

LIHORNE.COM

PHYS 234

QUANTUM PHYSICS I



DR. ROBERT HILL • SPRING 2014 • UNIVERSITY OF WATERLOO

Last Revision: July 22, 2014

Table of Contents

1 The Photoelectric and Compton Effects	1
1.1 Historical Background	1
1.2 Einstein's Theory of Photoelectric Effect	1
1.3 Compton Effect	2
2 De Broglie Wavelength and the Davisson-Germer Experiment	2
2.1 The De Broglie Postulate (1924)	2
2.2 The Davisson-Germer Experiment	3
2.3 Final Words	3
3 Linear Algebra Review	3
3.1 Vector Spaces	3
3.2 Matrices	5
4 Introduction to the Formalism and Structure of Quantum Mechanics	8
4.1 Angular Momentum and Spin	8
4.2 Stern Gerlach Experiments	9
Stern-Gerlach Experiment 1	10
Stern-Gerlach Experiment 2	11
Stern-Gerlach Experiment 3	11
Stern-Gerlach Experiment 4	12
4.3 Quantum State Vectors	12
4.4 Matrix Notation	17
4.5 General Quantum Systems	18
4.6 Quantum Mechanical Operators and Measurement	20
Operators, Eigenvalues, & Eigenvectors	20
Hermitian Operators	21
Completeness Relationship	21
Spectral Decomposition	21

4.7	More on Matrix Notation	22
4.8	Expectation Values	22
4.9	Stastical Operator / Density Matrix	24
4.10	Projection Operators and Measurements	26
4.11	Spin Components in Arbitrary Directions	27
4.12	Commuting Observables	28
4.13	Uncertainty in Measurement of Observables	29
5	Quantum Dynamics	30
5.1	Time Dependence in Quantum Mechanics	30
6	Continuous Observables in Quantum Mechanics	36
6.1	Transition to Infinite Dimensions	36
6.2	Infinite Square Well Potential	41
	Probability Density	43
	Zero Point Energy	43
	Completeness and Orthonormality	43
	Symmetry	43
6.3	Harmonic Oscillator Potential	44
6.4	Harmonic Oscillator - Algebraic Method	44
6.5	Time Dependance for Continuous Observables	48
7	Free Particle	51
8	Tutorials	52
8.1	Tutorial 1	52
8.2	Tutorial 2	53
8.3	Tutorial 3	53
8.4	Tutorial 4	53
8.5	Tutorial 5	55

Abstract

These notes are intended as a resource for myself; past, present, or future students of this course, and anyone interested in the material. The goal is to provide an end-to-end resource that covers all material discussed in the course displayed in an organized manner. If you spot any errors or would like to contribute, please contact me directly.

Robert Hill is a low temperature experimentalist, but this course will be mostly theoretical.

Albert Einstein once said, "Quantum mechanics is certainly imposing. But an inner voice tells me that it is not yet the real thing. The theory says a lot, but does not really bring us any closer to the secret of the 'old one'. I, at any rate, am convinced that He does not throw dice."

Richard Feynman said "I think I can safely say that nobody understand quantum mechanics."

So we're in for miserable experience with this course then? Well not really, there are some good reasons to study Quantum Physics:

- It's Extremely interesting!
 - Physically
 - Mathematically
 - Philosophically
- It is the science behind future technology!
- Waterloo is Quantum Valley!

1 The Photoelectric and Compton Effects

1.1 Historical Background

In classical physics we always observed things as behaving like waves or as particles. For example, there is

- Particle-like behaviour of radiation
- Wave-like behaviour of matter
- Wave-particle duality that combines the two

Let's explore the two sides of the coin. First, **what is a particle?** Some words that describe it are *point*, localised, mass, solid and similarly **what is a wave?** It can be described with words like *interference*, *oscillation*, *delocalised*, and *medium*. One such thing that we have had trouble with describing is **light**. Is it a wave or a particle?

1.2 Einstein's Theory of Photoelectric Effect

Radiant energy (light) is quantized into concentrated bundles (photons)

$$E = hf$$

His Photoelectric Equation (1905) states that

$$K_{\max} = hf - \omega_0$$

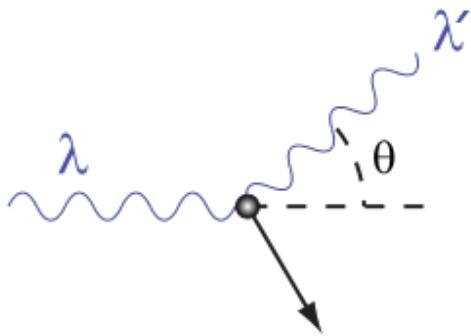


Figure 1.1: The Compton Effect. The scattered light has a different frequency; the frequency depends on the direction. A bigger deflection causes a bigger change in frequency.

1.3 Compton Effect

In the photoelectric effect, we treated light as being composed of individual light particles, called photons, that carry some energy. It then makes sense to think that the photons also have momentum.

Electromagnetic radiation is scattered by a target object. In classical theory, the charges in the target object will respond to the incoming wave and start to oscillate. All oscillating charges emit radiation at the frequency of oscillation, and this newly generated set of waves can also be detected at an angle θ with respect to the incoming wave. This classical model explains why the sky is blue and all that jazz. The scattering process itself, though, does not change the frequency of incoming and outgoing radiation.

However, an experimental problem occurred. In experiments with X-ray radiation on a graphene target, one observes that two separate frequencies at an angle θ result in different intensities. This effect is independent of the material, though intensities may vary.

Definition 1.1 (Compton Shift).

$$\Delta\lambda = \lambda_c(1 - \cos\theta)$$

Definition 1.2 (Compton wavelength).

$$\lambda_c = \frac{h}{m_0c}$$

2 De Broglie Wavelength and the Davisson-Germer Experiment

We have shown that wave phenomena can exhibit particle features. We can rewrite the momentum instead as $p = \frac{h}{\lambda}$ using a simple wave relationship. There is nothing in this reformed equation that has to do with light. This led to the following postulate.

2.1 The De Broglie Postulate (1924)

De Broglie's hypothesis was based on the grand symmetry of nature; if radiation has wave-particle duality, then so should matter.

Definition 2.1 (de Broglie Relation).

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

2.2 The Davisson-Germer Experiment

We must first understand the Bragg Grating; it is an optical filter that reflects particular wavelengths and transmits all others. Note that reflection, however, is common to both waves and particles.

2.3 Final Words

The observation of both phenomena in one and the same experiment leads us also to the concept of delocalization, which goes beyond the simple concept of "being extended", because single quantum objects seem to be able to simultaneously explore regions in space-time that cannot be explored by a single object in any classical way.

3 Linear Algebra Review

We're going to begin by reviewing some mathematics that will be needed in the course. This is a physics course so we're going to be a little loosey-goosey.

3.1 Vector Spaces

Definition 3.1 (Vector Space). A **vector space** consists of a set of vectors : $(|\alpha\rangle, |\beta\rangle, |\gamma\rangle, \dots)$ which is closed under vector addition and scalar multiplication.

