separately.

Even Parity Solutions: coefficient of $\sin(kx)$: $\quad A_2 = 0$

$$A_1 = B_3 = B_2 e^{\kappa L}\cos(kL)$$

$$\cot(kL) = \frac{k}{\kappa} \tag{11}$$

$$\phi_{\text{even}}(x) = B_2 \times \begin{cases} e^{\kappa(x+L)}\cos(kL), & x < -L, \\ \cos(kx), & -L \le x \le L, \\ e^{-\kappa(x-L)}\cos(kL), & x > L \end{cases} \tag{12}$$

The constant B_2 is determined by normalization.

Odd Parity Solutions: coefficient of $\cos(kx)$: $\quad B_2 = 0$

$$A_1 = -B_3 = -A_2 e^{\kappa L}\sin(kL)$$

$$\tan(kL) = -\frac{k}{\kappa} \tag{13}$$

$$\phi_{\text{odd}}(x) = A_2 \times \begin{cases} -e^{\kappa(x+L)}\sin(kL), & x < -L, \\ \sin(kx), & -L \le x \le L, \\ e^{-\kappa(x-L)}\sin(kL), & x > L \end{cases} \tag{14}$$

The constant A_2 is determined by normalization.

8.7 Energy Spectrum and Eigenfunctions

To find the spectrum of allowed energies, we need to find the values of E that satisfy eqns. (11) and (13).

> **Note 8.7.** We note that E appears in the argument of a trigonometric function on the left-hand side of these equations, and a polynomial form on the right-hand side.

Equations of this type are known as transcendental equations, and they have no algebraic solution. We can solve these equations graphically by plotting the right and left hand side and seeing where they cross. To plot the solutions, we need to pick an energy scale for the problem. We can then write all relevant functions in terms of the energy scales.

$$E_0 := \frac{\hbar^2}{2mL^2}$$
$$kL = \sqrt{\frac{E}{E_0}}$$
$$\kappa L = \sqrt{\frac{V_0 - E}{E_0}}$$
$$\frac{k}{\kappa} = \sqrt{\frac{E}{V_0 - E}}$$

For these plots, we've picked $E_0 = 0.01$ and $V_0 = 1$.

> **Discovery 8.4.** There are some important observations regarding the finite square well potential.
>
> 1. the energy of a state cannot exceed V_0. Therefore, unlike the infinite potential square well, the finite potential well supports a finite number of energy eigenstates.
> 2. you will notice that wavefunction for higher energy states extends further into the classically-forbidden region, i.e., regions 1 and 3 where $E < V_0$. The lengthscale that determines the penetration into the classically-forbidden region is
>
> $$\kappa = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$
>
> We can see that for higher energy states, the difference $V_0 - E$ becomes smaller, therefore κ is smaller, and the wavefunction decays slower.

Question 8.3.

Question: What happens if we place two finite potential wells close to each other, and place a particle into one of them?

Lecture 18 - Tuesday, March 17

In class review session today, I woke up but I didn't go.

8.8 Time Evolution of Superposition of Energy Eigenstates

Lecture 19 - Tuesday, March 24

8.8.1 Superposition of Energy Eigenstates

In this lecture, we will consider the time evolution of states that are not energy eigenstates.

We will consider the time-dependent probability density of superposition states and calculate the probability of observing the particle in a particular region of space as a function of time.

Suppose we are told that the wavefunction corresponding to a particle in an infinite potential square well at $t = 0$ is given by

$$|\phi(t=0)\rangle = \frac{1}{\sqrt{2}}\big(|\phi_1\rangle + |\phi_2\rangle\big)$$

where $|\phi_1\rangle$ and $|\phi_2\rangle$ are the $n = 1$ and $n = 2$ eigenstates corresponding to the infinite square well potential.

$$\langle x|\phi_n\rangle := \phi_n(x) = \begin{cases} 0, & x < 0, \\ \sqrt{\dfrac{2}{L}}\sin\Big(\dfrac{n\pi x}{L}\Big), & 0 \le x \le L, \\ 0, & x > L. \end{cases}$$

Question 8.4.

Given the state of the system at $t = 0$, $|\phi(t=0)\rangle$, what is the probability of finding the particle on the right half of the well at time t?

To solve this problem, we need to calculate the probability density inside the well as a function of time, and integrate it over the right half of the well to calculate the probability.

$$|\phi(t)\rangle = \frac{1}{\sqrt{2}}\left[|\phi_1\rangle e^{-iE_1 t/\hbar} + |\phi_2\rangle e^{-iE_2 t/\hbar}\right]$$

where

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}.$$

Hence,

$$\begin{aligned}\phi(x,t) := \langle x|\phi(t)\rangle &= \frac{1}{\sqrt{2}}\left[\langle x|\phi_1\rangle e^{-iE_1 t/\hbar} + \langle x|\phi_2\rangle e^{-iE_2 t/\hbar}\right] \\ &= \frac{1}{\sqrt{2}}\left[\phi_1(x) e^{-iE_1 t/\hbar} + \phi_2(x) e^{-iE_2 t/\hbar}\right]\end{aligned}$$

Use the projection operator in the position basis to express the probability density.

$$\begin{aligned}\langle\phi(t)|\phi(t)\rangle &= \int_{-\infty}^{\infty} \langle\phi(t)|x\rangle\langle x|\phi(t)\rangle\, dx \\ &= \int_{-\infty}^{\infty} \phi^*(x,t)\phi(x,t)\, dx = \int_{-\infty}^{\infty} |\phi(x,t)|^2\, dx = 1\end{aligned}$$

To calculate the probability of finding the particle in the right hand of the well, in the region

$$\frac{L}{2} \leq x \leq L,$$

we need to calculate the following integral:

$$\text{Prob.} = \int_{L/2}^{L} |\phi(x,t)|^2 \, dx$$

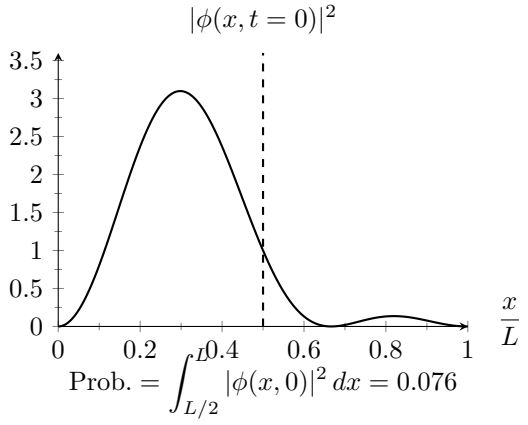
$$|\phi(x,t)|^2 = \frac{1}{2}\left(|\phi_1(x)|^2 + |\phi_2(x)|^2 + 2\,\mathrm{Re}\Big\{\phi_1^*(x)\phi_2(x)e^{i(E_1-E_2)t/\hbar}\Big\}\right)$$

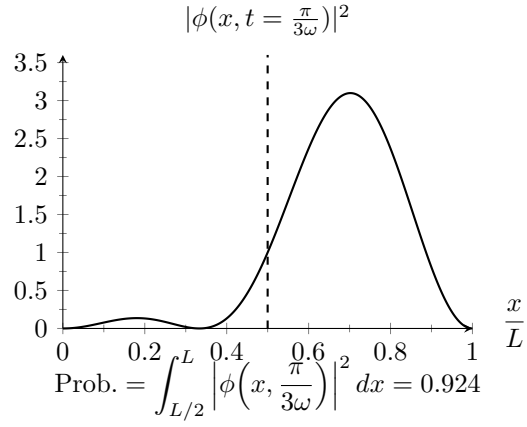
We evaluate the frequency of oscillation in the expression above as

$$\frac{(E_1 - E_2)t}{\hbar} = -\frac{3\pi^2\hbar t}{2mL^2} := -3\omega t, \qquad \omega = \frac{E_1}{\hbar}$$

Therefore,

$$\begin{aligned}\text{Prob.} &= \frac{1}{L}\int_{L/2}^{L}\left(\sin^2\Big(\frac{\pi x}{L}\Big) + \sin^2\Big(\frac{2\pi x}{L}\Big) + 2\sin\Big(\frac{\pi x}{L}\Big)\sin\Big(\frac{2\pi x}{L}\Big)\cos(3\omega t)\right) dx \\ &= \frac{1}{2} - \frac{4}{3\pi}\cos(3\omega t)\end{aligned}$$





8.8.2 Localization of a Particle Inside the Well

Discovery 8.5. We see that if we start from a state that is not an eigenstate of the Hamiltonian, then the system evolves in time.
In particular, we see that the probability of observing the particle in a given region of space changes in time.

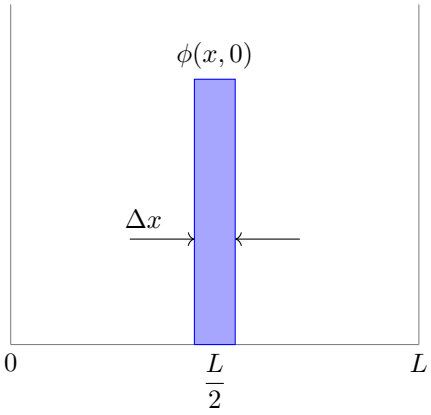
Let us now ask a slightly different question: suppose we use a measurement device to measure the location of the particle inside the box. The device is capable of resolving the location of the particle in a region Δx.

At $t = 0$ we observe the particle to be in the region

$$\frac{L - \Delta x}{2} \leq x \leq \frac{L + \Delta x}{2}.$$

The normalized wavefunction of the particle after measurement is

$$\phi(x, t = 0) = \begin{cases} 0, & x < \dfrac{L - \Delta x}{2}, \\ \dfrac{1}{\sqrt{\Delta x}}, & \dfrac{L - \Delta x}{2} \leq x \leq \dfrac{L + \Delta x}{2}, \\ 0, & x > \dfrac{L + \Delta x}{2}. \end{cases}$$



Calculate the probability density at $t > 0$. We need to express the initial state in the energy basis.

$$|\phi(t = 0)\rangle = \sum_{n=1}^{\infty} C_n \, |\phi_n\rangle$$

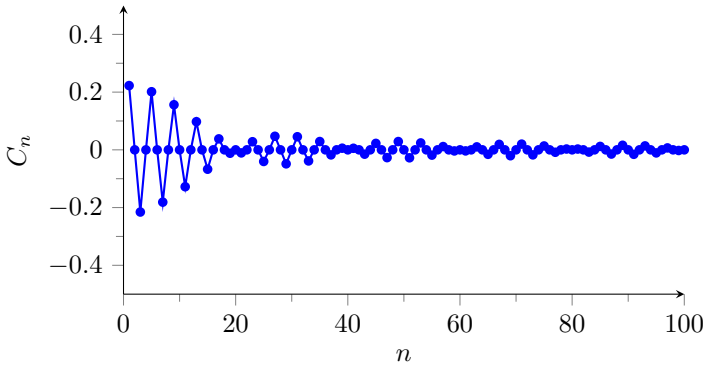
$$\langle \phi_m | \phi(0) \rangle = \sum_{n=1}^{\infty} C_n \, \langle \phi_m | \phi_n \rangle = \sum_{n=1}^{\infty} C_n \, \delta_{nm} = C_m$$

$$C_m = \langle \phi_m | \phi(0) \rangle = \int \phi_m^*(x) \phi(x, 0) \, dx$$

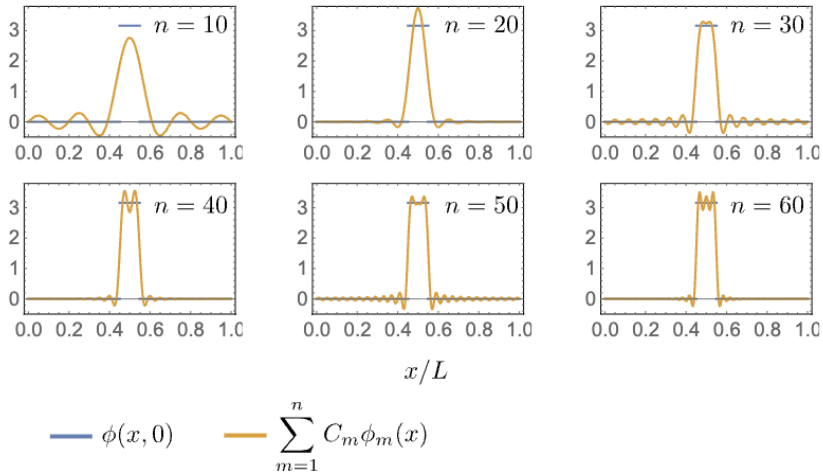
$$C_m = \sqrt{\frac{2}{L \Delta x}} \int_0^L \sin\Big(\frac{m \pi x}{L}\Big) \, \phi(x, 0) \, dx$$

$$C_m = \sqrt{\frac{2}{L \Delta x}} \int_{\frac{L - \Delta x}{2}}^{\frac{L + \Delta x}{2}} \sin\Big(\frac{m \pi x}{L}\Big) \, dx$$

Let us calculate the amplitudes $\{C\}$ for the first 100 coefficients for $\Delta x = 0.1L$.



Comment 8.6. It is instructive to observe how the representation of $\phi(x,0)$ improves as we include a larger number of coefficients.



Let us include the first 30 terms in the expansion of $\phi(x,0)$. The probability density at times $t > 0$ is

$$\phi(x,t) = \sum_{m=1}^{n} C_m e^{-iE_m t/\hbar} \phi_m(x)$$

$$|\phi(x,t)|^2 = \left| \sum_{m=1}^{n} C_m e^{-iE_m t/\hbar} \phi_m(x) \right|^2$$

We saw from our first example that the probability density will involve interference terms that are proportional to

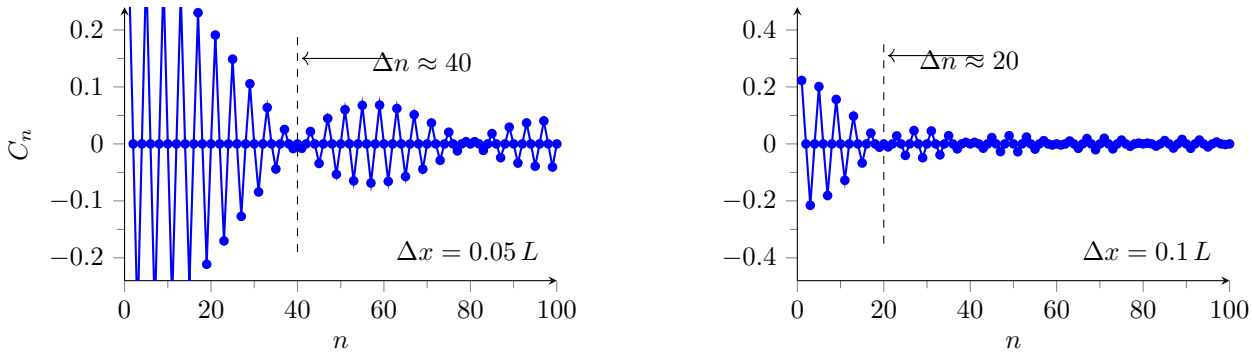
$$\cos\left(\frac{(E_n - E_m)t}{\hbar} \right),$$

where m and n are two different energy states in the sum.

If we include a large number of terms, we will get a very complicated evolution of the probability density.

Let us see what this looks like for $n = 30$.

8.8.3 Position-Momentum Uncertainty Relationship



We see that the number of non-zero terms required to represent $\phi(x, 0)$ is inversely proportional to the region Δx that the particle is localized. The range Δn can be related to a range of momentum values as follows.

$$p_n = \hbar k_n = \frac{\hbar \pi n}{L} \qquad \Delta p = \frac{\hbar \pi\, \Delta n}{L}$$

$$\Delta p\, \Delta x \approx 2\pi\hbar = h$$

We see in this example that the product $\Delta p\, \Delta x$ is constant.

This result shows that if we determine the position of the particle with greater certainty, i.e. make Δx small, then the uncertainty in momentum increases.

Conversely, if we make the uncertainty in momentum small, then the uncertainty in position becomes larger.

This uncertainty relationship between position and momentum is a consequence of the fact that position and momentum are non-commuting variables.

$$\Delta p\, \Delta x \geq \frac{1}{2} \left| \langle [\hat{p}, \hat{x}] \rangle \right|$$

$$\Delta p\, \Delta x \geq \frac{\hbar}{2}$$

Note 8.8. In quantum mechanics we cannot simultaneously determine the position and momentum of a particle with arbitrary certainty.