Vector Addition produces another vector, that is

$$|\alpha\rangle + |\beta\rangle = |\gamma\rangle$$

it is also commutative

$$|\alpha\rangle + |\beta\rangle = |\beta\rangle + |\alpha\rangle$$

and associative

$$|\alpha\rangle + (|\beta\rangle + |\gamma\rangle) = (|\alpha\rangle + |\beta\rangle) + |\gamma\rangle$$

The null vector exists such that $|\alpha\rangle + |0\rangle = |\alpha\rangle$, and of course there is the inverse vector such that $|\alpha\rangle + |- \alpha\rangle = |0\rangle$.

Scalar Multiplication: The product of a scalar with a vector is another vector ($a|\alpha\rangle = |\gamma\rangle$). Note that scalar multiplication is distributive with respect to vector addition

$$a(|\alpha\rangle + |\beta\rangle) = a|\alpha\rangle + a|\beta\rangle$$

Scalar multiplication is distributive with respect to scalar addition too

$$(a + b)|\alpha\rangle = a|\alpha\rangle + b|\alpha\rangle$$

and it is associative with respect to the product of scalars.

$$a(b|\alpha\rangle) = (ab)|\alpha\rangle$$

then multiplication by zero and by ± 1 has

$$0|\alpha\rangle = |0\rangle, \quad 1|\alpha\rangle = |\alpha\rangle, \quad -1|\alpha\rangle = -|\alpha\rangle = |- \alpha\rangle$$

Linear Combinations of Vectors: To generate a linear combination of vectors

$$|\lambda\rangle = a|\alpha\rangle + b|\beta\rangle + c|\gamma\rangle$$

- (I) Any vector is linearly independent of a set of vectors if it cannot be written as a linear combination of them.
- (II) A set of vectors is linearly independent if each is linearly independent of the rest.
- (III) A collection of vectors is said to **span** the space if every vector can be written as a linear combination of them.
- (IV) A set of linearly independent vectors that span a space is called a **basis**.
- (V) The number of vectors in the basis is called the **dimension** of the space.

Co-ordinate Representation: With respect to a given basis, $|e_1\rangle, |e_2\rangle, |e_3\rangle, \dots, |e_n\rangle$, any given vector $|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle + \dots + a_n|e_n\rangle$ is uniquely defined by the ordered n -tuple of its components.

$$|\alpha\rangle \iff \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

(the co-ordinate representation of $|\alpha\rangle$ with respect to the basis given by each $|e_i\rangle$.)

Coordinates depend on the chosen basis. In basis 1 $|\alpha\rangle = a_x|x\rangle + a_y|y\rangle \iff \begin{pmatrix} a_x \\ a_y \end{pmatrix}$ and then in basis 2 we see $|\alpha\rangle = a_{x'}|x'\rangle + a_{y'}|y'\rangle \iff \begin{pmatrix} a_{x'} \\ a_{y'} \end{pmatrix}$.

Addition of vectors by adding corresponding components (when in the same basis) works as you might expect, too:

$$|\alpha\rangle + |\beta\rangle \iff (a_1 + b_1, a_2 + b_2, \dots, a_n + b_n)$$

Also, scalar multiplication works by multiplying the scalar in each component

$$c|\alpha\rangle \iff (ca_1, ca_2, ca_3, \dots, ca_n)$$

so of course,

$$|0\rangle = (0, 0, 0, \dots, 0), \quad |- \alpha\rangle = (-a_1, -a_2, \dots, -a_n)$$

Inner Product: For every vector, $|\alpha\rangle$, in a vector space there exists a dual vector $\langle\alpha|$ in a corresponding dual vector space. Importantly, the dual vector to $c|\alpha\rangle$ is $C^* \langle\alpha|$ where $*$ denotes complex conjugation. So the inner product of $|\alpha\rangle$ and $|\beta\rangle$ is $\langle\alpha|\beta\rangle$ which is a scalar (complex number), hence $\langle\alpha|\beta\rangle$ is sometimes called **scalar product**.

- (I) $\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^*$
- (II) $\langle\alpha|\alpha\rangle \geq 0$ (real and positive), so $\langle\alpha|\alpha\rangle = 0$ if $|\alpha\rangle = |0\rangle$.

(III) The norm of a vector $\|\alpha\| = \sqrt{\langle \alpha | \alpha \rangle}$ generalized "length" of a vector.

(IV) Normalized $\|\alpha\| = 1$.

(V) Orthogonal if $\langle \alpha | \beta \rangle = 0$, then $|\alpha\rangle$ is orthogonal to $|\beta\rangle$.

(VI) Orthogonal set $\langle a_i | a_j \rangle = \delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$

Consider the orthonormal basis $|e_1\rangle, |e_2\rangle, \dots, |e_n\rangle$, and

$$|\alpha\rangle = a_1 |e_1\rangle + a_2 |e_2\rangle + \dots + a_n |e_n\rangle$$

$$|\beta\rangle = b_1 |e_1\rangle + b_2 |e_2\rangle + \dots + b_n |e_n\rangle$$

where we have the column vectors

$$|\alpha\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} \quad |\beta\rangle = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

then with dual vectors

$$|\alpha\rangle = a_1^* |e_1\rangle + a_2^* |e_2\rangle + \dots + a_n^* |e_n\rangle$$

$$|\beta\rangle = b_1^* |e_1\rangle + b_2^* |e_2\rangle + \dots + b_n^* |e_n\rangle$$

so that we have row vectors

$$|\alpha\rangle = (a_1^*, a_2^*, \dots, a_n^*) \quad |\beta\rangle = (b_1^*, b_2^*, \dots, b_n^*)$$

Now we can see that these results interact in a kind of cool way, check this out:

$$\langle \alpha | \beta \rangle = (a_1^*, a_2^*, \dots, a_n^*) \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix} = a_1^* b_1 + a_2^* b_2 + \dots + a_n^* b_n$$

which is a complex number. The components of the linear expansion are inner products too:

$$|\alpha\rangle = a_1 |e_1\rangle + a_2 |e_2\rangle + \dots + a_n |e_n\rangle$$

Consider also that

$$\langle e_1 | \alpha \rangle = \langle e_1 | (a_1 |e_1\rangle + a_2 |e_2\rangle + \dots + a_n |e_n\rangle) \rangle = a_1 \langle e_1 | e_1 \rangle + a_2 \langle e_1 | e_2 \rangle + \dots + a_n \langle e_1 | e_n \rangle = a_1$$

3.2 Matrices

Matrices represent linear transformations that take a vector in a vector space and map it to another vector.

$$|\alpha\rangle \longrightarrow |\alpha'\rangle = \hat{T} |\alpha\rangle$$

The transformation must be linear

$$\hat{T}(a |\alpha\rangle + b |\beta\rangle) = a \hat{T} |\alpha\rangle + b \hat{T} |\beta\rangle$$

Consider \hat{T} acting on n basic vectors, $|e_i\rangle$

$$\hat{T}|e_1\rangle = T_{11}|e_1\rangle + T_{21}|e_2\rangle + \dots + T_{n1}|e_n\rangle$$

That is, $|e_1\rangle$ is mapped to a new vector written as a linear combination of basis vectors, likewise

$$\begin{aligned}\hat{T}|e_2\rangle &= T_{12}|e_1\rangle + T_{22}|e_2\rangle + \dots + T_{n2}|e_n\rangle \\ &\vdots \\ \hat{T}|e_n\rangle &= T_{1n}|e_1\rangle + T_{2n}|e_2\rangle + \dots + T_{nn}|e_n\rangle\end{aligned}$$

which can be compactly expressed

$$\hat{T}|e_j\rangle = \sum_{i=1}^n T_{ij}|e_i\rangle \quad (j = 1, 2, \dots, n)$$

If $|\alpha\rangle$ is an arbitrary vector, expressed in terms of basis $|e_i\rangle$'s

$$|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle + \dots + a_n|e_n\rangle = \sum_{j=1}^n a_j|e_j\rangle$$

(and recall $a_i = \langle e_1 | \alpha \rangle$). Then the effect of \hat{T} on $|\alpha\rangle$ is

$$\hat{T}|\alpha\rangle = \sum_{j=1}^n a_j \hat{T}|e_j\rangle = \sum_{j=1}^n \sum_{i=1}^n a_j T_{ij}|e_i\rangle = \sum_{i=1}^n \left(\sum_{j=1}^n T_{ij} a_j \right) |e_i\rangle$$

Hence \hat{T} takes a vector $|\alpha\rangle$, with components a_1, a_2, \dots, a_n and maps to a new vector α' with components $a'_i = \sum_{j=1}^n T_{ij} a_j$. So \hat{T} is characterized by n^2 elements, T_{ij} , which depend on the chosen basis. Express \hat{T} as a matrix.

$$\begin{pmatrix} T_{11} & T_{12} & \dots & T_{1n} \\ T_{21} & T_{22} & \dots & T_{2n} \\ \vdots & \ddots & \ddots & \vdots \\ T_{n1} & T_{n2} & \dots & T_{nn} \end{pmatrix}$$

where T_{ij} is a matrix element, the row is i and column j . Now if we want to express \hat{T} with respect to a particular set of basis vectors, the i -th element will define the values of matrix elements T_{ij}

$$\hat{T}|e_j\rangle = \sum_{i=1}^n |e_i\rangle \quad (j = 1, 2, \dots, n)$$

multiply on left by basis vector $|e_k\rangle$,

$$\begin{aligned}\langle e_k | \hat{T} | e_j \rangle &= \langle e_k | \sum_{i=1}^n T_{ij} | e_i \rangle \\ &= \langle e_k | (T_{1j} | e_1 \rangle + T_{2j} | e_2 \rangle + \dots + T_{nj} | e_n \rangle) \\ &= (T_{1j} = \langle e_k | e_1 \rangle + T_{2j} \langle e_k | e_2 \rangle + \dots + T_{kj} \langle e_k | e_k \rangle + \dots + T_{nj} \langle e_k | e_n \rangle)\end{aligned}$$

where all terms except $\langle e_k | e_k \rangle$ go to 0. Now apply the orthonormal property of basis vectors $|e_i\rangle$ and thus

$$\langle e_k | \hat{T} | e_j \rangle = T_{kj} \quad \text{matrix element}$$

Once the basis is chosen, the i -th element will define the vector in coordinate representation and the linear transformation in matrix form.

Some matrix terminology,

Definition 3.2 (transpose). The interchange of rows and columns of the matrix. Transpose of column is row and vice versa. The transpose of a square matrix is to reflect elements in main diagonal.

Definition 3.3 (symmetric). A matrix is equal to its transpose (square matrices only).

Definition 3.4 (conjugate). The complex conjugate of every element.

Definition 3.5 (adjoint). The conjugate transpose of a matrix. Indicated by a dagger symbol \hat{T}^\dagger . A square matrix is **Hermitian** if matrix and adjoint are equal $\hat{T} = \hat{T}^\dagger$. Vector space and dual are related by adjoint.

$$|\alpha\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} = a \implies \text{DUAL} = a^\dagger = (a_1^*, a_2^*, \dots, a_n^*)$$

The inner product $\langle \alpha | \beta \rangle = a^\dagger b$.

Definition 3.6 (product). Multiplication may not be commutative : $\hat{T}\hat{S} \neq \hat{S}\hat{T}$. The difference between orders is commutator

$$[\hat{S}, \hat{T}] = \hat{S}\hat{T} - \hat{T}\hat{S} \quad (\text{will be zero if } \hat{T} \text{ and } \hat{S} \text{ commute})$$

Definition 3.7 (eigenvalues, eigenvectors). Every linear transformation has special vectors that transform into scalar multiples of themselves.

$$\hat{T} |\alpha\rangle = \lambda |\alpha\rangle$$

where $|\alpha\rangle$ is the eigenvector, and λ is the eigenvalue.

Example 3.1. Find the eigenvalues and normalized eigenvectors of $\begin{pmatrix} 5 & -2 \\ -2 & 2 \end{pmatrix}$.

$$\begin{vmatrix} 5 - \lambda & -2 \\ -2 & 2 - \lambda \end{vmatrix} = 0 \quad (\text{Characteristic Equation})$$

This resolves to solving

$$\begin{aligned} (5 - \lambda)(2 - \lambda) - (-2)(-2) &= 0 \\ (\lambda - 1)(\lambda - 6) &= 0 \end{aligned}$$

Therefore $\lambda = 1$ or $\lambda = 6$ are eigenvalues. Eigenvectors

$$\bullet \lambda_1 = 1 \implies |\lambda_1\rangle = \begin{pmatrix} x_1 \\ y_1 \end{pmatrix}$$

$$\begin{pmatrix} 5 & -2 \\ -2 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ y_1 \end{pmatrix} = 1 \begin{pmatrix} x_1 \\ y_1 \end{pmatrix} \implies 5x_1 - 2y_1 = x_1 \text{ and } -2x_1 + 2y_1 = y_1$$

Rearranging these equations gives us that $2x_1 - y_1 = 0$. This means that any vector on the line $2x_1 - y_1 = 0$ is an eigenvector. So one possible vector is $|\lambda_1\rangle = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$. Now we can normalize by introducing a normalization constant,

$$|\lambda_1\rangle = a \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

then

$$\sqrt{\langle\lambda_1|\lambda_1\rangle} = 1 \implies \left(a(1, 2) \begin{pmatrix} 1 \\ 2 \end{pmatrix}\right)^{\frac{1}{2}} = a\sqrt{5} = 1 \implies a = \frac{1}{\sqrt{5}} \implies |\lambda_1\rangle = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

4 Introduction to the Formalism and Structure of Quantum Mechanics

We're going to cover a few topics including Angular Momentum and Spin, the Stern-Gerlach Experiment, Quantum State Vectors, Computing Probabilities, and Operators and Measure.

4.1 Angular Momentum and Spin

Angular momentum and magnetic dipole moment (orbital). Consider an electron in a circular orbit, it has radius r , tangential velocity \vec{v} , and current going in the opposite direction of travel I , as well as dipole moment $\vec{\mu}_L$ and angular momentum \vec{L} . Now, to calculate the magnitude of the dipole moment,

$$\begin{aligned} |\vec{\mu}_L| &= IA \quad (\text{product of current and area}) \\ &= \frac{e}{T} \pi r^2 \quad (T = \text{period of electron}) \\ &= \frac{e}{\left(\frac{2\pi r}{v}\right)} \pi r^2 \\ &= \frac{e}{2} vr \\ &= \frac{e}{2m_e} m_e vr \\ &= \frac{e}{2m_e} |\vec{L}| \end{aligned}$$

The direction of $\vec{\mu}_L$ (follow the usual right hand rule)

$$\vec{\mu}_L = -\frac{e}{2m_e} \vec{L}$$

Next, we want to talk a little bit about **spin**. Spin is the intrinsic angular momentum \vec{S} which leads to an intrinsic dipole moment $\vec{\mu}_S$. This intrinsic property is a fundamental nature of particle and cannot be taken away (c.f., mass or charge). In analogy with orbital angular momentum,

$$\vec{\mu}_S = g \frac{q}{2m} \vec{S}$$

where g is the **gyromagnetic ratio**, q is the **charge**, and m is the **mass** of the particle.