8.9 Free Particle Eigenstates

Lecture 20 - Thursday, March 26

8.9.1 Free Particle Energy Eigenstates

We will now calculate the eigenstates of a particle moving in a region of space where

$$V(x) = 0.$$

The particle is not bound by any potential.

Comment 8.7. We assume the particle has kinetic energy E.

The Schrödinger equation for the free particle is

$$\begin{aligned}\mathcal{H}\phi_E(x) &= E\phi_E(x)\\ -\frac{\hbar^2}{2m}\frac{d^2\phi_E}{dx^2} &= E\phi_E(x)\\ \frac{d^2\phi_E}{dx^2} &= -\frac{2mE}{\hbar^2}\phi_E(x) = -k^2\phi_E(x)\end{aligned}$$

where

$$k = \pm\sqrt{\frac{2mE}{\hbar^2}}.$$

Theorem 8.1.

General solution:

$$\phi_E(x) = Ae^{ikx} + Be^{-ikx} \tag{1}$$

The solution to the time-dependent Schrödinger equation is

$$\mathcal{H}\phi_E(x,t) = E\phi_E(x,t) = i\hbar\frac{\partial\phi_E}{\partial t}$$

$$\phi_E(x,t) = \phi_E(x)e^{-iEt/\hbar} \tag{2}$$

Using the Plank-Einstein relationship $E = \hbar\omega$, we can express eq.(2) as

$$\phi_E(x,t) = Ae^{i(kx-\omega t)} + Be^{-i(kx+\omega t)} \tag{3}$$

We recall from classical mechanics that $e^{ik(x-vt)}$ represents a plane wave traveling in the $+\hat{x}$ direction with velocity v. Likewise, $e^{ik(x+vt)}$ represents a plane wave traveling in the $-\hat{x}$ direction.

$$\phi_E(x,t) = \underbrace{Ae^{ik(x-\omega t/k)}}_{\text{plane wave moving in the } +\hat{x} \text{ direction}} + \underbrace{Be^{-ik(x+\omega t/k)}}_{\text{plane wave moving in the } -\hat{x} \text{ direction}}$$

Waves moving with phase velocity

$$v_\phi = \frac{\omega}{k}.$$

8.9.2 Momentum Eigenstates in the Position Basis

We note that the Hamiltonian of a freely-moving particle

$$\mathcal{H} = \frac{\hat{p}^2}{2m}$$

commutes with momentum $\hat{p}$:

$$[\mathcal{H}, \hat{p}] = 0.$$

Therefore, the momentum and Hamiltonian operators share the same eigenbasis.

$$\langle x|\hat{p}|\phi_E\rangle = -i\hbar\frac{d}{dx}\phi_E(x) = -i\hbar\frac{d}{dx}Ae^{\pm ikx} = \pm\hbar k\, Ae^{\pm ikx}.$$

Thus

$$p = \pm\hbar k$$

are the two momentum eigenvalues, corresponding to a particle moving in the $+\hat{x}$ or the $-\hat{x}$ direction with momentum $\hbar k$. Both momentum states have the same energy

$$E = \frac{\hbar^2 k^2}{2m}.$$

Note 8.9. This is an example of degeneracy, which means that there are two or more eigenstates with the same eigenvalue. In this case, both energy eigenstates have the same energy eigenvalue.

We can label the free-particle states in terms of the momentum eigenvalue p. In the abstract bra-ket notation, the ket $|p\rangle$ represents a state with momentum p:

$$\hat{p}\,|p\rangle = p\,|p\rangle \tag{4}$$

From the solution to the Schrödinger equation, we saw that a free-particle state with momentum $p = \pm\hbar k$ is represented in the position basis as a plane wave:

$$\langle x|p\rangle := \phi_p(x) = Ae^{ipx/\hbar} \tag{5}$$

As we have done before, we now seek to find the normalization constant A corresponding to a particle with momentum p.

We note that a plane wave represents a particle having a definite momentum. By the uncertainty relationship,

$$\Delta p\,\Delta x \geq \frac{\hbar}{2},$$

such a state has infinite position uncertainty because $\Delta p = 0$.

Discovery 8.6. A state with $\Delta x = \infty$ is completely delocalized; that is, there is equal probability to find the particle in any region of space.

8.9.3 Normalization of Free Particle Momentum Eigenstates

Let us try to normalize a state of definite momentum.

$$\begin{aligned}\langle p|p\rangle &= \int_{-\infty}^{\infty}\langle p|x\rangle\langle x|p\rangle\,dx \\ &= \int_{-\infty}^{\infty}|\phi_p(x)|^2\,dx \\ &= A^2\int_{-\infty}^{\infty}dx \to \infty\end{aligned}$$

Free particle momentum eigenstates are normalized using the Dirac normalization, which relies on the orthogonality of momentum eigenstates having different momenta.

$$\begin{aligned}\langle p'|p\rangle &= \int_{-\infty}^{\infty} \langle p'|x\rangle\langle x|p\rangle\, dx \\ &= \int_{-\infty}^{\infty} \phi^*_{p'}(x)\phi_p(x)\, dx \\ &= A^2 \int_{-\infty}^{\infty} e^{i(p-p')x/\hbar}\, dx\end{aligned}$$

The Dirac-delta function is defined by

$$\delta(p-p') = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{i(p-p')x/\hbar}\, dx$$

so that

$$\langle p'|p\rangle = A^2(2\pi\hbar)\,\delta(p-p').$$

To impose Dirac normalization, we choose A so that

$$A^2(2\pi\hbar) = 1.$$

Hence

$$A = \frac{1}{\sqrt{2\pi\hbar}}.$$

Therefore,

$$\phi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \tag{6}$$

and

$$\langle p'|p\rangle = \int_{-\infty}^{\infty} \phi^*_{p'}(x)\phi_p(x)\, dx = \delta(p-p'). \tag{7}$$

8.9.4 Representation in the Position and Momentum Basis

Note 8.10. A note on representation:
The ket $|p\rangle$ represents a momentum eigenstate. The state itself is independent of representation.
The state $|p\rangle$ has a representation in both the position basis and the momentum basis:

$$\begin{aligned} \text{Position representation:} \qquad & \langle x|p\rangle = \phi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}, \\ \text{Momentum representation:} \qquad & \langle p'|p\rangle = \phi_p(p') = \delta(p - p'). \end{aligned}$$

Similarly, $|x\rangle$ is the position eigenket, and it also has representations in both the position and momentum bases:

$$\begin{aligned} \text{Position representation:} \qquad & \langle x'|x\rangle = \delta(x' - x), \\ \text{Momentum representation:} \qquad & \langle p|x\rangle = \big(\langle x|p\rangle\big)^* = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}. \end{aligned}$$

Suppose we are given the position-space representation of a state $|\psi\rangle$:

$$\langle x|\psi\rangle = \psi(x).$$

We can use the position-space representation of the momentum eigenkets to express $\psi(x)$ in terms of $\psi(p)$:

$$\begin{aligned} \psi(x) &= \langle x|\psi\rangle \\ &= \left\langle x \middle| \int_{-\infty}^{\infty} dp\, |p\rangle\langle p| \middle| \psi \right\rangle \\ &= \int_{-\infty}^{\infty} \langle x|p\rangle\langle p|\psi\rangle\, dp \\ &= \int_{-\infty}^{\infty} \phi_p(x)\, \psi(p)\, dp. \end{aligned}$$

Here $\psi(p)$ is the momentum-space representation of the state $|\psi\rangle$. Therefore,

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar} \psi(p)\, dp. \tag{8}$$

We can also determine $\psi(p)$ from $\psi(x)$. Starting from (8), we have

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ip'x/\hbar} \psi(p')\, dp'.$$

Multiplying both sides by $e^{-ipx/\hbar}$, we get

$$\psi(x) e^{-ipx/\hbar} = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{i(p'-p)x/\hbar} \psi(p')\, dp'.$$

Now integrate both sides over x:

$$\begin{aligned}\int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar}\, dx &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(p')\, dp' \int_{-\infty}^{\infty} e^{i(p'-p)x/\hbar}\, dx \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(p')\, (2\pi\hbar)\delta(p'-p)\, dp' \\ &= \sqrt{2\pi\hbar} \int_{-\infty}^{\infty} \psi(p')\delta(p'-p)\, dp' \\ &= \sqrt{2\pi\hbar}\, \psi(p).\end{aligned}$$

Hence,

$$\psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar}\, dx. \tag{9}$$

8.10 The Wave Packet

We saw in the previous lecture that free-particle momentum eigenstates cannot be normalized in the traditional sense.

This is a direct consequence of the uncertainty principle. The position-space representation of a momentum eigenstate is a plane wave, which has infinite extent. The momentum uncertainty for a plane wave is zero, which means that the position uncertainty is infinite.

In reality, a particle is never infinitely delocalized. For example, we can think of the probability density of a particle moving in space as being peaked in the region of space where the probability of finding the particle is largest, but may have some spread around this region.

The most natural way to model a free particle is as a wave packet, which we can think of as a plane wave multiplied by an envelope function that ensures that the probability density decays smoothly as we move away from the center of the probability density.

A wave packet is composed of a band of wavenumbers, corresponding to a band of momenta. Therefore, for a wave packet both Δx and Δp are non-zero.

We saw in the last lecture that, given a momentum-space representation $\psi(p)$, we can construct the position-space representation of the wavefunction:

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar} \psi(p)\, dp \tag{1}$$

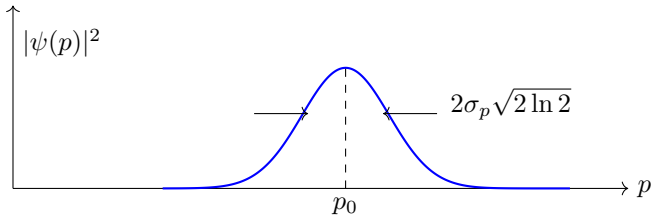
We can express the time-dependent state $\psi(x,t)$ as

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar} e^{-iE(p)t/\hbar} \psi(p)\, dp \tag{2}$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar} e^{-ip^2 t/2m\hbar} \psi(p)\, dp \tag{3}$$

Our goal is to construct a wave packet that represents a particle that is localized in some region of space. We will choose a momentum distribution $\psi(p)$ and calculate the corresponding $\psi(x)$.

Let us construct a wave packet moving in the $+\hat{x}$ direction with mean momentum p_0 and with a Gaussian envelope.



Normalized momentum distribution:

$$\psi(p) = \frac{1}{\sqrt{\sigma_p\sqrt{2\pi}}} e^{-(p-p_0)^2/4\sigma_p^2} \tag{4}$$

Indeed,

$$\int_{-\infty}^{\infty} |\psi(p)|^2\, dp = \frac{1}{\sigma_p\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-(p-p_0)^2/2\sigma_p^2}\, dp = 1.$$

Calculate the expectation value of momentum and the uncertainty in momentum, based on the distribution $\psi(p)$:

$$\langle p\rangle = \int_{-\infty}^{\infty} p\,|\psi(p)|^2\, dp = p_0 \tag{5}$$

$$\langle p^2\rangle = \int_{-\infty}^{\infty} p^2\,|\psi(p)|^2\, dp = p_0^2 + \sigma_p^2 \tag{6}$$

$$\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \sigma_p \tag{7}$$

From eq. (3),

$$\begin{aligned}\psi(x,t) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(p) e^{-ip^2t/2m\hbar} e^{ipx/\hbar}\, dp \\ &= \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{\sqrt{\sigma_p\sqrt{2\pi}}} \int_{-\infty}^{\infty} e^{-(p-p_0)^2/4\sigma_p^2} e^{ipx/\hbar} e^{-ip^2t/2m\hbar}\, dp.\end{aligned}$$

The integral is straightforward to do, although tedious. The result of the integration is

$$\psi(x,t) = \left(\frac{1}{2\pi\alpha^2}\right)^{1/4} \frac{1}{\sqrt{\gamma}} \exp\left\{\frac{ip_0}{\hbar}\left(x - \frac{p_0 t}{2m}\right)\right\} \exp\left\{-\frac{1}{4\alpha^2\gamma}\left(x - \frac{p_0 t}{m}\right)^2\right\} \tag{8}$$

where

$$\gamma := 1 + \frac{it}{\tau}, \qquad \tau := \frac{m\hbar}{2\sigma_p^2}, \qquad \alpha := \frac{\hbar}{2\sigma_p}.$$

The term

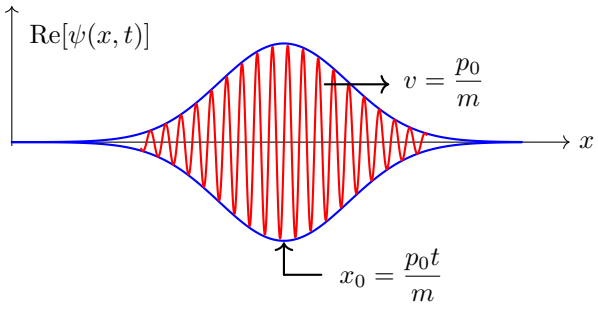
$$\exp\left\{\frac{ip_0}{\hbar}\left(x - \frac{p_0 t}{2m}\right)\right\}$$

represents a plane wave traveling in the $+\hat{x}$ direction with wavenumber

$$k = \frac{p_0}{\hbar},$$

with phase velocity

$$v_\phi = \frac{p_0}{2m}.$$



The term

$$\exp\left\{-\frac{1}{4\alpha^2\gamma}\left(x - \frac{p_0 t}{m}\right)^2\right\}$$

represents a Gaussian envelope that modulates the amplitude of the plane wave.

The center of the Gaussian

$$x_0 = \frac{p_0 t}{m}$$

advances in time with the classical velocity

$$v = \frac{p_0}{m},$$

also known as the group velocity. The group velocity is given by

$$E = \frac{\hbar^2 k^2}{2m} = \hbar\omega, \qquad \omega(k) = \frac{\hbar k^2}{2m} \tag{9}$$

$$\frac{\partial \omega}{\partial k} = \frac{\hbar k}{m} = \frac{p_0}{m}. \tag{10}$$

We note that the wave packet is a sum of different momenta, determined by the distribution $\psi(p)$, each with corresponding phase velocity

$$v_\phi = \frac{\omega}{k} = \frac{p}{2m}.$$

Because the phase velocity is momentum dependent, we expect the wave packet to spread out in time.

To visualize the wave packet in time, it is useful to construct the time-dependent probability density, which represents the probability of finding the particle in a given region of space as a function of time:

$$|\psi(x,t)|^2 = \frac{1}{\alpha\sqrt{2\pi}}\frac{1}{\sqrt{\gamma\gamma^*}}\exp\left\{-\frac{1}{4\alpha^2\gamma}\left(x - \frac{p_0 t}{m}\right)^2\right\}\exp\left\{-\frac{1}{4\alpha^2\gamma^*}\left(x - \frac{p_0 t}{m}\right)^2\right\}.$$

Let

$$\Gamma(t) := \sqrt{|\gamma|^2} = \sqrt{1 + \frac{t^2}{\tau^2}}.$$

Then

$$|\psi(x,t)|^2 = \frac{1}{\alpha\,\Gamma(t)\sqrt{2\pi}} \exp\left\{ -\frac{1}{2\alpha^2\Gamma^2(t)} \left(x - \frac{p_0 t}{m} \right)^2 \right\}. \tag{11}$$

Thus $|\psi(x,t)|^2$ is a normalized Gaussian of the form

$$|\psi(x,t)|^2 = \frac{1}{\sigma_x(t)\sqrt{2\pi}} \exp\left\{ -\frac{(x - x_0(t))^2}{2\sigma_x^2(t)} \right\}, \qquad \text{with } \sigma_x(t) = \alpha\,\Gamma(t).$$

Hence

$$\sigma_x(t) = \frac{\hbar}{2\sigma_p}\sqrt{1 + \frac{t^2}{\tau^2}} = \frac{\hbar}{2\sigma_p}\sqrt{1 + \left(\frac{2\sigma_p^2 t}{m\hbar} \right)^2}. \tag{12}$$

Calculate the expectation value of position and the uncertainty in position based on the distribution $\psi(x,t)$:

$$\langle x \rangle = \int_{-\infty}^{\infty} x\,|\psi(x,t)|^2\,dx = x_0(t) = \frac{p_0 t}{m} \tag{13}$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2\,|\psi(x,t)|^2\,dx = x_0^2(t) + \sigma_x^2(t) \tag{14}$$

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sigma_x(t). \tag{15}$$

We know from the uncertainty relationship

$$\Delta x\,\Delta p \geq \frac{\hbar}{2}.$$

For the Gaussian momentum distribution discussed above,

$$\Delta p = \sigma_p, \qquad \text{time independent} \tag{16}$$

$$\Delta x = \sigma_x(t) = \frac{\hbar}{2\sigma_p}\sqrt{1 + \left(\frac{2\sigma_p^2 t}{m\hbar} \right)^2} \tag{17}$$

$$\Delta x\,\Delta p = \frac{\hbar}{2}\sqrt{1 + \left(\frac{2\sigma_p^2 t}{m\hbar} \right)^2}. \tag{18}$$

At $t = 0$, we have the minimum uncertainty of $\hbar/2$.

As t increases, the uncertainty product grows due exclusively to the increase in Δx as a function of

time:

$$\lim_{t\to\infty} \Delta x\, \Delta p \to \frac{\sigma_p^2\, t}{m}.$$

If the wave packet has a broad distribution of momenta, i.e. large σ_p, then $|\psi(x, t = 0)|^2$ is sharply peaked, and disperses quickly as time increases.

We have seen that a state of definite momentum $|p_0\rangle$ has a delta-function representation in momentum space, and is represented by a plane wave in position:

$$\langle p|p_0\rangle = \delta(p - p_0),$$
$$\langle x|p_0\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ip_0 x/\hbar}.$$

A state of definite momentum $|p_0\rangle$ is infinitely localized in the momentum domain, and infinitely delocalized in the position domain.

Similarly, a state of definite position $|x'\rangle$ has a delta-function representation in the position space, and is also represented as a plane wave in the momentum space:

$$\langle x|x'\rangle = \delta(x - x'),$$
$$\langle p|x'\rangle = \big(\langle x'|p\rangle\big)^* = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx'/\hbar}.$$

A state of definite position $|x'\rangle$ is infinitely localized in the position domain, and infinitely delocalized in the momentum domain.

We can understand the dynamics of a wave packet as follows.

As the initial probability distribution $|\psi(x, t = 0)|^2$ advances in time, the plane-wave contributions having different momenta move with different phase velocities

$$v_\phi = \frac{p}{2m},$$

with the higher-momentum components moving faster than the smaller-momentum ones.

As a result, a wave packet that has a narrow distribution of momenta (small σ_p) spreads out less than one that has a broader distribution of momenta (large σ_p).

A wave packet with large σ_p, however, is more delocalized in momentum, and therefore has a sharper initial spatial distribution.

8.10.1 Example 1. Momentum and position representation of a wave packet

Example 8.2. Consider a wave packet defined by

$$\psi(p) = \langle p \mid \psi \rangle = \begin{cases} 0, & p < -\dfrac{p_0}{2}, \\ N, & -\dfrac{p_0}{2} < p < \dfrac{p_0}{2}, \\ 0, & p > \dfrac{p_0}{2}. \end{cases}$$

(a) Determine a value for N such that $\langle \psi \mid \psi \rangle = 1$ using the momentum-space wave function directly.

We are given the momentum space representation of the state $|\psi\rangle$. We can therefore expand $|\psi\rangle$ in the momentum basis, and carry out the normalization.

$$\begin{aligned} \langle \psi \mid \psi \rangle &= \int_{-\infty}^{\infty} dp \, \langle \psi \mid p \rangle \langle p \mid \psi \rangle = \int_{-\infty}^{\infty} dp \, |\langle p \mid \psi \rangle|^2 \\ &= \int_{-p_0/2}^{p_0/2} N^2 \, dp = N^2 p_0 = 1 \end{aligned}$$

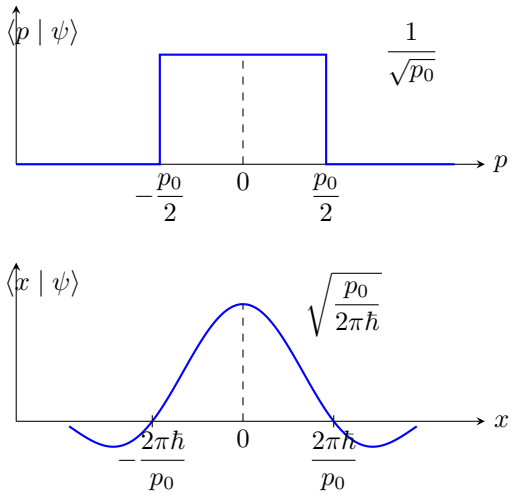
$$\boxed{N = \frac{1}{\sqrt{p_0}}}$$

(b) Determine $\psi(x) = \langle x \mid \psi \rangle$.

$$\begin{aligned} \langle x \mid \psi \rangle = \int_{-\infty}^{\infty} dp \, \langle x \mid p \rangle \langle p \mid \psi \rangle &= \frac{1}{\sqrt{p_0}} \frac{1}{\sqrt{2\pi\hbar}} \int_{-p_0/2}^{p_0/2} e^{ipx/\hbar} \, dp \\ &= \frac{1}{\sqrt{2\pi\hbar \, p_0}} \left(\frac{\hbar}{ix} \right) \left[e^{ipx/\hbar} \right]_{-p_0/2}^{p_0/2} \\ &= \frac{1}{\sqrt{2\pi\hbar \, p_0}} \left(\frac{2i\hbar}{ix} \right) \sin\left(\frac{p_0 x}{2\hbar} \right) = \sqrt{\frac{p_0}{2\pi\hbar}} \left(\frac{2\hbar}{p_0 x} \right) \sin\left(\frac{p_0 x}{2\hbar} \right) \end{aligned}$$

$$\boxed{\langle x \mid \psi \rangle = \sqrt{\frac{p_0}{2\pi\hbar}} \, \frac{\sin\left(\dfrac{p_0 x}{2\hbar} \right)}{\dfrac{p_0 x}{2\hbar}}}$$

(c) Sketch $\langle p \mid \psi \rangle$ and $\langle x \mid \psi \rangle$. *Estimate* Δp from $\langle p \mid \psi \rangle$ and Δx from $\langle x \mid \psi \rangle$; you do not have to calculate the uncertainties, only estimate them from the width of the distributions. Use these values to estimate $\Delta x \Delta p$. Show that your answer is independent of p_0.



Our uncertainty in momentum is given by the width of the momentum distribution $\Delta p = p_0$.

Note 8.11. We note the the functional form of $\langle x \mid \psi \rangle$ is a sinc function

$$\langle x \mid \psi \rangle \propto \frac{\sin(ax)}{ax} = \text{sinc}(ax).$$

We can estimate the uncertainty in position by either picking the full width at half max of the function, or picking the first zero of the function. The problem is only asking for an estimate of the uncertainty, so it isn't important how you estimate the width of the distribution.

I will estimate Δx from the first zeros of the function

$$\sin\left(\frac{p_0 x_0}{2\hbar}\right) = 0 \quad \Rightarrow \quad \frac{p_0 x_0}{2\hbar} = \pm\pi$$

$$\Delta x \approx 2x_0$$

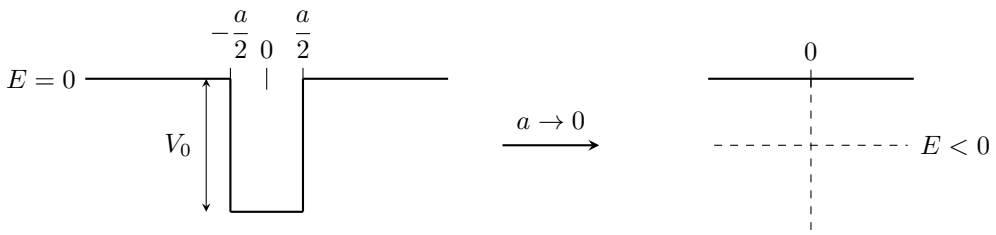
$$\boxed{\Delta p \Delta x \approx p_0 \frac{4\pi\hbar}{p_0} = 4\pi\hbar}$$

8.10.2 Example 2. Bound state of a delta function potential

An interesting limiting case of the finite square well is the case where the well depth approaches infinity but the width of the well goes to zero such that $V_0 a$ remains finite. Such a well may be represented by the potential energy satisfying

$$V(x) = -\frac{\hbar^2 \alpha}{2m}\,\delta(0)$$

where α is a constant with units of inverse length m^{-1}.



We wish to consider bound states of the delta function potential, i.e., the spectrum of energy eigenstates for which $E < 0$.

The potential is only non-zero at the point $x = 0$. Away from this point, we know that the solutions must be of the form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi(x) = -|E|\psi(x)$$

$$\frac{d^2\psi}{dx^2} = \frac{2m|E|}{\hbar^2}\psi(x) \tag{1}$$

$$\psi(x) = \begin{cases} Ae^{-\kappa x}, & x > 0, \\ Ae^{\kappa x}, & x < 0, \end{cases}$$

where

$$\kappa = \sqrt{\frac{2m|E|}{\hbar^2}}.$$

Comment 8.8. I have chosen constant multiplicative constant for the $x > 0$ and $x < 0$ solutions to be the same constant A to ensure that $\psi(x)$ is continuous at $x = 0$.

To determine the allowed values of κ, we need one more boundary condition for $\psi(x)$.

We have noted that for any finite potential, the first derivative of $\psi(x)$ must be continuous. However, the delta function potential is infinite at $x = 0$. Therefore, we expect

$$\left[\frac{d\psi}{dx}\right]_{x=0}$$

to be discontinuous.

To determine the discontinuity, we must integrate the time-independent Hamiltonian over an infinitesimal range $x \in [-\epsilon, \epsilon]$, on either side of the delta function.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \frac{\hbar^2\alpha}{2m}\delta(x)\psi(x) = E\psi(x)$$

$$\frac{d^2\psi}{dx^2} = -\left[\alpha\delta(x) + \frac{2mE}{\hbar^2}\right]\psi(x)$$

$$\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon}\frac{d^2\psi}{dx^2}\,dx = -\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon}\alpha\delta(x)\psi(x)\,dx - \lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon}\frac{2mE}{\hbar^2}\psi(x)\,dx$$

$$\lim_{\epsilon\to 0}\left\{\left[\frac{d\psi}{dx}\right]_{x=\epsilon} - \left[\frac{d\psi}{dx}\right]_{x=-\epsilon}\right\} = -\alpha\psi(0) - \lim_{\epsilon\to 0}\underbrace{\frac{2mE}{\hbar^2}\psi(0)(2\epsilon)}_{\to 0}$$

$$\lim_{\epsilon\to 0}\left\{\left[\frac{d\psi}{dx}\right]_{x=\epsilon}-\left[\frac{d\psi}{dx}\right]_{x=-\epsilon}\right\}=-\alpha\psi(0)$$

We apply the boundary condition above to the general solution:

$$\lim_{\epsilon\to 0}\left(-2A\kappa e^{\kappa\epsilon}\right)=-\alpha A$$

$$\boxed{\kappa=\frac{\alpha}{2}}$$

There is only a single bound state with energy (eq.(1)).

$$\boxed{|E|=\frac{\hbar^2\kappa^2}{2m}=\frac{\hbar^2\alpha^2}{8m}}$$

Normalization:

$$\int_{-\infty}^{\infty}|\psi(x)|^2\,dx=2\int_0^{\infty}A^2e^{-2\kappa x}\,dx=1$$

$$\frac{2A^2}{2\kappa}\left[e^{-2\kappa x}\right]_0^{\infty}=1$$

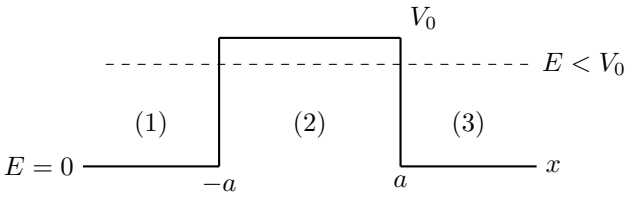
$$A=\sqrt{\kappa}=\sqrt{\frac{\alpha}{2}}$$

$$\boxed{\psi(x)=\sqrt{\frac{\alpha}{2}}\begin{cases}e^{-\alpha x/2}, & x>0,\\ e^{\alpha x/2}, & x<0.\end{cases}}$$

8.11 Tunneling

8.11.1 Tunneling Through a Step Potential

In this lecture, we will consider a free particle incident on a step potential shown below.



$$V(x)=\begin{cases}0, & x<-a,\\ V_0, & -a<x<a,\\ 0, & x>a.\end{cases}$$

The Schrödinger in the three regions is

$$\text{Regions 1 and 3:}\qquad \frac{d^2\phi_{1,3}}{dx^2}=-\frac{2mE}{\hbar^2}\phi_{1,3}(x)=-k^2\phi_{1,3}(x)$$

$$\text{Region 2:} \qquad \frac{d^2\phi_2}{dx^2} = \frac{2m(V_0 - E)}{\hbar^2}\phi_2(x) = \kappa^2\phi_2(x)$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}}, \qquad \kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

We will consider a particle traveling from the $+\hat{x}$ direction that is incident on the step potential. The solution to the differential equations for this case take the form

$$\phi_1(x) = Ae^{ikx} + Be^{-ikx}$$

$$\phi_2(x) = Ce^{\kappa x} + De^{-\kappa x}$$

$$\phi_3(x) = Fe^{ikx}$$

> **Comment 8.9.** As before, the boundary conditions must satisfy the continuity of $\phi(x)$ and $\frac{d\phi}{dx}$ at $x = \pm a$.

From the four equations we get by applying the boundary conditions, we find the following relationship for the reflection coefficient.

$$R = \left|\frac{B}{A}\right|^2 = \frac{1}{1 + \dfrac{4E(V_0 - E)}{V_0^2 \sinh^2\left(2a\sqrt{\dfrac{2m(V_0 - E)}{\hbar^2}}\right)}}, \qquad E < V_0$$

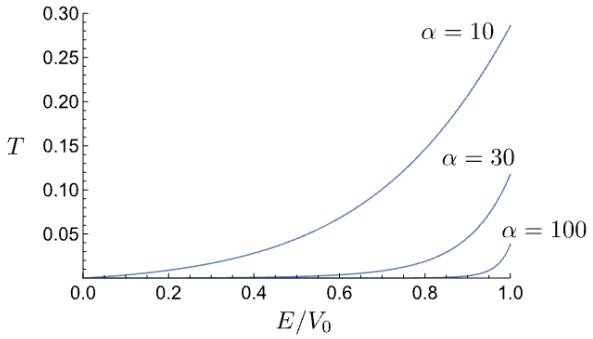
The transmission coefficient is

$$T = \left|\frac{F}{A}\right|^2 = 1 - R.$$

We can express T in dimensionless energy units $\epsilon = \dfrac{E}{V_0}$. Then

$$T = \frac{1}{1 + \dfrac{1}{4\epsilon(1-\epsilon)} \sinh^2\left(2a\sqrt{\frac{2mV_0(1-\epsilon)}{\hbar^2}}\right)}.$$

Let's plot T vs. ϵ for the case where $\alpha := \frac{8ma^2V_0}{\hbar^2} \gg 1$.



We see that as E approaches V_0, T increases exponentially.

8.11.2 Scanning Tunneling Microscopy

We would like to evaluate T in the limit $E \lesssim V_0$.

$$\epsilon = 1 - \delta\epsilon \quad \text{with } \delta\epsilon \ll 1$$

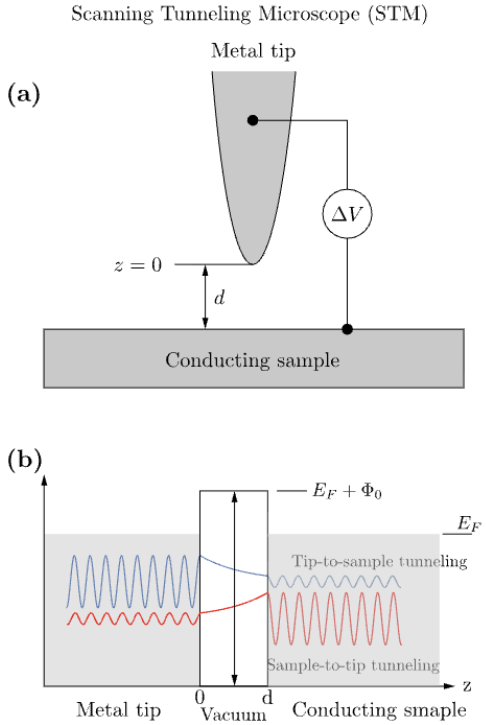
$$\begin{aligned} T \approx \frac{4\delta\epsilon}{\sinh\left(\sqrt{\alpha\delta\epsilon}\right)^2} &= \frac{4\delta\epsilon}{\left(\frac{1}{2}\left(e^{\sqrt{\alpha\delta\epsilon}} - e^{-\sqrt{\alpha\delta\epsilon}}\right)\right)^2} \\ &\approx \frac{16\delta\epsilon}{e^{2\sqrt{\alpha\delta\epsilon}}} \\ &\approx 16\delta\epsilon\, e^{-2\sqrt{\alpha\delta\epsilon}} = 16\delta\epsilon\, \exp\left(-2a\sqrt{\frac{2mV_0\delta\epsilon}{\hbar^2}}\right) \end{aligned}$$

We see that for energies near but below V_0, the tunneling probability varies exponentially with the width $2a$ of the barrier, and the height V_0.