For an electron, $g \approx 2$, $q = -e$, $m = m_e$, which means

$$\vec{\mu}_S = -\frac{e}{m_e} \vec{S}$$

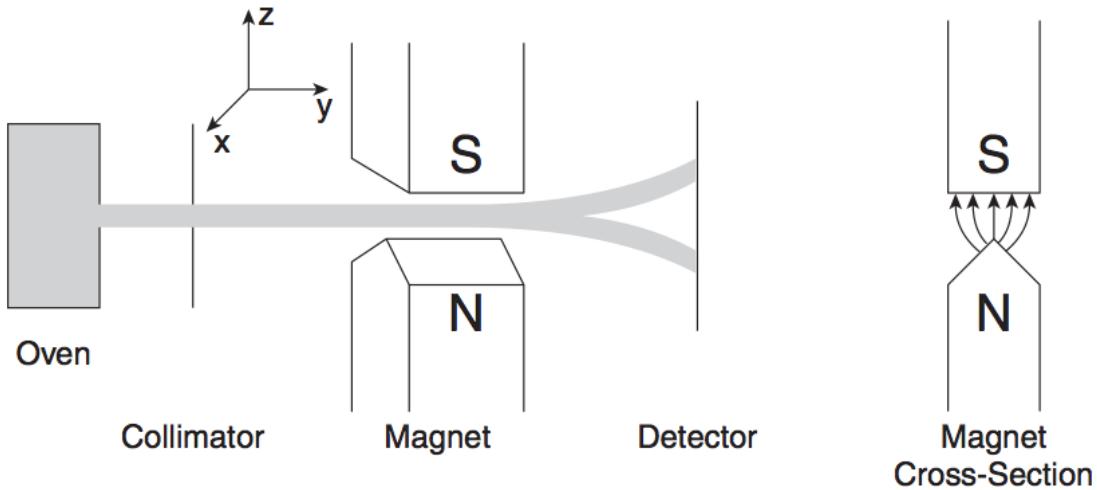


Figure 4.1: Stern-Gerlach experiment to measure the spin component of neutral particles along the z -axis. The magnet cross section at right shows the inhomogeneous field used in the experiment.

4.2 Stern Gerlach Experiments

This experiment was designed to measure the magnetic dipole moment of a particle (atom). A beam of atoms is passed through a magnetic field gradient and observations are made as to what happens to the trajectory.

So what are the physics in this experiment?

Potential energy of the magnetic dipole moment $\vec{\mu}$, in external field \vec{B}

$$E_{magn} = -\vec{\mu} \cdot \vec{B}$$

The force is negative of the gradient of the potential energy

$$\vec{F} = -\vec{\nabla}(-\vec{\mu} \cdot \vec{B})$$

In the Stern Gerlach experiment, the field gradient is in the z -direction, so only $\frac{dB_z}{dz} \neq 0$, so

$$\vec{F} = \mu_z \frac{dB_z}{dz} \hat{z} \quad (\hat{z} \text{ is unit vector in } z\text{-direction})$$

Atoms experience a force in the z -direction proportional to the z -component of magnetic dipole moment μ_z because we designed an experiment where only $\frac{dB_z}{dz} \neq 0$.

What is the classical expectation for silver atoms? ($47e^-$, 47 photons, 60/62 neutrons). Note that

$$-\mu_L \text{ or } \mu_S \propto \frac{1}{m}, \quad \text{so only consider electrons } (m_p \approx 2000m_e)$$

and there is only one non-closed (tell electron that contributes to angular momentum), it is in an s-shell ($\vec{L} = 0$), leaving only intrinsic angular momentum. For silver atoms,

$$\vec{\mu} = -g \frac{e}{2m_e} \vec{S} \quad (\text{with } g \approx 2)$$

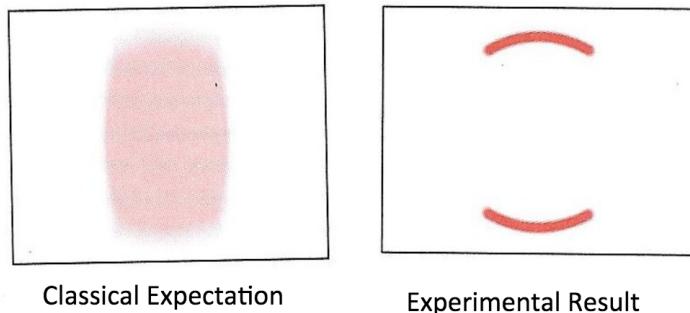


Figure 4.2: Space quantization as it appears in the experimental results of the Stern Gerlach experiment.

For a random gas of atoms, $\vec{\mu}$ is in all directions, so μ_z will have all possible values. So the force will range,

$$-\mu \frac{dB_z}{dz} \leq |\vec{F}| \leq +\mu \frac{dB_z}{dz}$$

which implies a circular beam spread in the z -direction.

It turns out that experimental results reveal that the beam is split into two. This is known as **space quantization**. This indicates that S_z has two possible values,

$$S_z = \pm \frac{\hbar}{2} \quad \left(\hbar = \frac{h}{2\pi} \right)$$

Splitting is associated with the field gradient $\frac{dB_z}{dz}$ since it can change direction and splitting tracks the direction of field gradient. The weird thing here is that **there is no bias to atom deflection**. There is a 50% deflection up rate and 50% deflection down rate. An individual atom is deflected in a probabilistic way. So there is no way of determining precisely what happens to an individual atom.

No what we'd like to do is strip down the experiment to the essentials and introduce language for additional study. First, there are **two possible outcomes**

$$S_z = +\frac{\hbar}{2} \text{ "spin up"} \quad S_z = -\frac{\hbar}{2} \text{ "spin down"}$$

Definition 4.1 (observable). The Quantum Mechanics term for the quantity being measured (S_z in this case.)

Definition 4.2 (analyser). Stern Gerlach device is some form of an analyser ($(x, y, z, \theta, \hat{n})$)

These are being called the essence of quantum mechanics, and there are a number of experiments involved, we're going to analyze each experiment, one by one.

Stern-Gerlach Experiment 1

In this experiment, no atoms are deflected down at the second analyzer. Also, each analyzer plays a different role; the first analyzer **prepared** the beam in a specific quantum state ($|+\rangle$) and so it is a **state preparation device**. The second analyzer **measures** the prepared beam.