Quantum mechanical tunneling is important in many process, including molecular bonding, nuclear fusion, and integrated circuits.

The tunneling phenomenon is also used as a tool for imaging the surface of materials with atomic resolution.

Discovery 8.7. Scanning Tunneling Microscopy (STM) relies on the exponential dependence of the tunneling probability on the width and height of the energy barrier.



To a very good approximation, electrons inside a metal behave as free particles. They are bound to the metal with energy Φ_0, also referred to as the work function.

We can think of Φ_0 as the work done on an electron to remove it from the metal. Inside the metal tip and surface, electrons travel as free particles

$$\psi_{\text{metal}}(z) \sim e^{\pm ikz}, \qquad k = \sqrt{\frac{2mE_F}{\hbar^2}}$$

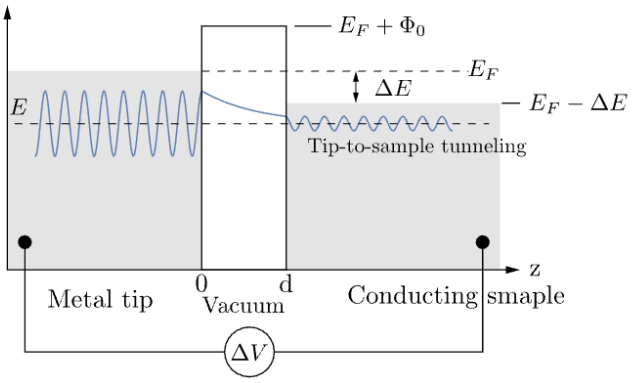
E_F is the Fermi energy, which is the energy of electrons inside the metal. Inside the gap

$$\psi_{\text{gap}}(z) \sim e^{-\kappa z}, \qquad \kappa = \sqrt{\frac{2m\Phi_0}{\hbar^2}}$$

In the absence of an applied potential ΔV between the tip and surface, the probability of an electron to tunnel from the tip to the surface is

$$P \propto |\psi(0)|^2 e^{-2\kappa d}.$$

If the electron energy in the tip and surface is the same, then the probability of tunneling in either direction is the same. Hence, on average, equal number of electrons tunnel from the tip-to-surface as from the surface-to-tip. Thus, the net tunneling current is zero.



By applying a small voltage difference ΔV between the tip and surface, we can increase the energy of electrons in the tip by an amount

$$\Delta E = e\Delta V$$

relative to the electrons in the sample.

This increases the probability for electrons to tunnel from the tip-to-surface relative to the tunneling from the surface-to-tip, and produces a net tunneling current.

9 Quantum Harmonic Oscillator

In this chapter, we will solve for the energy spectrum of the quantum harmonic oscillator (QHO).

Lecture 21 - Tuesday, March 31

If you recall from classical mechanics, we encounter the harmonic oscillator potential in system that have a linear restoring force.

An example is Hooke's law, which states that the restoring force is proportional to the displacement x of a mass m away from its equilibrium position. The constant of proportionality k is called the spring constant. The negative sign signifies that the force is in the opposite direction to the displacement, ensuring that the force returns the mass to its equilibrium position

$$F_{\text{restoring}} = -kx = -\frac{\mathrm{d}V}{\mathrm{d}x}$$

Because the restoring force is conservative, we can express the potential energy as

$$V(x) = \frac{1}{2}kx^2$$

More often, the potential energy is expressed in terms of the mass and oscillation frequency of the harmonic oscillator

$$V(x) = \frac{1}{2}m\omega^2 x^2$$

where $\omega = \sqrt{\frac{k}{m}}$ is the frequency of oscillation.

The harmonic potential applies to many quantum systems. For example, the restoring force between two atoms that form a diatomic molecule is well approximated by Hooke's Law, for small displacement of the atoms away from equilibrium. Likewise, atoms in solids can be thought of as little masses coupled together by a network of springs.

9.1 The Quantum Harmonic Oscillator

Unlike a classical harmonic oscillator which can have any energy, we will see that a QHO has a discrete spectrum of allowed energies. Importantly, we will find that the minimum energy of a QHO is not zero, which is a consequence of the uncertainty principle.

The Hamiltonian for the QHO is

$$\mathcal{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \tag{1}$$

To solve for the eigenfunctions and energy spectrum, we can either solve the differential equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi(x) = E\psi(x)$$

which can be done using special functions, or there is another way that involves the complex factoring of $\mathcal{H}$ and introducing two new operators.

Comment 9.1. Here, we will use the complex factoring approach.

We notice that the Hamiltonian has a special form. Namely, it is quadratic in both $\hat{p}$ and $\hat{x}$. We can factor $\mathcal{H}$ into the product of two terms as follows:

$$\mathcal{H} = \frac{1}{2}m\omega^2\left(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2}\right)$$

Consider the following factorization:

$$\begin{aligned}\frac{1}{2}m\omega^2\left(\hat{x} - \frac{i\hat{p}}{m\omega}\right)\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right) &= \frac{1}{2}m\omega^2\left(\hat{x}^2 + \frac{i}{m\omega}\underbrace{[\hat{x}\hat{p} - \hat{p}\hat{x}]}_{[\hat{x},\hat{p}]=i\hbar} + \frac{\hat{p}^2}{m^2\omega^2}\right)\\ &= \frac{1}{2}m\omega^2\left(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2}\right) - \frac{\hbar\omega}{2} = \mathcal{H} - \frac{\hbar\omega}{2}\end{aligned}$$

Hence we obtain that

$$\mathcal{H} = \frac{1}{2}m\omega^2\left(\hat{x} - \frac{i\hat{p}}{m\omega}\right)\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right) + \frac{\hbar\omega}{2}$$

Let

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right) \tag{2}$$

We note that $\hat{x}$ and $\hat{p}$ are Hermitian operators, therefore $\hat{x} = \hat{x}^\dagger$, $\hat{p} = \hat{p}^\dagger$, and

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i\hat{p}}{m\omega}\right) \tag{3}$$

We can express $\mathcal{H}$ in terms of the operators $\hat{a}$ and $\hat{a}^\dagger$.

$$\boxed{\mathcal{H} = \hbar\omega\,\hat{a}^\dagger\hat{a} + \frac{1}{2}\hbar\omega} \tag{4}$$

Let's analyze the commutator algebra of the operators $\hat{a}^\dagger$ and $\hat{a}$.

$$\begin{aligned}[\hat{a}, \hat{a}^\dagger] &= \frac{m\omega}{2\hbar}\left[\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right), \left(\hat{x} - \frac{i\hat{p}}{m\omega}\right)\right]\\ &= \frac{m\omega}{2\hbar}\left(\underbrace{[\hat{x}, \hat{x}]}_{=0} - \frac{i}{m\omega}\underbrace{[\hat{x}, \hat{p}]}_{i\hbar} + \frac{i}{m\omega}\underbrace{[\hat{p}, \hat{x}]}_{-i\hbar} + \frac{1}{m^2\omega^2}\underbrace{[\hat{p}, \hat{p}]}_{=0}\right)\\ &= 1\end{aligned}$$

Hence we obtain that

$$\boxed{[\hat{a}, \hat{a}^\dagger] = 1} \tag{5}$$

In particular,

$$\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = 1$$

Consider the action of $\hat{a}$ and $\hat{a}^\dagger$ on an energy eigenstate:

$$\mathcal{H}\,|E\rangle = E\,|E\rangle$$

Let's calculate the energy corresponding to the state $\hat{a}\,|E\rangle$.

$$\mathcal{H}(\hat{a}\,|E\rangle) = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\hat{a}\,|E\rangle$$

Using eq. (5), we can express $\hat{a}^\dagger\hat{a} = \hat{a}\hat{a}^\dagger - 1$.

$$\begin{aligned}
\Rightarrow \quad \mathcal{H}(\hat{a}\,|E\rangle) &= \hbar\omega\left(\hat{a}\hat{a}^\dagger - 1 + \frac{1}{2}\right)\hat{a}\,|E\rangle \\
&= \hbar\omega\,\hat{a}\left(\hat{a}^\dagger\hat{a} - \frac{1}{2}\right)|E\rangle \qquad \text{(factoring } \hat{a} \text{ to the left.)} \\
&= \hat{a}(\mathcal{H} - \hbar\omega)\,|E\rangle \\
&= (E - \hbar\omega)\hat{a}\,|E\rangle
\end{aligned}$$

We see that the action of $\hat{a}$ on $|E\rangle$ produces a state that has an energy that is lower by $\hbar\omega$.

Definition 9.1. **[Lowering Operator]**

The operator $\hat{a}$ is called the lowering operator.

Let's consider the action of $\hat{a}^\dagger$ on the state $|E\rangle$.

$$\begin{aligned}
\mathcal{H}(\hat{a}^\dagger\,|E\rangle) &= \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\hat{a}^\dagger\,|E\rangle \\
&= \hbar\omega\,\hat{a}^\dagger\left(\hat{a}\hat{a}^\dagger + \frac{1}{2}\right)|E\rangle \qquad \text{(factoring } \hat{a}^\dagger \text{ to the left.)}
\end{aligned}$$

Using eq. (5), we express $\hat{a}\hat{a}^\dagger = \hat{a}^\dagger\hat{a} + 1$.

$$\begin{aligned}
\Rightarrow \quad \mathcal{H}(\hat{a}^\dagger\,|E\rangle) &= \hbar\omega\,\hat{a}^\dagger\left(\hat{a}^\dagger\hat{a} + \frac{3}{2}\right)|E\rangle \\
&= \hat{a}^\dagger(\mathcal{H} + \hbar\omega)\,|E\rangle \\
&= (E + \hbar\omega)\hat{a}^\dagger\,|E\rangle
\end{aligned}$$

We see that the action of $\hat{a}^\dagger$ on $|E\rangle$ produces a state that has an energy that is higher by $\hbar\omega$.

Definition 9.2. **[Raising Operator]**

The operator $\hat{a}^\dagger$ is called the raising operator.

9.2 The Energy Spectrum of the QHO

Note 9.1. There exists a minimum energy state of the QHO, which we refer to as the ground state $|E_0\rangle$.

While we do not yet know the energy E_0, it is reasonable to enforce the condition:

$$\hat{a}\,|E_0\rangle = 0 \tag{6}$$

This condition states that if we apply the lowering operator on the ground state, it returns zero because, by definition, there are no states with energy lower than E_0.
We can use eq. (6) to find the ground state energy.

$$\begin{aligned}\mathcal{H}\,|E_0\rangle &= \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)|E_0\rangle \\ &= \hbar\omega\,\hat{a}^\dagger\underbrace{\hat{a}\,|E_0\rangle}_{=0} + \frac{1}{2}\hbar\omega\,|E_0\rangle\end{aligned}$$

hence

$$\boxed{\mathcal{H}\,|E_0\rangle = \frac{1}{2}\hbar\omega\,|E_0\rangle} \tag{7}$$

Theorem 9.1.

The minimum energy of a QHO is $\frac{1}{2}\hbar\omega$.

Comment 9.2. Our goal now is to find the energy spectrum of the QHO.

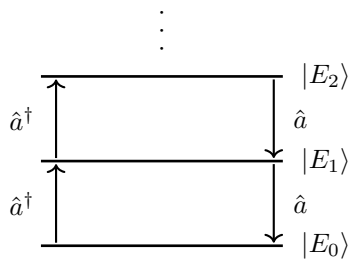
Suppose the QHO is in a state with energy E: $|E\rangle$. We can produce a state of lower energy by applying the lowering operator to $|E\rangle$.

$$\hat{a}\,|E\rangle = \text{const.}\;|E - \hbar\omega\rangle$$

We don't yet know the constant that multiplies the state $|E - \hbar\omega\rangle$.

If we repeatedly apply the lowering operator to $|E\rangle$, we will ultimately reach the ground state $|E_0\rangle$.

Because we lower the energy in units of $\hbar\omega$, it must be true that the energy spectrum is quantized in units of $\hbar\omega$, starting from a ground state energy of $\frac{1}{2}\hbar\omega$.



The energy spectrum of the QHO is

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \qquad n = 0, 1, 2, \cdots \tag{8}$$

We label the energy eigenstates with the index n.

$$\mathcal{H}\,|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle \tag{9}$$

By expressing eq. (9) in terms of the Hamiltonian, we discover a useful identity

$$\hbar\omega\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)|n\rangle=\hbar\omega\left(n+\frac{1}{2}\right)|n\rangle$$

Notice that the operator $\hat{a}^\dagger\hat{a}=n$. We define the number operator

$$\hat{N}:=\hat{a}^\dagger\hat{a} \tag{10}$$

which counts the number of quanta of excitation n in the QHO.

$$\mathcal{H}|n\rangle=\hbar\omega\left(\hat{N}+\frac{1}{2}\right)|n\rangle \tag{11}$$

9.3 Approach to Solving for Eigenfunctions

In this lecture, we will derive the eigenfunctions of the QHO. To do this, we will again be using the raising and lowering operators $\hat{a}$ and $\hat{a}^\dagger$.

We first need to determine the constant factors c and c'.

$$\hat{a}|n\rangle=c|n-1\rangle$$

$$\hat{a}^\dagger|n\rangle=c'|n+1\rangle$$

Recall that the number operator $\hat{N}=\hat{a}^\dagger\hat{a}$, with

$$\hat{N}|n\rangle=n|n\rangle$$

Consider

$$\langle n|\hat{a}^\dagger\hat{a}|n\rangle=n=(\hat{a}|n\rangle)^\dagger\hat{a}|n\rangle$$

Hence

$$(c|n-1\rangle)^\dagger c|n-1\rangle=|c|^2\langle n-1|n-1\rangle=n$$

This implies that

$$|c|^2=n$$

which gives us that

$$\boxed{|c|=\sqrt{n}}$$

In order to evaluate c', we note

$$\langle n|\hat{a}^\dagger\hat{a}|n\rangle=n$$

and

$$\boxed{\hat{a}^\dagger\hat{a}=\hat{a}\hat{a}^\dagger-1}$$

so

$$\langle n|\hat{a}\hat{a}^\dagger-1|n\rangle=n\qquad\Rightarrow\qquad(\hat{a}^\dagger|n\rangle)^\dagger\hat{a}^\dagger|n\rangle=n+1$$

$$(c'|n+1\rangle)^\dagger c'|n+1\rangle=n+1$$

$$|c'|^2\langle n+1|n+1\rangle = n+1$$

$$|c'|^2 = n+1$$

$$\boxed{|c'| = \sqrt{n+1}}$$

We will drop overall phase factors that multiply c and c'.

$$\hat{a}\,|n\rangle = \sqrt{n}\;|n-1\rangle \tag{1}$$

$$\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\;|n+1\rangle \tag{2}$$

9.3.1 Solving for the Ground State Wavefunction

We will use the position representation of the raising and lowering operators to find the energy eigenfunctions, starting from the ground state.

$$\hat{a}\,|0\rangle = 0$$

From

$$\hat{a}\,|0\rangle = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right)|0\rangle = 0,$$

we obtain the ground-state wavefunction in the position basis. Writing $\phi_0(x) := \langle x \mid 0\rangle$, we have

$$\begin{aligned} 0 &= \left\langle x\middle|\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right)\middle|0\right\rangle \\ &= \left(x + \frac{\hbar}{m\omega}\frac{d}{dx}\right)\phi_0(x). \end{aligned}$$

Hence

$$\begin{aligned} \frac{d\phi_0}{dx} &= -\frac{m\omega}{\hbar}\,x\,\phi_0(x), \\ \phi_0(x) &= \text{const.}\,e^{-\alpha x^2}, \\ \frac{d\phi_0}{dx} &= -2\alpha x\,\phi_0(x) = -\frac{m\omega}{\hbar}\,x\,\phi_0(x), \end{aligned}$$

so

$$\boxed{\alpha = \frac{m\omega}{2\hbar}}.$$

Therefore

$$\phi_0(x) = \text{const.}\,\exp\left(-\frac{m\omega x^2}{2\hbar}\right).$$

Normalization gives

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} |\phi_0(x)|^2\,dx \\ &= |\text{const.}|^2 \int_{-\infty}^{\infty} \exp\left(-\frac{m\omega x^2}{\hbar}\right)\,dx. \end{aligned}$$

Using

$$\int_{-\infty}^{\infty} e^{-\gamma x^2}\, dx = \sqrt{\frac{\pi}{\gamma}}, \qquad \Re(\gamma) > 0,$$

we get

$$|\text{const.}|^2 \sqrt{\frac{\pi\hbar}{m\omega}} = 1.$$

Thus

$$\boxed{\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar}\right)}.$$

We can find the wavefunction corresponding to the nth eigenstate by repeatedly applying $\hat{a}^\dagger$ on $|0\rangle$. In particular,

$$\hat{a}^\dagger |n-1\rangle = \sqrt{n}\, |n\rangle\,,$$
$$|n\rangle = \frac{1}{\sqrt{n}}\, \hat{a}^\dagger |n-1\rangle\,.$$

Example 9.1. For example, by applying the raising operator repeatedly, we obtain

$$\begin{aligned} |3\rangle &= \frac{1}{\sqrt{3}}\, \hat{a}^\dagger |2\rangle \\ &= \frac{1}{\sqrt{3}}\, \hat{a}^\dagger \left(\frac{1}{\sqrt{2}}\, \hat{a}^\dagger |1\rangle\right) \\ &= \frac{1}{\sqrt{3\cdot 2\cdot 1}}\, (\hat{a}^\dagger)^3 |0\rangle \\ &= \frac{1}{\sqrt{3!}}\, (\hat{a}^\dagger)^3 |0\rangle\,. \end{aligned}$$

This suggests the general formula

$$|n\rangle = \frac{1}{\sqrt{n!}}\, (\hat{a}^\dagger)^n |0\rangle\,.$$

Passing to the position representation, we therefore obtain

$$\boxed{\phi_n(x) = \frac{1}{\sqrt{n!}} \left[\sqrt{\frac{m\omega}{2\hbar}} \left(x - \frac{\hbar}{m\omega}\frac{d}{dx}\right)\right]^n \phi_0(x)}$$

We define the dimensionless quantity

$$\xi := \sqrt{\frac{m\omega}{\hbar}}\, x.$$

The general form of the solution to eq. (3) is

$$\phi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}}\, H_n(\xi) e^{-\xi^2/2},$$

where $H_n(\xi)$ are Hermite polynomials. The first few Hermite polynomials are

$$
\begin{aligned}
H_0(\xi) &= 1, \\
H_1(\xi) &= 2\xi, \\
H_2(\xi) &= 4\xi^2 - 2, \\
H_3(\xi) &= 8\xi^3 - 12\xi, \\
H_4(\xi) &= 16\xi^4 - 48\xi^2 + 12, \\
&\vdots
\end{aligned}
$$

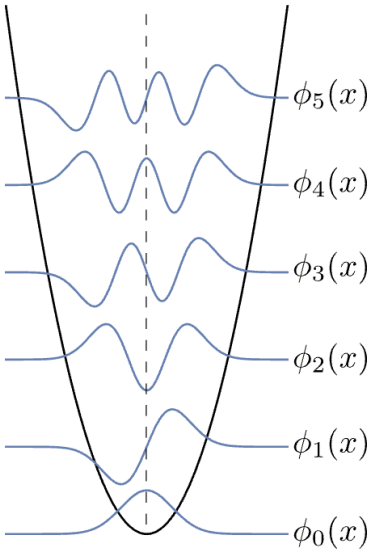


Figure: QHO Eigenfunctions

9.3.2 Position & Momentum Uncertainty Relationship for a QHO

Let's calculate the uncertainty in the position and momentum for the different energy eigenstates. The uncertainty relation states

$$\Delta p\, \Delta x \geq \frac{1}{2} \left| \langle [\hat{x}, \hat{p}] \rangle \right| \tag{5}$$

$$\Delta p\, \Delta x \geq \frac{\hbar}{2}. \tag{6}$$

where

$$\Delta p = \sqrt{\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2}, \qquad \Delta x = \sqrt{\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2},$$

and

$$[\hat{x}, \hat{p}] = i\hbar.$$

We will first express $\hat{x}$ and $\hat{p}$ in terms of $\hat{a}$ and $\hat{a}^\dagger$, then use these expressions to evaluate the expectation values in Δp and Δx. The expectation values will be evaluated for an arbitrary state $|n\rangle$.

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right) \tag{7}$$

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i\hat{p}}{m\omega}\right) \tag{8}$$

We can express $\hat{x}$ and $\hat{p}$ as linear combinations of $\hat{a}$ and $\hat{a}^\dagger$:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\,(\hat{a} + \hat{a}^\dagger) \tag{9}$$

$$\hat{p} = i\sqrt{\frac{m\hbar\omega}{2}}\,(\hat{a}^\dagger - \hat{a}). \tag{10}$$

In evaluating the expectation values, we utilize the orthogonality of the energy eigenstates:

$$\langle n|m\rangle = \delta_{nm}.$$

Hence

$$\begin{aligned}\langle n|\hat{x}|n\rangle &\propto \langle n|(\hat{a} + \hat{a}^\dagger)|n\rangle \\ &\propto \langle n|n-1\rangle + \langle n|n+1\rangle \\ &= 0.\end{aligned}$$

Likewise,

$$\langle n|\hat{p}|n\rangle = 0.$$

Now compute $\langle n|\hat{x}^2|n\rangle$:

$$\begin{aligned}\langle n|\hat{x}^2|n\rangle &= \left(\frac{\hbar}{2m\omega}\right)\langle n\big|\hat{a}^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + (\hat{a}^\dagger)^2\big|n\rangle \\ &= \left(\frac{\hbar}{2m\omega}\right)\left((\sqrt{n+1})^2 + n\right) \\ &= \left(\frac{\hbar}{m\omega}\right)\left(n + \frac{1}{2}\right).\end{aligned}$$

Similarly,

$$\begin{aligned}\langle n|\hat{p}^2|n\rangle &= -\left(\frac{m\hbar\omega}{2}\right)\langle n\big|(\hat{a}^\dagger)^2 - \hat{a}^\dagger\hat{a} - \hat{a}\hat{a}^\dagger + \hat{a}^2\big|n\rangle \\ &= \left(\frac{m\hbar\omega}{2}\right)\left(n + (\sqrt{n+1})^2\right) \\ &= m\hbar\omega\left(n + \frac{1}{2}\right).\end{aligned}$$

Therefore,

$$\Delta p = \sqrt{\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2} = \sqrt{m\hbar\omega \left(n + \frac{1}{2} \right)},$$
$$\Delta x = \sqrt{\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2} = \sqrt{\left(\frac{\hbar}{m\omega} \right) \left(n + \frac{1}{2} \right)}.$$

Thus,

$$\Delta p \, \Delta x = \hbar \left(n + \frac{1}{2} \right).$$

The minimum uncertainty allowed by the uncertainty principle is

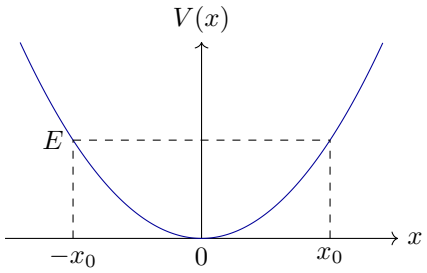
$$\Delta p \, \Delta x = \frac{\hbar}{2}.$$

The minimum uncertainty is realized only for the ground state. All other states have larger uncertainty.

9.4 Quantum vs. Classical

9.4.1 Classical Harmonic Oscillator

Let's compare the behavior of the QHO to the classical HO.



The total energy of the oscillator is the sum of the kinetic and potential energy.

$$E = \frac{1}{2} m \dot{x}^{\,2} + \frac{1}{2} m\omega^2 x^2(t)$$

Let the position and velocity of the particle at time t be given by

$$x(t) = x_0 \cos(\omega t),$$
$$\dot{x}(t) = -x_0 \omega \sin(\omega t),$$

where x_0 is the peak oscillation amplitude. At times

$$t_0 = \frac{n\pi}{\omega}, \qquad n \in \mathbb{Z},$$

the velocity of the oscillator is zero $\big(\dot{x}(t_0) = 0\big)$, and the energy of the oscillator is stored as potential energy.

$$E = \frac{1}{2} m\omega^2 x_0^2$$

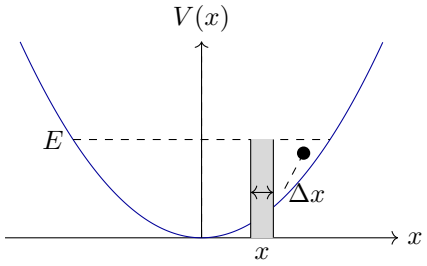
The positions $x = \pm x_0$ are the classical turning points.

$$x_0 = \pm\sqrt{\frac{2E}{m\omega^2}}$$

9.4.2 Classical Probability Density

Let ΔP be the probability of finding the particle in an interval Δx centered at position x.

To calculate this probability, we simply need to calculate the fraction of the time per half cycle that the particle spends in an interval Δx about some position x.



The amount of time that the particle spends passing through the region Δx in one-half cycle is

$$\Delta t = \frac{\Delta x}{|\dot{x}|} = \frac{\Delta x}{x_0\omega|\sin(\omega t)|}.$$

In terms of the particle's position, we can express

$$|\sin(\omega t)| = \sqrt{1 - \frac{x^2(t)}{x_0^2}},$$
$$\Delta t = \frac{\Delta x}{\omega\sqrt{x_0^2 - x^2(t)}}.$$

The probability of observing the particle at location x is

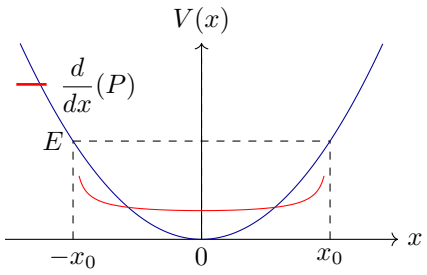
$$\Delta P = \frac{\Delta t}{T/2}, \qquad \text{where } T = \frac{2\pi}{\omega}.$$

Hence the classical probability density is

$$\frac{\Delta P}{\Delta x} \to \frac{d}{dx}(P) = \frac{1}{\pi\sqrt{x_0^2 - x^2}}.$$

The classical probability density is normalized:

$$\int_{-x_0}^{x_0} \frac{1}{\pi\sqrt{x_0^2 - x^2}}\, dx = 1.$$



Near the classical turning points, the velocity of the particle approaches zero. Therefore, the amount of time spent by the oscillator in a region Δx around $x = \pm x_0$ is the highest anywhere on its trajectory, which corresponds to the high probability density at these locations. The probability density near $x = 0$ is the lowest since here it is moving the fastest.

9.4.3 Correspondence Between Classical and Quantum Probability Densities

For the QHO, the probability density corresponding to the n^{th} eigenstate is

$$P_n = |\phi_n(x)|^2.$$

Notice that the ground state probability density $|\phi_0(x)|^2$ is peaked at $x = 0$, which is exactly the opposite of the classical harmonic oscillator.

This behavior is directly related to the uncertainty principle, which prevents the particle from having zero energy.

As the quantum number n increases, P_n behaves more and more like the classical distribution—both are peaked near the classical turning points.

In the large n limit, the quantum and classical oscillators behave essentially identically.

For example, although the spacing between adjacent quantum energy levels is always

$$E_{n+1} - E_n = \hbar\omega,$$

the total energy of the n^{th} state is

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right).$$

Hence the relative spacing between neighboring energy levels is

$$\frac{E_{n+1} - E_n}{E_n} = \frac{\hbar\omega}{\hbar\omega\left(n + \frac{1}{2}\right)} = \frac{1}{n + \frac{1}{2}}.$$

As $n \to \infty$, this ratio tends to 0. Thus, for very large quantum numbers, adjacent energy levels become extremely close compared to the total energy, so the discrete quantum spectrum appears almost continuous.

This is an example of the correspondence principle, introduced by Niels Bohr, which states that the predictions of quantum mechanics should agree with those of classical physics in regimes where classical physics is valid.

For $n = 10^5$, the states $|n\rangle$ and $|n+1\rangle$ look essentially the same, so quantization effects are virtually impossible to observe.

10 Tutorials

10.1 Tutorial 1 — Review of Linear Algebra

Tutorial 1 - Monday, January 12

Question Consider the matrices given below:

$$M_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad M_2 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}, \quad M_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \quad M_4 = \begin{pmatrix} i & 1 \\ 0 & 0 \end{pmatrix}$$

1. Diagonalize the above matrices by finding their eigenvalues and (normalized) eigenvectors. If your matrix is real, check if the calculated eigenvalues and eigenvectors are consistent with the geometric interpretation of the matrix as a linear map on $\mathbb{R}^2$.

2. Find the inner product between the eigenvectors of each matrix, and also determine whether $M^\dagger M = MM^\dagger$ for each of them. What do you find?

Quiz We define

$$v = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad u = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{i\theta} \end{pmatrix}$$

Find $|\langle v|u\rangle|^2$.

Proof. We first compute

$$\langle v|u\rangle = \frac{1}{2}(1 + e^{i\theta}) = \frac{1}{2}(1 + \cos\theta + i\sin\theta)$$

and now we can compute

$$\begin{aligned} |\langle v|u\rangle|^2 &= \left|\frac{1}{2}(1 + \cos\theta + i\sin\theta)\right|^2 \\ &= \frac{1}{4}[(1 + \cos\theta)^2 + (\sin\theta)^2] \\ &= \frac{1}{4}(2 + 2\cos\theta) \\ &= \cos^2\left(\frac{\theta}{2}\right) \end{aligned}$$

as desired. □

10.2 Tutorial 2

Tutorial 2 - Monday, January 19

Consider a spin-$\frac{1}{2}$ particle whose spin is *down* along the direction specified by the unit vector

$$\hat{\mathbf{n}} = \cos\varphi \, \sin\theta \, \hat{\mathbf{x}} + \sin\varphi \, \sin\theta \, \hat{\mathbf{y}} + \cos\theta \, \hat{\mathbf{z}}, \tag{1}$$

where (θ, φ) are the usual spherical angles (see Fig. 1). Equivalently, the state is an eigenstate of $\hat{\mathbf{n}} \cdot \mathbf{S}$ with eigenvalue $-\hbar/2$, so a measurement of $\hat{\mathbf{n}} \cdot \mathbf{S}$ returns $-\hbar/2$ with probability 1.

Note 10.1. We use

$$\hat{\mathbf{n}} \cdot \mathbf{S} = n_x S_x + n_y S_y + n_z S_z.$$

(a) Show that the particle's state vector can be written as

$$|-\rangle_{\hat{\mathbf{n}}} = \sin\left(\frac{\theta}{2}\right) |+\rangle - e^{i\varphi} \cos\left(\frac{\theta}{2}\right) |-\rangle \, . \tag{2}$$

In other words, calculate the eigenvector of $\hat{\mathbf{n}} \cdot \mathbf{S}$ corresponding to the eigenvalue $\frac{-\hbar}{2}$.

Hint. Recall that, in the S_z eigenbasis, we have the matrix representations

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

(b) What outcomes are possible when measuring S_z? For each outcome, compute its probability in the state $|-\rangle_{\hat{\mathbf{n}}}$. Sketch (or plot) these probabilities as functions of θ.

(c) Give a qualitative reason the probabilities in part (b) do not depend on φ.

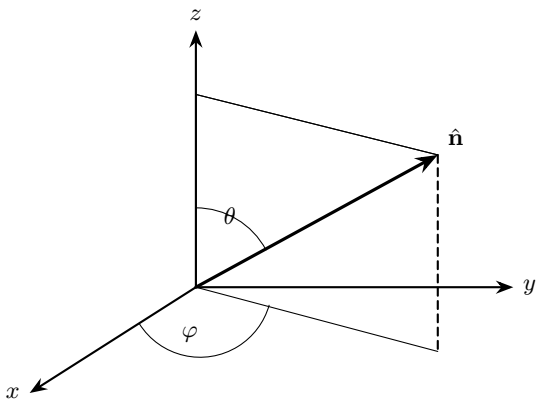


Figure 8: Direction of the spin in spherical coordinates.