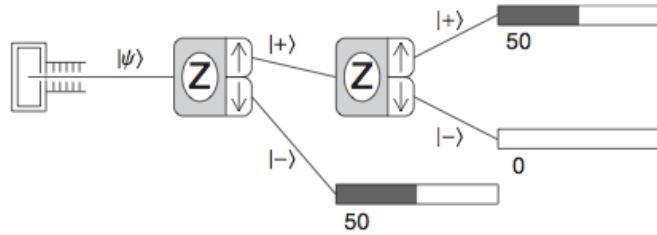


Figure 4.3: Experiment 1

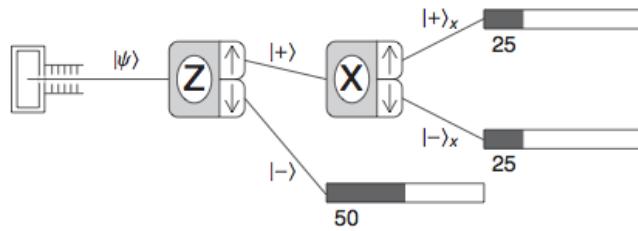


Figure 4.4: Experiment 2

Stern-Gerlach Experiment 2

The X analyzer has field gradient in the x -direction, (90° with respect to the z -direction). Also, atoms leaving spin-up / spin-down part of the X -analyzer have

$$S_x = +\frac{\hbar}{2} \quad / \quad S_x = -\frac{\hbar}{2}$$

For input beam $S_z = +\frac{\hbar}{2} [|+\rangle]$, then 50% are measured to have $S_x = +\frac{\hbar}{2}$. There is the same result for any two different X , Y , or Z analyser combinations.

Stern-Gerlach Experiment 3

Classically, we expect to be able to measure X , Y , and Z components and figure out the total spin direction. Experiment 3 shows this is not possible in quantum mechanics, as information is reset or lost when new measurements are made. This is a very generic and key feature of quantum mechanics and comes down to really the statement that **measurement disturbs the system**. By making a measurement, we change the information of the system. Every time we make a measurement, the system isn't what it was before you made the measurement.

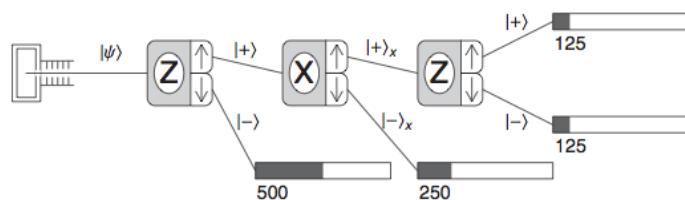


Figure 4.5: Experiment 3

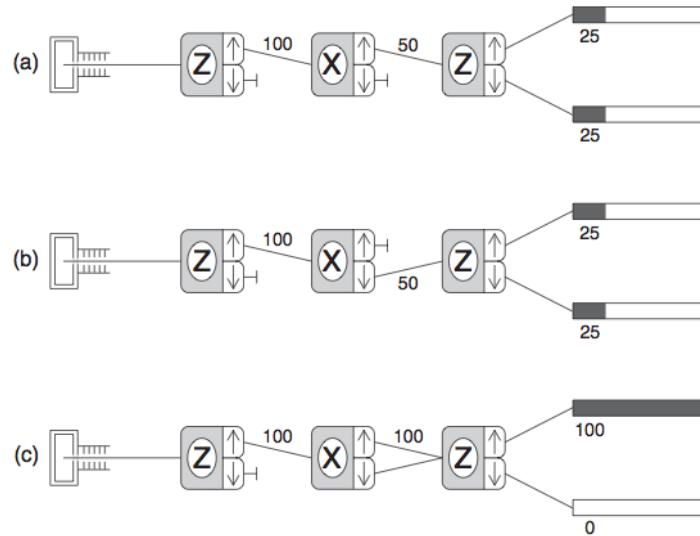


Figure 4.6: Experiment 4

This is a key feature of quantum mechanics. We cannot have simultaneous knowledge of more than one spin component; this is a fundamental incompatibility of knowing spin components along two or more directions. We can say that in quantum mechanics, S_x , S_y , S_z are **incompatible observables**. More specifically then, the state represented by $|+\rangle_z = |S_z = +\frac{\hbar}{2}\rangle$ or $|+\rangle_x = |S_x = +\frac{\hbar}{2}\rangle$ but **not** $|S_z = +\frac{\hbar}{2}, S_x = +\frac{\hbar}{2}\rangle$.

Stern-Gerlach Experiment 4

The first two demonstrate experiment 3 for both parts of the middle X analyzer independently. The third one gives a surprising result, allowing both parts into the Z analyzer simultaneously then it is as if the middle measurement had not occurred. This is reminiscent of interference; adding two outputs results in enhancement in one sector and reduction or cancellation in the other.

In summary,

- Experiment 1: State preparation. If we know the input state and choose an appropriate experiment, we remeasure the state with certainty.
- Experiment 2: Probabilistic nature of quantum measurement when the measurement is not matched to the input state.
- Experiment 3: Measurement disturbs the system leading to incompatible observables.
- Experiment 4: Quantum mechanical interference effects can be observed.

4.3 Quantum State Vectors

Definition 4.3 (Postulate 1). We label the input state with a left **ket**, ($|\Psi\rangle$), and label the output states with $|+\rangle$ for spin up and $|-\rangle$ for spin down.

Thus the ket, $|\Psi\rangle$ is part of a vector space called a **Hilbert Space**. The dimensionality of the Hilbert Space depends on the **observable**. For the S_z observable (z -component of angular momentum), it has two possible values,

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

Each value is associated with a state vector $|+\rangle$, $|-\rangle$ (note that no subscript will in general mean the z -direction, which is just our notation here), so the Hilbert Space is 2D.

- Much like $\hat{x}, \hat{y}, \hat{z}$ vectors span 3D geometric space, the kets $|+\rangle$ and $|-\rangle$ span the 2D Hilbert Space associated with observable S_z .
- They are **complete** (only 2 possible outcomes).
- They are **orthogonal**; the result is either spin up or spin down.
- They are also **normalised**; All Quantum state vectors can (or should be) normalized such that $\langle\Psi|\Psi\rangle = 1$.

Orthonormal properties are characterised mathematically as

$$\begin{aligned}\langle +|+ \rangle &= 1 & \langle +|- \rangle &= 0 \\ \langle -|- \rangle &= 1 & \langle -|+ \rangle &= 0\end{aligned}$$

Completeness ensures that $|+\rangle, |-\rangle$ can be used as a basis to express any general Quantum Mechanical state as a linear combination of them

$$\text{General State Vector} \quad |\Psi\rangle = a|+\rangle + b|-\rangle \quad \text{with } a, b \text{ complex scalars}$$

The coefficients are inner products, for example consider multiplying on the left by $|+\rangle$,

$$\begin{aligned}\langle +|\Psi \rangle &= \langle +|(a|+ \rangle + b|-\rangle) \rangle \\ &= a\langle +|+ \rangle + b\langle +|- \rangle \\ &= a(1) + b(0) \\ &= a\end{aligned}$$

Likewise, $\langle -|\Psi \rangle = b$. Therfore,

$$|\Psi\rangle = (\langle +|\Psi \rangle)|+ \rangle + (\langle -|\Psi \rangle)|- \rangle$$

As an aside, the $\langle +|$ is the bra to the $|+$, so together $\langle +|+$ is a bra-ket. \therefore .

The dual vector (bra) to the Quantum Mechanical ket $|\Psi\rangle$:

$$\begin{aligned}\langle \Psi| &= a^* \langle +| + b^* \langle -| \\ \langle \Psi|+ \rangle &= a^* \langle +|+ \rangle + b^* \langle -|+ \rangle = a^*\end{aligned}$$

Hence,

$$\langle \Psi|+ \rangle = a^* = (a)^* = (\langle +|\Psi \rangle)^* = \langle +|\Psi \rangle^*$$

Finally,

$$\langle \Psi| = (\langle \Psi|+ \rangle)\langle +| + (\langle +|- \rangle)\langle -|$$

In Quantum Mechanics we require that all kets (vectors) are normalized.

Example 4.1. Given a general quantum state vector expressed as a linear combination of the basis kets for the 2D Hilbert Space associated with the S_z observable:

$$|\Psi\rangle = a|+\rangle + b|-\rangle$$

Derive an expression for the coefficients, a and b , which when satisfied ensure that $|\Psi\rangle$ is normalized.

First we normalize $|\Psi\rangle$, so

$$\begin{aligned}\langle\Psi|\Psi\rangle &= 1 \\ &= (a^* \langle+| + b^* \langle-|)(a|+\rangle + b|-\rangle) \\ &= a^*a \langle+|+ + a^*b \langle+|-\rangle + b^*a \langle-|+ + b^*b \langle-|- \\ &= a^*a + b^*b \\ &= 1 \quad (\text{requires normalization}) \\ &= |a|^2 + |b|^2\end{aligned}$$

or since

$$\begin{aligned}a &= \langle+|\Psi\rangle & a^* &= \langle\Psi|+\\ b &= \langle-|\Psi\rangle & b^* &= \langle\Psi|-\\ \end{aligned}$$

which implies

$$|\langle+|\Psi\rangle|^2 + |\langle-|\Psi\rangle|^2 = 1$$

Definition 4.4 (Postulate 4). The probability of obtaining the value $\pm\frac{\hbar}{2}$ in a measurement of the observable S_z on a system in the state $|\Psi\rangle$ is

$$P_{\pm} = |\langle\pm|\Psi\rangle|^2$$

where $|\pm\rangle$ is the basis ket of S_z corresponding to the result $\pm\frac{\hbar}{2}$.

- (i) $\langle+|\Psi\rangle$ is the **Probability Amplitude**, it must be "squared" (multiply by the complex conjugate) to get a probability.
- (ii) Convention is usually to put order of the inner product as $\langle\text{out}|\text{in}\rangle$ but since

$$P = |\langle\text{out}|\text{in}\rangle|^2 = \langle\text{out}|\text{in}\rangle \langle\text{in}|\text{out}\rangle$$

it doesn't really matter.

$|\text{in}\rangle$ is the input state, and $|\text{out}\rangle$ is the output state, whose probability for measurement we are calculating.

Example 4.2. A Z-analyzer is used to prepare atoms in the state "spin-up". The spin state if these atoms is then measured using a 2nd Z-analyzer. What is the probability that these atoms are measured as "spin-up" and "spin-down"?

$$P = |\langle\text{out}|\text{in}\rangle|^2 \quad \text{Postulate 4}$$

The first analyzer prepares the input state to the 2nd analyzer : $|\text{in}\rangle = |+\rangle$. The probability when $|\text{out}\rangle = |+\rangle$ implies that

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

then similary for when $|out\rangle = |-\rangle$ we get

$$P_- = |\langle -|+\rangle|^2 = 0$$

This agrees perfectly with our observations for Stern Gerlach Experiment 1.

Quantum State Tomography is a way of determining the quantum state based on results of measurement and is the name of this method.

With regards to Stern Gerlach Experiment 2, let's apply this method:

The input state is $|+\rangle$ and we measure S_x with output states $|+\rangle_x$ with probability $\frac{1}{2}$ and $|-\rangle_x$ with probability $\frac{1}{2}$ (giving a sum probability of 1). Next we formulate mathematically using [Postulate 4](#) :

$$P = |\langle \text{out}|\text{in}\rangle|^2$$

So,

$$|\text{in}\rangle = |+\rangle \implies P_{+x} = |_x\langle +|+\rangle|^2 = \frac{1}{2} \quad (1)$$

$$P_{-x} = |_x\langle -|+\rangle|^2 = \frac{1}{2} \quad (2)$$

and the result should be the same if $|\text{in}\rangle = |-\rangle$ (Experiment 4b)

$$|\text{in}\rangle = |-\rangle \implies P_{+x} = |_x\langle +|- \rangle|^2 = \frac{1}{2} \quad (3)$$

$$P_{-x} = |_x\langle -|- \rangle|^2 = \frac{1}{2} \quad (4)$$

Since $|+\rangle$ and $|-\rangle$ are basis states that SPAN the 2D Hilbert Space then kets for outputs of other Stern Gerlach measurements can be expressed as linear combinations of them. For example, S_x output states

$$|+\rangle_x = a|+\rangle + b|-\rangle$$

$$|-\rangle_x = c|+\rangle + d|-\rangle$$

for $a, b, c, d \in \mathbb{C}$. Now,

$$\begin{aligned} P_{+x} &= |_x\langle +|+\rangle|^2 = |(a^*\langle +| + b^*\langle -|)|+\rangle|^2 \\ &= |a^*\langle +|+\rangle + b^*\langle -|+\rangle|^2 \\ &= |a|^2 \\ &= \frac{1}{2} \quad (\text{from experiment}) \end{aligned}$$

Similary we can use (2), (3), and (4) to show that $|b|^2 = |c|^2 = |d|^2 = \frac{1}{2}$.

The coefficients a, b, c, d are complex numbers implying that the amplitude of the phase is

$$re^{i\theta}$$

Note. The overall phase (global phase) of a quantum state vector is not physically meaningful - this means it doesn't affect the computation of probabilities (Assignment 3).

Only the relative phase between components of a ket (vector) is important, that is between a and b or c and d . This means that we chose one component to be real ($\theta = 0$) and one complex ($\theta \neq 0$).

Say $a = r_1 e^{i\theta_1}$ and $b = r_2 e^{i\theta_2}$, then only $\theta_2 - \theta_1$ matters for quantum mechanics so we rotate the vectors to make one real.

This means we can solve for a , b , c , and d in the following way

$$\begin{aligned} |+\rangle_x &= \frac{1}{\sqrt{2}} |+\rangle + \frac{1}{\sqrt{2}} e^{i\alpha} |-\rangle \\ |-\rangle_x &= \frac{1}{\sqrt{2}} |+\rangle + \frac{1}{\sqrt{2}} e^{i\beta} |-\rangle \end{aligned}$$

We still need to determine the phases α and β . We can check,

$$P_{+x} = |\langle \text{out} | \text{in} \rangle|^2 = \left| \left(\frac{1}{\sqrt{2}} |+\rangle + \frac{1}{\sqrt{2}} e^{i\alpha} |-\rangle \right) |+\rangle \right|^2 = \frac{1}{2}$$

If we consider experiment 1 with an X -analyser, we would establish orthonormal properties of $|+\rangle_x$ and $|-\rangle_x$. That is,

$$\begin{aligned} {}_x \langle +|+ \rangle_x &= {}_x \langle -| - \rangle_x = 1 \quad (\text{normalized}) \\ {}_x \langle +|- \rangle_x &= {}_x \langle -|+ \rangle_x = 0 \quad (\text{orthogonal}) \end{aligned}$$