Proof. For part (a). We first compute

$$\begin{aligned}\hat{\mathbf{n}} \cdot \mathbf{S} &= \cos\varphi \sin\theta \cdot \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \sin\varphi \sin\theta \cdot \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \cos\theta \cdot \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ &= \frac{\hbar}{2}\begin{pmatrix} \cos\theta & \cos\varphi\sin\theta - i\sin\varphi\sin\theta \\ \cos\varphi\sin\theta + i\sin\varphi\sin\theta & -\cos\theta \end{pmatrix}\end{aligned}$$

To find the eigenvector corresponding to eigenvalue $-\frac{\hbar}{2}$, we solve for x and y in the following equation:

$$(\hat{\mathbf{n}} \cdot \mathbf{S} + I)\begin{pmatrix} x \\ y \end{pmatrix} = 0$$

which is equivalent to solving

$$\begin{cases} (\cos\theta + 1)x + \sin\theta e^{-i\varphi} y & = 0 \\ \sin\theta e^{i\varphi} x + (-\cos\theta + 1)y & = 0 \end{cases}$$

One solution could be $x = -\cos\theta + 1$ and $y = -\sin\theta e^{i\varphi}$. Recall that we know

$$\begin{aligned} 1 - 2\sin^2\left(\frac{\theta}{2}\right) &= \cos\theta \\ 2\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right) &= \sin\theta \end{aligned}$$

Hence we can rewrite x and y:

$$\begin{aligned} x &= 2\sin^2\left(\frac{\theta}{2}\right) \\ y &= -2\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right)e^{i\varphi} \end{aligned}$$

Cancelling out $2\sin\frac{\theta}{2}$ in both x and y we obtain:

$$x = \sin\left(\frac{\theta}{2}\right), \qquad y = -\cos\left(\frac{\theta}{2}\right)e^{i\varphi}$$

as desired. □

Comment 10.1. Let the particle be in the state $|-\rangle_{\hat{\mathbf{n}}}$ (Eq. (2)). Let $\hat{\mathbf{n}}_{\text{perp}}$ be any unit vector orthogonal to $\hat{\mathbf{n}}$. Before computing anything, what do you expect for the probabilities of measuring $\hat{\mathbf{n}}_{\text{perp}} \cdot \mathbf{S} = \pm\hbar/2$? Then verify your expectation by calculation.

10.3 Tutorial 3

Tutorial 3 - Monday, February 2

Question Consider a spin-1/2 system. The operator A has a matrix representation

$$A = \begin{pmatrix} 1 & 2i \\ c & 1 \end{pmatrix}$$

in the S_z eigenbasis.

1. Find the constant c such that A can represent a physical observable. Use this constant for all subsequent questions.
2. What are the possible measurement outcomes of A?
3. Find the matrix representation of A in the S_y eigenbasis.
4. If the system is in the $|+\rangle_y$ state, what is the probability distribution for the measurement outcomes of A.
5. Find the expectation value of A for both the $|+\rangle$ and $|+\rangle_y$ states.
6. Find the standard deviation (uncertainty) of A for the $|+\rangle_y$ state.

Hint: Recall that the S_y eigenstates are $|\pm\rangle_y = (|+\rangle \pm i\,|-\rangle)/\sqrt{2}$.

> **Note 10.2.** Something to think about: Suppose a spin-1/2 particle is in the $\dot{\mathbf{n}} \cdot \mathbf{S}$ eigenstate $|+\rangle_{\dot{\mathbf{n}}}$. Show that the probability of a measurement of $\dot{\mathbf{n}}' \cdot \mathbf{S}$ yielding $\hbar/2$ is $\cos^2(\alpha/2)$ where α is the angle between the two vectors $\dot{\mathbf{n}}$ and $\dot{\mathbf{n}}'$.

Hint: A clever choice of basis will make the algebra a lot less tedious.

Quiz Let $|\pm\rangle$ denote the S_x eigenstates for a spin-1/2 particle. Given the vector

$$|\psi\rangle = \frac{e^{i\theta}}{\sqrt{2}}(|+\rangle + e^{i\varphi}\,|-\rangle), \qquad \theta, \varphi \in \mathbb{R}$$

For each of the following, identify whether it is true or false. Justify your answer.

1. $|\psi\rangle$ is not a physically-valid state since it is not normalized;
2. For arbitrary φ, $|\psi\rangle$ is an eigenstate of the S_x operator;
3. The probability of measuring different values of S_x is independent of θ.

Proof. (1) is false, because ψ is normalized:

$$\begin{aligned}\langle\psi|\psi\rangle &= \frac{e^{-i\theta}}{\sqrt{2}}(\langle+| + e^{-i\varphi}\langle-|)\frac{e^{i\theta}}{\sqrt{2}}(|+\rangle + e^{i\varphi}|-\rangle)\\ &= \frac{1}{2}(\langle+|+\rangle + \langle-|-\rangle)\\ &= 1\end{aligned}$$

For (2), it is also false because the eigenvalues correspond to $|+\rangle$ and $|-\rangle$ are different. The third statement is correct:

$$\begin{aligned}P(+) &= |\langle+|\psi\rangle|^2 & P(-) &= |\langle-|\psi\rangle|^2\\ &= \left|\frac{e^{i\theta}}{\sqrt{2}}\right|^2 & &= \left|\frac{e^{i\theta}e^{i\varphi}}{\sqrt{2}}\right|^2\\ &= \frac{1}{2} & &= \frac{1}{2}\end{aligned}$$

as desired. □

10.4 Tutorial 4

Tutorial 4 - Monday, February 09

Question Consider a quantum system described by a 3-dimensional Hilbert space. The state of the system is given by

$$|\psi\rangle \propto |1\rangle + 2\,|2\rangle + 3\,|3\rangle$$

where $\{|1\rangle, |2\rangle, |3\rangle\}$ is an orthonormal basis for the Hilbert space. Suppose we have an operator

$$A = |1\rangle\langle 1| + i\,|1\rangle\langle 3| + 3\,|2\rangle\langle 2| + a\,|3\rangle\langle 1|$$

1. Normalize the state $|\psi\rangle$.
2. What should the value of a be for A to represent an observable?
3. Calculate the expectation value $\langle A\rangle$ using the inner product formula $\langle\psi|\,A\,|\psi\rangle$.
4. Find the uncertainty $\Delta A = \sqrt{\langle A^2\rangle - \langle A\rangle^2}$ in measuring the observable A.
5. Calculate $\langle A\rangle$ and ΔA using the probability distribution of the measurement outcomes of A, and show that they match the results of parts 3 and 4.

Note 10.3. Something to think about: For the same quantum system and observable A above, characterize all states $|\phi\rangle$ for which $\Delta A = 0$. What special property do these states have with respect to the observable A?

Quiz Answer the following multiple-choice questions. No need to justify your answer.

1. Which of the following is the matrix representation of the z component of the spin angular momentum for a spin-1/2 system?

   (a) $\frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$ (b) $\frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$ (c) $\frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$ (d) Depends on the basis

2. In a d-dimensional Hilbert space, the object $|\psi\rangle\langle\phi|$ is represented by a

   (a) $d \times 1$ matrix (b) $1 \times d$ matrix (c) $d \times d$ matrix (d) 1×1 matrix

3. For an observable A and state $|\psi\rangle$, the object $\langle A\rangle = \langle\psi|\,A\,|\psi\rangle$ is

   (a) the average of the matrix elements of A in a given basis;
   (b) the trace of the operator A;
   (c) the average of the vector $A\,|\psi\rangle$ over its components;
   (d) the average of outcomes in a large number of ientical measurement of A, all starting from state $|\psi\rangle$.

10.5 Tutorial 5

Tutorial 5 - Monday, February 23

Question Consider the following thought experiment. Alice prepares a large ensemble of spin-1/2 particles as follows: for each particle she flips a fair coin. If it comes up heads, she prepares the state $|+\rangle$. If it comes up tails, she prepares the state $|+\rangle_x$. She then hands the ensembles to Bob, who performs the same measurement on each particle.

1. Bob measures S_z on each particle. Compute the probabilities of the two measurement outcomes using conditional probabilities.
2. Express the ensemble state (before measurement) as a density matrix ρ in the S_z eigenbasis. Show that ρ describes a mixed ensemble by confirming that $\mathrm{tr}[\rho^2] < 1$.
3. Calculate the same outcome probabilities as part 1 using the density matrix. Confirm that your answer agrees with part 1.
4. Alice now uses a different precedure: she does not flip a coin. Instead, for each particle she always prepares the pure state
$$|\psi\rangle \propto |+\rangle + |+\rangle_x$$
Compute the S_z probabilities again. Is the answer same as part 1.

Note 10.4. Something to think about: For the coin-flip state preparation procedure, there is classible ignorance about which of the $|+\rangle$ or $|+\rangle_x$ states was prepared on a given particle, so the ensemble is described by a statistical mixture. For the second procedure, Alice prepares a coherent superposition on every trial, and the ensemble is pure. To make this distinction concrete, show that in the pure case there exists a direction $\hat{\mathbf{n}}$ such that measuring $\hat{\mathbf{n}} \cdot \mathbf{S}$ has a definite outcome (probability 1), whereas for the mixed state there is no such direction.

Quiz

1. Which of the following is *always* true for a density matrix ρ?
   (a) ρ is Hermitian.
   (b) All entries of ρ are real numbers.
   (c) $\rho^2 = \rho$.
   (d) $\mathrm{Tr}[\rho^2] = 1$.
2. Consider an ensemble prepared in a 40/60 *statistical mixture* of $|+\rangle$ and $e^{i\varphi}|-\rangle$. For this ensemble, the probability distribution for measuring an arbitrary observable is
   (a) independent of φ for all observables.
   (b) dependent on φ for some observables, but not all.
   (c) dependent on φ for all observables.

3. Consider an ensemble prepared in a 40/60 *superposition* of $|+\rangle$ and $e^{i\varphi}|-\rangle$, i.e. the state

$$|\psi\rangle = \sqrt{0.4}\,|+\rangle + \sqrt{0.6}\,e^{i\varphi}|-\rangle$$

For this ensemble, the probability distribution for measuring an arbitrary observable is

(a) independent of φ for all observables.

(b) dependent on φ for some observables, but not all.

(c) dependent on φ for all observables.

10.6 Tutorial 6

Tutorial 6 - Monday, March 02

Question Consider a spin-1/2 particle with gyromagnetic ratio $\gamma > 0$ in the state $|\psi(0)\rangle = |+\rangle$ at time $t = 0$. The Hamiltonian of the system is

$$H = -\gamma \mathbf{S} \cdot \mathbf{B},$$

where $\mathbf{B}$ is the magnetic field.

1. A magnetic field $\mathbf{B} = B\hat{\mathbf{y}}$ is applied to the particle for a time T. What is the smallest $T > 0$ for which the spin ends up in $|-\rangle_x$?
2. The field is now abruptly switched to $\mathbf{B} = B\hat{\mathbf{z}}$, and the spin evolves for time $2T$, where T is the time calculated in part 1. What is the resulting state?
3. Using the results of part 1-2, sketch the trajectory of the expectation value of the spin angular momentum vector $\langle \mathbf{S} \rangle$ over the interval $[0, 3T]$.
4. Say we measure S_y at time $t = 3T$. What are the possible measurement outcomes? What are the corresponding probabilities?
5. Immediately after the measurement, the field is switched back to $\mathbf{B} = B\hat{\mathbf{y}}$ for another T duration. How does the system eolve after this?

Note 10.5. Something to think about: After measuring S_y in part 4, the state becomes probabilistic depending on the measurement outcome. Suppose the person doing the measurement does not inform you of the outcome they have measured. So for you, the state of the particle is unknown. Describe the state of the particle at $t = 4T$ using a density operator.

Proof. 1. For $\mathbf{B} = B\hat{\mathbf{y}}$, the Hamiltonian is

$$H_y = -\gamma B S_y = -\frac{\hbar\omega}{2}\sigma_y, \qquad \omega = \gamma B.$$

Hence the time-evolution operator is

$$U_y(t) = e^{-iH_y t/\hbar} = e^{i\omega t\sigma_y/2}.$$

Acting on $|+_z\rangle$ gives

$$U_y(t)\,|+_z\rangle = \cos\left(\frac{\omega t}{2}\right)|+_z\rangle - \sin\left(\frac{\omega t}{2}\right)|-_z\rangle\,.$$

Since

$$|-_x\rangle = \frac{1}{\sqrt{2}}\big(|+_z\rangle - |-_z\rangle\big),$$

we require

$$\cos\left(\frac{\omega T}{2}\right) = \sin\left(\frac{\omega T}{2}\right) = \frac{1}{\sqrt{2}}.$$

Therefore

$$\frac{\omega T}{2} = \frac{\pi}{4} \quad \Longrightarrow \quad T = \frac{\pi}{2\gamma B}.$$

Thus the smallest such time is

$$\boxed{T = \frac{\pi}{2\gamma B}}.$$

2. After time T, the state is $|-_x\rangle$. Now switch to $\mathbf{B} = B\hat{\mathbf{z}}$. Then

$$H_z = -\gamma B S_z = -\frac{\hbar\omega}{2}\sigma_z, \qquad U_z(t) = e^{-iH_z t/\hbar} = e^{\,i\omega t\sigma_z/2}.$$

Using

$$|-_x\rangle = \frac{1}{\sqrt{2}}\big(|+_z\rangle - |-_z\rangle\big),$$

after an additional time $2T$ we get

$$U_z(2T)\,|-_x\rangle = \frac{1}{\sqrt{2}}\left(e^{i\omega(2T)/2}\,|+_z\rangle - e^{-i\omega(2T)/2}\,|-_z\rangle\right).$$

Since $\omega T = \frac{\pi}{2}$, we have $\omega(2T) = \pi$, so

$$U_z(2T)\,|-_x\rangle = \frac{1}{\sqrt{2}}\left(e^{i\pi/2}\,|+_z\rangle - e^{-i\pi/2}\,|-_z\rangle\right) = i\frac{1}{\sqrt{2}}\big(|+_z\rangle + |-_z\rangle\big) = i\,|+_x\rangle\,.$$

Hence the resulting state is

$$\boxed{|\psi(3T)\rangle = i\,|+_x\rangle},$$

which is physically the same as $|+_x\rangle$ up to a global phase.

3. The expectation value $\langle\mathbf{S}\rangle$ has constant magnitude $\hbar/2$ and follows the Bloch-sphere precession.

For $0 \le t \le T$, the field is along $\hat{\mathbf{y}}$, so

$$\langle\mathbf{S}\rangle(t) = \frac{\hbar}{2}\big(-\sin(\omega t),\, 0,\, \cos(\omega t)\big).$$

Thus it moves from

$$\frac{\hbar}{2}\hat{\mathbf{z}} \quad \text{to} \quad -\frac{\hbar}{2}\hat{\mathbf{x}}.$$

For $T \le t \le 3T$, let $\tau = t - T$. The field is now along $\hat{\mathbf{z}}$, so

$$\langle\mathbf{S}\rangle(t) = \frac{\hbar}{2}\big(-\cos(\omega\tau),\, \sin(\omega\tau),\, 0\big), \qquad \tau = t - T.$$

Thus it moves from

$$-\frac{\hbar}{2}\hat{\mathbf{x}} \quad \text{to} \quad \frac{\hbar}{2}\hat{\mathbf{x}},$$

passing through $+\frac{\hbar}{2}\hat{\mathbf{y}}$ halfway through this interval.

So the trajectory is:

- from $+\hat{\mathbf{z}}$ to $-\hat{\mathbf{x}}$ along a quarter-circle in the xz-plane;
- then from $-\hat{\mathbf{x}}$ to $+\hat{\mathbf{x}}$ along a half-circle in the xy-plane.