Also, orthogonality shows

$$\begin{aligned} {}_x \langle +|+ \rangle_x &= \frac{1}{\sqrt{2}} (|+\rangle + e^{-i\beta} |-\rangle) \cdot \frac{1}{\sqrt{2}} (|+\rangle + e^{i\alpha} |-\rangle) = 0 \\ &= \frac{1}{2} \left(\cancel{\langle +|+ \rangle^1} + e^{-i\beta} \cancel{\langle -|+ \rangle^0} + e^{-i\alpha} \cancel{\langle +|- \rangle^0} + e^{i(\alpha-\beta)} \cancel{\langle -|- \rangle^1} \right) = 0 \\ &\implies \frac{1}{2} (1 + e^{i(\alpha-\beta)}) = 0 \\ &\implies e^{i\alpha} = -e^{i\beta} \end{aligned}$$

This is all the information we have to determine α and β . So, we choose $\alpha = 0$, so $e^{i\alpha}$ and $e^{i\beta} = -1$. Thus,

$$\begin{aligned} |+\rangle_x &= \frac{1}{\sqrt{2}} (|+\rangle + |-\rangle) \\ |-\rangle_x &= \frac{1}{\sqrt{2}} (|+\rangle - |-\rangle) \end{aligned}$$

Similar analysis leads to,

$$\begin{aligned} |+\rangle_y &= \frac{1}{\sqrt{2}} (|+ \rangle + i |-\rangle) \\ |-\rangle_y &= \frac{1}{\sqrt{2}} (|+ \rangle - i |-\rangle) \end{aligned}$$

4.4 Matrix Notation

If an ordered set of vectors is chosen as a basis, then we can express a general state as a linear combination of them.

$$|\Psi\rangle = a |+\rangle + b |-\rangle$$

or as an ordered array of coefficients a, b in co-ordinate representation.

$$|+\rangle \xrightarrow[\text{basis}]{S_z} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \langle +|\Psi\rangle \\ \langle -|\Psi\rangle \end{pmatrix} \quad (\text{column vector})$$

$$\begin{aligned} |\Psi\rangle &= |+\rangle_x = \frac{1}{\sqrt{2}} |+\rangle + \frac{1}{\sqrt{2}} |-\rangle \xrightarrow[\text{basis}]{S_z} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ |\Psi\rangle &= |-\rangle_y = \frac{1}{\sqrt{2}} |+\rangle - \frac{i}{\sqrt{2}} |-\rangle \xrightarrow[\text{basis}]{S_z} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} \end{aligned}$$

Note. Basis vectors are unit vectors when expressed in co-ordinate representation with respect to their own basis. For example,

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

For the dual space,

$$|\Psi\rangle = a^* \langle +| + b^* \langle -| \xrightarrow[\text{basis}]{S_z} (a^*, b^*) \quad \text{row vector}$$

remember that the bra is the conjugate transpose of ket. So for the inner product,

$$\langle \Psi | \Psi \rangle = (a^* \ b^*) \begin{pmatrix} a \\ b \end{pmatrix} = |a|^2 + |b|^2$$

Let's revisit $|\pm\rangle_y$ in Matrix Notation, first consider experiment 2, but with X , replaced by Y (the probabilities measured will be the same).

Then, if $|in\rangle = |+\rangle$,

$$\begin{aligned} Prob_{+y} &= |_y \langle +| + \rangle|^2 = \frac{1}{2} \\ Prob_{-y} &= |_y \langle -| + \rangle|^2 = \frac{1}{2} \end{aligned}$$

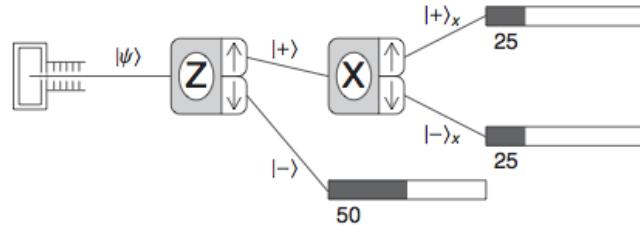


Figure 4.7: Experiment 2

otherwise if $|\text{in}\rangle = |-\rangle$,

$$\begin{aligned} \text{Prob}_{+y} &= |_y \langle +|-\rangle|^2 = \frac{1}{2} \\ \text{Prob}_{-y} &= |_y \langle -|-\rangle|^2 = \frac{1}{2} \end{aligned}$$

Then if we use $|+\rangle_y = r|+\rangle + s|-\rangle$ and $|-\rangle_y = t|+\rangle + u|-\rangle$ and orthonormality of $|\pm\rangle_y$ to get

$$\begin{aligned} |+\rangle_y &= \frac{1}{\sqrt{2}} (|+\rangle + e^{i\theta} |-\rangle) \xrightarrow[\text{basis}]{S_z} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{i\theta} \end{pmatrix} \\ |-\rangle_y &= \frac{1}{\sqrt{2}} (|+\rangle - e^{i\theta} |-\rangle) \xrightarrow[\text{basis}]{S_z} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -e^{i\theta} \end{pmatrix} \end{aligned}$$

To determine the phase angle θ we need to consider Experiment 2 but with state preparation $|\pm\rangle_x$ (not $|\pm\rangle$, (z -analyzer))

$$|\text{in}\rangle = |+\rangle_x \quad \text{Prob}_{+y} = |_y \langle +|+\rangle_x|^2 = \frac{1}{2}$$

compute the inner product using Matrix notation

$$\begin{aligned} |_y \langle +|+\rangle_x &= \frac{1}{\sqrt{2}} (1 \ e^{-i\theta}) \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{2} (1 + e^{-i\theta}) \\ |_y \langle +|+\rangle_x|^2 &= \frac{1}{2} (1 + e^{-i\theta}) \frac{1}{2} (1 + e^{i\theta}) = \frac{1}{4} (1 + e^{-i\theta} + e^{i\theta} + 1) \end{aligned}$$

then using Euler,

$$|_y \langle +|+\rangle_x|^2 = \frac{1}{2} (1 + \cos \theta) = \frac{1}{2} \quad \leftarrow \text{from experiment}$$

which implies $\cos \theta = 0$ and so $\theta = \pm \frac{\pi}{2}$. So the two possible oputcomes correspond to RH or LH orientation of Y with respect to X and Z . Let's choose the RH slution $\theta = \frac{\pi}{2}$ then

$$|+\rangle_y \xrightarrow[\text{basis}]{S_z} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |-\rangle_y \xrightarrow[\text{basis}]{S_z} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

4.5 General Quantum Systems

Consider a measurement of observable A , which yields results a_1, a_2, \dots, a_n (discrete and finite). The states associated with each outcome are described by kets, $|a_1\rangle, |a_2\rangle, \dots, |a_n\rangle$. These kets are orthogonal (in the sense

that any single measurement on a single particle yields only 1 outcome).

$$\text{Mathematically, } \langle a_i | a_j \rangle = \delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}.$$

The set of kets is complete (they span the Hilbert Space associated with observable A). They can be used to express any arbitrary state as a linear combination.

$$|\Psi\rangle = \alpha_1 |\alpha_1\rangle + \alpha_2 |\alpha_2\rangle + \cdots + \alpha_n |\alpha_n\rangle$$

with $\alpha_i = \langle a_1 | \Psi \rangle$. So, given $|\Psi\rangle$ as an input state to a measurement of observable A with results a_i and associates states $|a_i\rangle$, the probability for obtaining result a_i is given by

$$Prob(a_i) = |\langle a_i | \Psi \rangle|^2 \quad [\text{Postulate 4}]$$

Example 4.3. Consider a quantum system with an observable A that has three possible measurement outcomes, with values a_1, a_2 and a_3 . The quantum state associated with each of these outcomes is described by the three orthonormal kets:

$$|a_1\rangle, |a_2\rangle, |a_3\rangle$$

A system is prepared in the state that is a superposition of the three basis kets:

$$|\Psi\rangle = 2|a_1\rangle - 3|a_2\rangle + 4i|a_3\rangle$$

Calculate the probability for each of the possible outcomes if a measurement of A is made on the state.