4. At time $t = 3T$, the state is $|+_x\rangle$ (up to phase). Measuring S_y gives the eigenvalues

$$\boxed{+\frac{\hbar}{2} \quad \text{and} \quad -\frac{\hbar}{2}}.$$

Since $|+_x\rangle$ has equal overlap with $|+_y\rangle$ and $|-_y\rangle$,

$$P\left(S_y = +\frac{\hbar}{2}\right) = \frac{1}{2}, \qquad P\left(S_y = -\frac{\hbar}{2}\right) = \frac{1}{2}.$$

Therefore

$$\boxed{P\left(S_y = +\frac{\hbar}{2}\right) = \frac{1}{2}, \qquad P\left(S_y = -\frac{\hbar}{2}\right) = \frac{1}{2}.}$$

5. Immediately after the measurement, the state collapses to either $|+_y\rangle$ or $|-_y\rangle$.

Switching the field back to $\mathbf{B} = B\hat{\mathbf{y}}$ means the Hamiltonian is again

$$H_y = -\gamma B S_y.$$

Since $|\pm_y\rangle$ are eigenstates of S_y, they are stationary states under this Hamiltonian and only acquire phase factors.

If the outcome was $+\hbar/2$, then

$$|+_y\rangle \longrightarrow e^{-iE_+T/\hbar}\,|+_y\rangle\,, \qquad E_+ = -\gamma B\frac{\hbar}{2} = -\frac{\hbar\omega}{2}.$$

Hence

$$|+_y\rangle \longrightarrow e^{\,i\omega T/2}\,|+_y\rangle = e^{i\pi/4}\,|+_y\rangle\,.$$

If the outcome was $-\hbar/2$, then

$$|-_y\rangle \longrightarrow e^{-iE_-T/\hbar}\,|-_y\rangle\,, \qquad E_- = +\frac{\hbar\omega}{2},$$

so

$$|-_y\rangle \longrightarrow e^{-i\omega T/2}\,|-_y\rangle = e^{-i\pi/4}\,|-_y\rangle\,.$$

Therefore the post-measurement evolution is

$$\boxed{|+_y\rangle \to e^{i\pi/4}\,|+_y\rangle \quad \text{with probability } \frac{1}{2},}$$

$$\boxed{|-_y\rangle \to e^{-i\pi/4}\,|-_y\rangle \quad \text{with probability } \frac{1}{2}.}$$

Physically, the spin remains aligned along $\pm\hat{\mathbf{y}}$.

□

Quiz Mark each statement with True/False. No need to justify your answers. Assume tha Hamiltonian in question is *time-independent* for all parts.

1. For a time-independent Hamiltonian, the state of the system is always time-independent.
2. If a system starts in an energy eigenstate, the probability of measuring the same energy at a later time is 1.
3. If a system is in a superposition of two energy eigenstates with different energies, the state is time-independent.
4. If the Hamiltonian is 0 ($H = 0$), the state of the ststem is time-independent.
5. If a system is in a superposition of two energy eigenstates with different energies, the probabilies of measuring those energies are time-independent.

Answer. ✗✓✗✓✓ □

10.7 Tutorial 7

Tutorial 7 - Monday, March 09

Question In the lectures on magnetic resonance, you have seen the evolution of a spin-1/2 system in the presence of a static field and an orthogonal circularly polarized field that is time dependent. In this tutorial, we will see how the system evolves if the static and time-dependent fields are parallel.

Consider the initial state $|\psi(0)\rangle = |+\rangle_x$ for the system evolving in the presence of the magnetic field

$$\mathbf{B}(t) = [B_0 + B_{\mathrm{RF}} \cos(wt)]\hat{\mathbf{z}}$$

wheere B_0 and B_{RF} reresent the static and time-dependent fields, respectively.

1. Calculate the Hamiltonian in terms of the gyromagnetic ratio γ;
2. Write the unknown evolved state $|\psi(t)\rangle$ in the $|\pm\rangle$ basis and substitute it into the Schrödinger equation along with the Hamiltonian from part 1. Find $|\psi(t)\rangle$ by solving the resulting differential equation.
3. What is the trajectory of the expectation value $\langle \mathbf{S} \rangle$ in space? Specify the trajectory in terms of spherical coordinates $\theta(t)$, $\varphi(t)$.
4. Simplify $\varphi(t)$ in the limit of large RF frequencies ($w \gg \gamma B_{\mathrm{RF}}$). What is the physical interpretation of this result?

Note 10.6. Something to think about: Extend the above analysis to a general tume dependence for the field rather than just a sinusoidal one.

Quiz Answer the following multiple-choice questions. No need to justify your answers.

1. A system has a time-independent Hamiltonian H, which of the following statements is always true?
   (a) Every state is stationary;
   (b) Every energy eigenstate is stationary;
   (c) The expectation value of every observable is constant in time;
   (d) The state vector can always be chosen real for all time.
2. Now suppose the Hamiltonian depends explicitly on time, $H(t)$. Which statement is always true?
   (a) The system's energy is conserved;
   (b) An eigenstate of $H(t)$ at $t = 0$ is a stationary state;
   (c) The state vector still satisfies the Schrödinger equation $i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle$;
   (d) An eigenstate of $H(t)$ at $t = 0$ is also an eigenstate for later times.

10.8 Tutorial 8

Tutorial 8 - Monday, March 16

Question Consider the problem of a particle in a 1D infinite potential well spanning $0 \leq x \leq l$. At time $t = 0$, the particle is in the state $|\psi_0\rangle$, with position representation

$$\psi_0(x) = \langle x|\psi_0\rangle = \begin{cases} A\sin^3(\pi x/l), & x \in [0, l], \\ 0, & x \notin [0, l]. \end{cases}$$

1. Calculate A such that $|\psi_0\rangle$ is a valid quantum state.

   Hint: Recall the identity
   $$\sin^3(x) = \frac{3}{4}\sin x - \frac{1}{4}\sin(3x).$$

2. Find the evolved state $|\psi(t)\rangle$ at an arbitrary time t. Specify the state using its position-basis representation
   $$\psi(x, t) = \langle x|\psi(t)\rangle\,.$$

3. Calculate the expectation value of the kinetic energy
   $$\langle T\rangle = \frac{\langle P^2\rangle}{2m}$$
   as a function of time. How do you interpret the resulting time dependence?

4. Calculate the expectation value of momentum as a function of time.

> **Note 10.7.** Something to think about: Show that the expectation value of the kinetic energy for a particle in 1D is always strictly positive.

Quiz Answer the following multiple-choice questions. No need to justify your answers.

1. A particle is in a 1D infinite potential well on $0 \leq x \leq l$. At $t = 0$, its wavefunction is

$$\psi(x, 0) = \begin{cases} A, & x \in [0, l], \\ 0, & x \notin [0, l]. \end{cases}$$

What is the value of A?

(a) $\sqrt{2/l}$

(b) $1/\sqrt{l}$

(c) $1/l$

(d) $2/l$

2. For the same state, which statement is correct?

(a) The state is a single energy eigenstate.

(b) The state is a superposition of exactly two energy eigenstates.

(c) The state is a superposition of infinitely many energy eigenstates.

(d) The state cannot be written as a superposition of energy eigenstates.

3. For the same state, which statement is correct?

(a) $\langle X \rangle$ varies with time because the state is not an energy eigenstate.

(b) $\langle X \rangle = l/2$ for all t, because the state is symmetric about the center of the box.

(c) $\langle X \rangle = 0$ for all t, because the wavefunction is real at $t = 0$.

(d) $\langle X \rangle$ is undefined because the potential goes to infinity outside the well.

10.9 Tutorial 9

Tutorial 9 - Monday, March 23

Questions Consider a particle of mass m in a 1D infinite potential well. For $t < 0$, the well spans $[0, l]$, and the particle is in the ground state:

$$\psi(x, 0^-) = \begin{cases} \sqrt{\frac{2}{l}} \sin\left(\frac{\pi x}{l}\right), & x \in [0, l], \\ 0, & x \notin [0, l]. \end{cases} \tag{1}$$

At time $t = 0$, the right wall is suddenly moved so that the new well spans $[0, 2l]$. Assume the wall is moved so quickly that the wavefunction does not change during the expansion, i.e. $\psi(x, 0^+) = \psi(x, 0^-)$.

1. Calculate the wavefunction $\psi(x, t)$ for $t > 0$.
2. For $t > 0$, calculate the probability that an energy measurement returns the same value as the particle's energy before the wall was moved.
3. For $t > 0$, show that the wavefunction is periodic in time, i.e. $\psi(x, t + T) = \psi(x, t)$. Find the period T.

Something to think about: If the Hamiltonian of a quantum system changes discontinuously from H_1 to H_2 at time $t = t_0$, and $H(t)|\psi(t)\rangle$ remains finite across the jump, show directly from the Schrodinger equation that

$$|\psi(t_0^-)\rangle = |\psi(t_0^+)\rangle,$$

i.e. the state is continuous at $t = t_0$.

Quiz Answer the following multiple-choice questions. No need to justify your answers.

1. Consider a particle in 1D. The wave function $\psi(x, t)$ of this particle has units of

(a) Length (b) $\sqrt{\text{Length}}$ (c) 1/Length (d) $1/\sqrt{\text{Length}}$

2. For a quantum particle in 1D with state vector $|\psi\rangle$, the quantity $\psi(x) = \langle x|\psi\rangle$ is

(a) The position representation of the particle's state;

(b) The coefficient of $|\psi\rangle$ when decomposed in the position eigenbasis;

(c) The wavefunction;

(d) All of the above.

3. What is the result of the following integral?

$$\int_0^\infty \delta(x - 2) \frac{e^{\sin(2\pi x)}}{x^2 + 1} \, \mathrm{d}x$$

(a) Undefined; (b) 0; (c) 1/5; (d) 1/3

10.10 Tutorial 10

Tutorial 10 - Monday, March 30

Questions In this tutorial, we will study the energy eigenstates of a particle in the 1D finite rectangular barrier

$$V(x) = \begin{cases} V_0 & x \in [0, l], \\ 0 & x \notin [0, l], \end{cases}$$

where $V_0 > 0$.

1. Write down the time-independent Schrodinger equation (i.e. the eigenvalue problem for the Hamiltonian) and solve it separately in the three regions $x < 0$, $0 < x < l$, and $x > l$.

   Show that the form of the solutions depends on whether $0 < E < V_0$ or $E > V_0$. In each case, determine whether the corresponding eigenstates are scattering states or bound states.

2. By requiring that the wavefunction and its first derivative are continuous at $x = 0$ and $x = l$, relate the unknown coefficients in the three regions. What is the general form of an energy eigenstate?

3. Consider an energy eigenstate describing a particle incident on the barrier from the right, i.e. for $x > l$, the wavefunction contains an incident left-moving term proportional to e^{-ikx} and a reflected right-moving term proportional to e^{ikx}, while for $x < 0$, it contains only a transmitted left-moving term proportional to e^{-ikx}.

   (a) What form should the wavefunction take in each of the three regions?

   (b) Calculate the reflection and transmission probabilities and sketch them as a function of E.

Quiz Answer the following multiple-choice questions. No need to justify your answers.

1. For a free particle of mass m in 1D, the Hamiltonian operator in the position representation is

   (a) $-i\hbar\dfrac{d}{dx}$ (b) $-\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx^2}$ (c) $\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx^2}$ (d) 0

2. Consider the free-particle wavefunction $\psi(x) = Ae^{ikx}$ where A is a constant and k is real. This state has a definite value of

   (a) Position only
   (b) Momentum only
   (c) Energy only
   (d) Both momentum and energy

3. For a free particle in 1D, the states e^{ikx} and e^{-ikx} have

   (a) The same momentum and the same energy
   (b) Opposite momentum and the same energy
   (c) Opposite momentum and opposite energy
   (d) The same momentum and opposite energy

A Appendix: Linear Algebra

A.1 Invert Matrices

Theorem A.1. Invertibility of a Matrix

for an $n \times n$ matrix A over a field (e.g., $\mathbb{R}$, $\mathbb{C}$),

$$A \text{ is invertible} \quad \Longleftrightarrow \quad \det(A) \neq 0$$

Theorem A.2. Inverse of a 2×2 Matrix

We have

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \qquad A^{-1} = \frac{1}{\det(A)} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix},$$

provided that $\det(A) \neq 0$.

Input : $A \in \mathbb{F}^{n \times n}$
Output: A^{-1} if it exists, otherwise `FAIL`

$M \leftarrow [\, A \mid I_n \,]$
Row-reduce M to RREF: $M \to [\, R \mid B \,]$
if $R \neq I_n$ **then**
  return *FAIL*
return B

Algorithm 1: Inverse(A) via Gauss–Jordan elimination

A.2 Diagonalize Matrices

Theorem A.3. Diagonalization via an Eigenbasis

Let $A \in M_n(\mathbb{F})$. Suppose $\mathbb{F}^n$ has a basis of eigenvectors $\vec{v}_1, \ldots, \vec{v}_n$ for A for some scalars $c_1, \ldots, c_n \in \mathbb{F}$. Let

$$S \;=\; \begin{bmatrix} \vec{v}_1 & \vec{v}_2 & \cdots & \vec{v}_n \end{bmatrix}$$

be the matrix whose columns are $\vec{v}_1, \ldots, \vec{v}_n$. Then S is invertible and

$$S^{-1}AS \;=\; \operatorname{diag}(c_1, \ldots, c_n) \;=\; \begin{pmatrix} c_1 & & 0 \\ & \ddots & \\ 0 & & c_n \end{pmatrix}.$$

Input : $A \in \mathbb{F}^{n \times n}$
Output: (P, D) with $P^{-1}AP = D$ diagonal, or `FAIL`

Compute $p(\lambda) = \det(A - \lambda I)$ and factor $p(\lambda) = \prod_{j=1}^{k} (\lambda - \lambda_j)^{a_j}$ in $\mathbb{F}$
$V \leftarrow [\,],\ L \leftarrow [\,]$
for $j = 1$ **to** k **do**
    $B_j \leftarrow \text{basis}(\ker(A - \lambda_j I))$
    foreach $v \in B_j$ **do**
        append v to V; append λ_j to L;
if $|V| < n$ **then**
    return *FAIL*
Take n independent vectors from V as columns of P and their labels from L for D
$D \leftarrow \text{diag}(L_1, \ldots, L_n)$
return (P, D)

Algorithm 2: Diagonalize(A)

B Special Topic — Generators of Transformations in Hilbert Space

Our goal in this lecture to describe the action of operators on quantum states.

We have seen that when an operator $\hat{A}$ acts on a arbitrary state $|\psi\rangle$ that is not an eigenstate of the operator it produces a new state $|\psi'\rangle$.

$$|\psi\rangle = \sum_n c_n |a_n\rangle$$
$$|\psi'\rangle = \hat{A}\,|\psi\rangle = \sum_n c_n a_n |a_n\rangle \neq \text{const. } |\psi\rangle$$

We will study the new state that is produced in the context of spin-1/2 system. We will start by constructing the spin operator in an arbitrary direction $\hat{n}$.

$$\hat{n} = \cos\varphi\,\sin\theta\,\hat{x} + \sin\varphi\,\sin\theta\,\hat{y} + \cos\theta\,\hat{z}$$

where (φ, θ) are the polar angles. We define the spin-1/2 operator in an arbitrary direction as

$$\begin{aligned}
\hat{S}_n &:= \hat{\mathbf{S}}\cdot\hat{n} = \hat{S}_x\cos\varphi\,\sin\theta + \hat{S}_y\sin\varphi\,\sin\theta + \hat{S}_z\cos\theta. \\
\hat{S}_n &:= \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\cos\varphi\,\sin\theta + \frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\sin\varphi\,\sin\theta + \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\cos\theta \\
&= \frac{\hbar}{2}\begin{pmatrix}\cos\theta & e^{-i\varphi}\sin\theta\\ e^{i\varphi}\sin\theta & -\cos\theta\end{pmatrix}
\end{aligned}$$

Note B.1. The eigenvalues of $\hat{S}_n$ are $\pm\frac{\hbar}{2}$ with corresponding eigenstates:

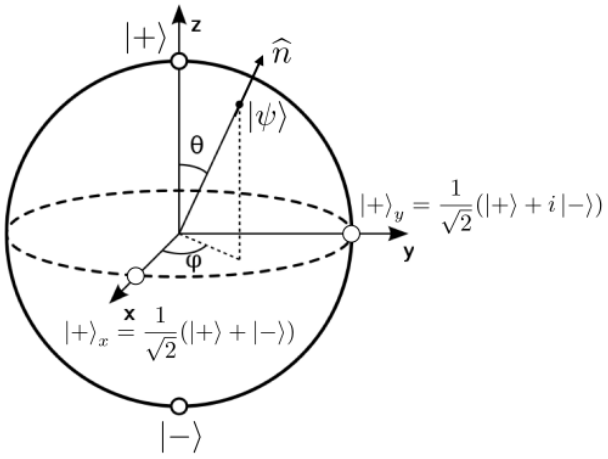
$$|\psi_+(\theta,\phi)\rangle = \cos\left(\frac{\theta}{2}\right)|+\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\phi}\,|-\rangle$$

$$|\psi_-(\theta,\phi)\rangle = \sin\left(\frac{\theta}{2}\right)|+\rangle - \cos\left(\frac{\theta}{2}\right)e^{i\phi}\,|-\rangle$$

The 2-dimensional Hilbert space of the spin-1/2 system can be represented as a the points on the surface of a sphere of radius 1 in 3-dimensional Euclidean space.

Definition B.1. **[Bloch Sphere]**

This representation is referred to as the Bloch Sphere, named after the Physicist Felix Bloch.



Let $|\psi'\rangle = S_n|\psi\rangle$, which is another state in the 2-dimensional Hilbert space of the spin-$\frac{1}{2}$ system. What is the relationship between $|\psi\rangle$ and $|\psi'\rangle$? Let's consider the following example:

$$\hat{S}_x|+\rangle = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}0\\1\end{pmatrix} = \frac{\hbar}{2}|-\rangle$$

We see that up to a multiplicative factor of $\frac{\hbar}{2}$ the action of $\hat{S}_x$ on the state $|+\rangle$ rotates the state by an angle π about the x-axis. We can also consider another example:

$$\hat{S}_z|+\rangle_y = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix} = \frac{\hbar}{2}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} = \frac{\hbar}{2}|-\rangle_y$$

We see again that the state $|\psi'\rangle$ is a rotated version of the state $|+\rangle_y$ by an angle π about the z-axis.

B.1 Infinitesimal Rotation

We see that angular momentum operators "generate" rotations of states on the Bloch sphere. The rotation axis is defined by the direction of the spin operator. The component of the state vector that is perpendicular to the rotation axis rotates by π. It is also possible to generate arbitrary rotations about any axis. To do this we start by first constructing an operator that generates an infinitesimal rotation.

We begin by considering an infinitesimal rotation $d\phi$ about the z-axis.

$$\hat{R}_z(d\phi) := \mathbb{1} - \frac{i}{\hbar}\hat{S}_z\, d\phi \tag{1}$$

The matrix representation of $\hat{R}_z(d\phi)$ in the z-basis is

$$\hat{R}_z(d\phi) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \frac{i\,d\phi}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 - \dfrac{i\,d\phi}{2} & 0 \\ 0 & 1 + \dfrac{i\,d\phi}{2} \end{pmatrix} \tag{2}$$

Let $\zeta = 1 - i\,\dfrac{d\phi}{2}$.

$$\hat{R}_z(d\phi) = \begin{pmatrix} \zeta & 0 \\ 0 & \zeta^* \end{pmatrix}$$

$$\zeta = e^{-i\gamma}\sqrt{1 + \left(\frac{d\phi}{2}\right)^2}, \qquad \gamma = \tan^{-1}\left(\frac{d\phi}{2}\right)$$

We take the limit $d\phi \to 0$

$$\lim_{d\phi \to 0} \zeta = e^{-i\,d\phi/2}$$

$$\hat{R}_z(d\phi) \;\to\; \begin{pmatrix} e^{-i\,d\phi/2} & 0 \\ 0 & e^{i\,d\phi/2} \end{pmatrix} \tag{3}$$

Therefore, we compute that

$$\begin{aligned} \hat{R}_z(d\phi)\,|\psi_+(\theta,\phi)\rangle &= e^{-i\,d\phi/2}\begin{pmatrix} 1 & 0 \\ 0 & e^{i\,d\phi} \end{pmatrix}\begin{pmatrix} \cos\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) e^{i\phi} \end{pmatrix} \\ &= e^{-i\,d\phi/2}\begin{pmatrix} \cos\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) e^{i(\phi + d\phi)} \end{pmatrix} \end{aligned}$$

$$\boxed{\begin{aligned} \hat{R}_z(d\phi)\,|\psi_+(\theta,\phi)\rangle &= e^{-i\,d\phi/2}\,|\psi_+(\theta,\phi + d\phi)\rangle \qquad (4) \\ \hat{R}_z(d\phi)\,|\psi_-(\theta,\phi)\rangle &= e^{-i\,d\phi/2}\,|\psi_-(\theta,\phi + d\phi)\rangle \qquad (5) \end{aligned}}$$

Discovery B.1. We see that up to an overall phase factor $\hat{R}_z(d\phi)$ rotates the states $|\psi_\pm(\theta,\phi)\rangle$ counterclockwise about the z-axis by an angle $d\phi$.

The operator $\hat{R}_z^\dagger(d\phi)$ is the inverse of $\hat{R}_z(d\phi)$ up to order $\mathcal{O}((d\phi)^2)$.

$$\hat{R}_z^\dagger(d\phi) = \mathbb{1} + \frac{i}{\hbar}\hat{S}_z\,d\phi \tag{6}$$

We note that $\hat{S}_z$ is a Hermitian operator, therefore $\hat{S}_z^\dagger = \hat{S}_z$.

$$\begin{aligned} \hat{R}_z(d\phi)\,\hat{R}_z^\dagger(d\phi) &= \left(\mathbb{1} - \frac{i}{\hbar}\hat{S}_z\,d\phi\right)\left(\mathbb{1} + \frac{i}{\hbar}\hat{S}_z\,d\phi\right) \\ &= \mathbb{1} + \left(\frac{d\phi}{\hbar}\right)^2 S_z^2 \end{aligned}$$

As a result,

$$\lim_{d\phi\to 0}\ \hat{R}_z(d\phi)\,\hat{R}_z^\dagger(d\phi) \to \mathbb{1}.$$

Discovery B.2. In the limit that $d\phi \to 0$, $\hat{R}_z^\dagger(d\phi)$ produces a clockwise rotation by an angle $d\phi$ about the z-axis.

B.2 Angular Momentum as the Generator of Rotation

We can produce a larger rotation by an angle ϕ, by applying $\hat{R}_z(d\phi)$ back-to-back a large number N times.

$$\hat{R}_z(\phi) = \lim_{N\to\infty}\left(\mathbb{1} - \frac{i}{\hbar}\left[\frac{\phi}{N}\right]\hat{S}_z\right)^N \tag{7}$$

To evaluate eq. (7), consider the Taylor series expansion of the following polynomial for $x/N < 1$:

$$\left(1+\frac{x}{N}\right)^N = 1 + x + \frac{1}{2!}\left(\frac{N-1}{N}\right)x^2 + \frac{1}{3!}\left(\frac{(N-1)(N-2)}{N^2}\right)x^3 + \cdots$$

In the limit $N \to \infty$, the above expression reduces to the following

$$\lim_{N\to\infty}\left(1+\frac{x}{N}\right)^N \to 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots = \sum_{n=0}^{\infty}\frac{x^n}{n!} = e^x \tag{8}$$

If we replace the term x in eq. (8) by $-\dfrac{i\phi}{\hbar}\hat{S}_z$, then eq. (7) may be written as

$$\hat{R}_z(\phi) = \mathbb{1} - i\left(\frac{\phi}{\hbar}\right)\hat{S}_z - \frac{1}{2!}\left(\frac{\phi}{\hbar}\right)^2\hat{S}_z^2 + \frac{i}{3!}\left(\frac{\phi}{\hbar}\right)^3\hat{S}_z^3 + \cdots \tag{9}$$

$$= e^{-i\phi\hat{S}_z/\hbar} \tag{10}$$

The exponential of an operator may look a bit strange, however we can use the power series expansion form of the exponential (eq. (9)) to evaluate its action on a state vector.

$$e^{-i\phi\hat{S}_z/\hbar}|+\rangle = \left[\mathbb{1} - i\left(\frac{\phi}{\hbar}\right)\hat{S}_z - \frac{1}{2!}\left(\frac{\phi}{\hbar}\right)^2\hat{S}_z^2 + \frac{i}{3!}\left(\frac{\phi}{\hbar}\right)^3\hat{S}_z^3 + \cdots\right]|+\rangle$$

Note B.2.

$$\hat{S}_z^n|\pm\rangle = \left(\pm\frac{\hbar}{2}\right)^n|\pm\rangle$$

$$e^{-i\phi\hat{S}_z/\hbar}|+\rangle = \left[1 - i\left(\frac{\phi}{\hbar}\right)\frac{\hbar}{2} - \frac{1}{2!}\left(\frac{\phi}{\hbar}\right)^2\left(\frac{\hbar}{2}\right)^2 + \frac{i}{3!}\left(\frac{\phi}{\hbar}\right)^3\left(\frac{\hbar}{2}\right)^3 + \cdots\right]|+\rangle$$

$$= e^{-i\phi/2}|+\rangle$$

We see that if the exponential operator acts on an eigenvector of the operator in the exponent, then we simply replace the operator by the corresponding eigenvalue.

$$\therefore \quad e^{-i\phi\hat{S}_z/\hbar}|+\rangle = e^{-i\phi/2}|+\rangle.$$

We can now see what happens when $\hat{R}_z(\phi)$ acts on the state $|\psi_+(\theta,\phi)\rangle$.

$$\begin{aligned}
\hat{R}_z(\phi)|\psi_+(\theta,\phi)\rangle &= e^{-i\phi\hat{S}_z/\hbar}\left[\cos\left(\frac{\theta}{2}\right)|+\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\phi}|-\rangle\right] \\
&= \left[\cos\left(\frac{\theta}{2}\right)e^{-i\phi/2}|+\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\phi/2}e^{i\phi}|-\rangle\right] \\
&= e^{-i\phi/2}\left[\cos\left(\frac{\theta}{2}\right)|+\rangle + \sin\left(\frac{\theta}{2}\right)e^{i(\phi+\phi)}|-\rangle\right] \\
\Rightarrow \quad \hat{R}_z(\phi)|\psi_+(\theta,\phi)\rangle &= e^{-i\phi/2}|\psi_+(\theta,\phi+\phi)\rangle.
\end{aligned}$$

We see that up to an overall phase factor the operator $\hat{R}_z(\phi)$ produces a rotation of the state by an angle ϕ about the z-axis. Furthermore, $\hat{R}_z(\phi)$ corresponds to an unitary operator:

$$\hat{R}_z(\phi)\hat{R}_z^\dagger(\phi) = e^{-i\phi\hat{S}_z/\hbar}\,e^{i\phi\hat{S}_z/\hbar} = \mathbb{1} \tag{11}$$

$$\hat{R}_z^\dagger(-\phi) = \hat{R}_z(\phi) \tag{12}$$

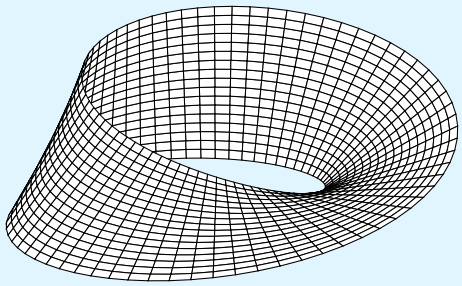
Matrix representation of $\hat{R}_z(\phi)$. See the appendix at the end of the lecture for the derivation.

$$\boxed{e^{-i\phi\hat{S}_z/\hbar} = \mathbb{1}\cos\left(\frac{\phi}{2}\right) - \frac{2i\hat{S}_z}{\hbar}\sin\left(\frac{\phi}{2}\right)} \tag{13}$$

Discovery B.3. A 2π rotation of the spin-1/2 state vector does not reproduce the original state. Rather, it produces the negative of the state.

$$\hat{R}_z(\phi = 2\pi)\ |\psi_+(\theta,\phi)\rangle = e^{-i\pi}\,|\psi_+(\theta,\phi)\rangle = -\,|\psi_+(\theta,\phi)\rangle\,.$$

A 4π rotation is required to recover the original state. This property of the quantum state of spin-1/2 particles is referred to as the "spinor" property.
We can make a correspondence with spinors and a Möbius strip.



Comment B.1. We have said many times in this course that the overall phase factor of a quantum state does not change the probability of measurement outcomes.
While strictly speaking this is true, it is also possible to measure this overall phase if we devise an experiment that interferes two quantum states with different overall phase factors. Such an experiment has been done using the technique of magnetic resonance. We will study how magnetic resonance works when we discuss time-dependent quantum processes.

B.2.1 Additional A: Matrix Representation of the Rotation Operator

We seek to find a matrix representation of the rotation operator. I will use the following notation for the operator $\hat{S}_z$ in this derivation:

$$\hat{S}_z = \frac{\hbar}{2}\sigma_z, \qquad \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$\sigma_z^2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1}.$$

Now,

$$\begin{aligned}
e^{-i\phi\hat{S}_z/\hbar} &= e^{-i\phi\sigma_z/2} \\
&= \mathbb{1} - i\left(\frac{\phi}{2}\right)\sigma_z - \frac{1}{2!}\left(\frac{\phi}{2}\right)^2\sigma_z^2 + \frac{i}{3!}\left(\frac{\phi}{2}\right)^3\sigma_z^3 + \frac{1}{4!}\left(\frac{\phi}{2}\right)^4\sigma_z^4 + \cdots \\
&= \mathbb{1} - i\left(\frac{\phi}{2}\right)\sigma_z - \frac{1}{2!}\left(\frac{\phi}{2}\right)^2\mathbb{1} + \frac{i}{3!}\left(\frac{\phi}{2}\right)^3\sigma_z + \frac{1}{4!}\left(\frac{\phi}{2}\right)^4\mathbb{1} + \cdots \\
&= \mathbb{1}\left\{1 - \frac{1}{2!}\left(\frac{\phi}{2}\right)^2 + \frac{1}{4!}\left(\frac{\phi}{2}\right)^4 + \cdots\right\} - i\sigma_z\left\{\frac{\phi}{2} - \frac{1}{3!}\left(\frac{\phi}{2}\right)^3 + \frac{1}{5!}\left(\frac{\phi}{2}\right)^5 + \cdots\right\} \\
&= \mathbb{1}\sum_{n=0}^{\infty}\frac{(-1)^n(\phi/2)^{2n}}{(2n)!} - i\sigma_z\sum_{n=0}^{\infty}\frac{(-1)^n(\phi/2)^{2n+1}}{(2n+1)!} \\
&= \mathbb{1}\cos\left(\frac{\phi}{2}\right) - i\sigma_z\sin\left(\frac{\phi}{2}\right) \\
&= \cos\left(\frac{\phi}{2}\right)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - i\sin\left(\frac{\phi}{2}\right)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\
&= \begin{pmatrix} \cos(\phi/2) - i\sin(\phi/2) & 0 \\ 0 & \cos(\phi/2) + i\sin(\phi/2) \end{pmatrix} \\
&= \begin{pmatrix} e^{-i\phi/2} & 0 \\ 0 & e^{i\phi/2} \end{pmatrix}.
\end{aligned}$$

B.2.2 Additional B: Generators of Infinitesimal Transformations

Operators corresponding to observables, such as angular momentum, linear momentum, position and energy all generate transformations on states in Hilbert space.

Angular momentum, for example rotates kets. We will see later that the linear momentum operator will produce translations, and the energy operator will produce a translation of states in time. We can build continuous transformations by applying a series of infinitesimal transformations.

The infinitesimal transformation operator has the basic form

$$U(\epsilon) = \mathbb{1} - i\epsilon G$$

where G is a Hermitian operator corresponding to the particular observable in question, e.g., angular momentum, and ϵ is the infinitesimal quantity, e.g., $d\phi$ for the case of rotations.

There are two reasons for choosing $U(\epsilon)$ to have this mathematical form. First, we require

$$\lim_{\epsilon \to 0} U(\epsilon) = \mathbb{1}.$$

Second, $U(\epsilon)$ should be unitary, that is, it should transform a state without changing its norm. Another way of saying this is that it should conserve probability. We therefore require that $UU^\dagger = \mathbb{1}$.

$$\begin{aligned} UU^\dagger &= (\mathbb{1} - i\epsilon G)(\mathbb{1} + i\epsilon G^\dagger) \\ &= \mathbb{1} + i\epsilon G - i\epsilon G + \epsilon^2 G^2 \end{aligned}$$

We see that terms of $\mathcal{O}(\epsilon)$ cancel. Neglecting terms of order $\mathcal{O}(\epsilon^2)$, $UU^\dagger = \mathbb{1}$, as required.

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