So,

$$|in\rangle = |\Psi\rangle = 2|a_1\rangle - 3|a_2\rangle + 4i|a_3\rangle \quad \text{with } |a_1\rangle, |a_2\rangle, |a_3\rangle \text{ orthogonal, normalised basis set}$$

First we normalize the state vector. Let $|\Psi\rangle = C(2|a_1\rangle - 3|a_2\rangle + 4i|a_3\rangle)$, then

$$\begin{aligned} 1 &= \langle \Psi | \Psi \rangle \\ &= C^*(2\langle a_1 | - 3\langle a_2 | - 4i\langle a_3 |)C(2|a_1\rangle - 3|a_2\rangle + 4i|a_3\rangle) \\ &= |C|^2(4\langle a_1 | a_1 \rangle + 9\langle a_2 | a_2 \rangle + 16\langle a_3 | a_3 \rangle) \\ |C|^2 &= \frac{1}{29} \end{aligned}$$

So, $C = \frac{1}{\sqrt{29}}$. Note that I skipped the full expansion, but remember that mismatched bra and ket pairs have inner product 0, and same pairs have inner product 1. Okay then, let's get the probabilities.

$$\begin{aligned}
 Prob_{a_1} &= |\langle \text{out} | \text{in} \rangle|^2 = Prob_{a_1} = |\langle a_1 | \Psi \rangle|^2 \\
 &= \left| \left\langle a_1 \left| \frac{1}{\sqrt{29}} (2|a_1\rangle - 3|a_2\rangle + 4i|a_3\rangle) \right. \right\rangle \right|^2 \\
 &= \left| \frac{1}{\sqrt{29}} \langle a_1 | (2\langle a_1 | a_1 \rangle - 3\langle a_1 | a_2 \rangle + 4i\langle a_1 | a_3 \rangle) \rangle \right|^2 \\
 &= \left| \frac{2}{\sqrt{29}} \right|^2 \\
 &= \frac{4}{29}
 \end{aligned}$$

Likewise, $Prob_{a_2} = \frac{9}{29}$, $Prob_{a_3} = \frac{16}{29}$ (check $Prob_{a_1} + Prob_{a_2} + Prob_{a_3} = 1$)

4.6 Quantum Mechanical Operators and Measurement

The goal is to be able to make prediction about measurements that haven't been done yet.

Operators, Eigenvalues, & Eigenvectors

Definition 4.5 (Postulate 2). A physical observable is represented mathematically by an operator A that acts on kets.

$$A |\Psi\rangle = \phi$$

where A is an operator that represents a physical observable.

For each operator there are "special" (eigen) kets that are not transformed by the operator except for being multiplied by a scalar constant, which has no measureable effect on the state (we will normalize anyway). So,

Eigenvector = unchanged ket (eigenstate, eigenket)

Eigenvalue = multiplicative constant

So, the Eigen-equation is

$$A |\Psi\rangle = a |\Psi\rangle$$

where A is an **operator**, a is an **eigenvalue**, and $|\Psi\rangle$ is an **eigenstate**.

Definition 4.6 (Postulate 3). The only possible result of a measurement of an observable is one of the eigenvalues a_n of the corresponding operator A . Eigenvalues are the outputs of measurements.

Example 4.4. Define operator S_z associated with measurement of the observable that is the z -component of intrinsic angular momentum.

$$\begin{aligned}
 S_z |+\rangle &= +\frac{\hbar}{2} |+\rangle \\
 S_z |-\rangle &= -\frac{\hbar}{2} |-\rangle
 \end{aligned}$$

We are using Abstract notation here. Note that the eigenvalues are $\pm \frac{\hbar}{2}$ and the eigenvectors of S_z are $|\pm\rangle$.

Hermitian Operators

Operators used in Quantum Mechanics are Hermitian operators. This means that the operator is equal to its adjoint (conjugate transpose), that is

$$A = A^\dagger$$

Why Hermitian?

- (i) Eigenvalues of Hermitian operators are real. (Quantum Mechanics interpretation is that they are results of measurements, to they must be real numbers (Energy, position, component of span))
- (ii) Eigenvectors of Hermitian operators form a complete set of basis vectors.
- (iii) Same operator for the dual space vectors. So,

$$A |\alpha\rangle = |\beta\rangle \quad \text{operator } A \text{ acts to right on ket } |\alpha\rangle$$

$$\langle \alpha | B = \langle \gamma | \quad \text{operator } B \text{ acts to left on bra } |\alpha\rangle$$

For $\langle \gamma | = |\beta\rangle$, then $B = A^\dagger$. So if $A = A^\dagger$ then the operator can act to the left or the right to give appropriate dual space relationship. Note that the dual space is transformed in the same way as original space.

$$A |\alpha\rangle = |\beta\rangle$$

$$\langle \alpha | A = \langle \beta |$$

Completeness Relationship

We have already seen operators, but didn't realize it.

$$|\Psi\rangle = a |+\rangle + b |-\rangle \quad \text{with } a = \langle +|\Psi\rangle, b = \langle -|\Psi\rangle$$

$$\begin{aligned} |\Psi\rangle &= \langle +|\Psi\rangle |+\rangle + \langle -|\Psi\rangle |-\rangle \\ &= |+\rangle \langle +|\Psi\rangle + |-\rangle \langle -|\Psi\rangle \\ &= (|+\rangle \langle +|) |\Psi\rangle + (|-\rangle \langle -|) |\Psi\rangle \\ &= (|+\rangle \langle +| + |-\rangle \langle -|) |\Psi\rangle \end{aligned}$$

Hence $|+\rangle \langle +| + |-\rangle \langle -| = \mathbb{1}$, the identity operator. This is known as the completeness relation. Note that $|+\rangle \langle +|$ and $|-\rangle \langle -|$ are projection operators, and are an example of an outer product.

More generally for any orthonormal basis, $|e_1\rangle, |e_2\rangle, \dots, |e_n\rangle$,

$$\sum_{i=1}^n |e_i\rangle \langle e_i| = \mathbb{1} \quad \text{identity}$$

Spectral Decomposition

Clearly there exists a very close relationship between an operator, its eigenvalues, and its eigenvectors. In general, any operator is related to its eigenvectors and eigenvalues by

$$\text{Operator } A = \sum_i a_i |a_i\rangle \langle a_i|$$

where a_i is an eigenvalue and $\langle a_i |$ and $|a_i\rangle$ are eigenvectors (eigenkets).

Example 4.5. Use the eigen-equations for the S_z operator to verify the spectral decomposition relationship.

$$S_z |+\rangle = +\frac{\hbar}{2} |+\rangle, \quad S_z |-\rangle = -\frac{\hbar}{2} |-\rangle \quad \text{are eigen-equations}$$

So we multiply by the appropriate bra,

$$S_z |+\rangle \langle +| = +\frac{\hbar}{2} |+\rangle \langle +|, \quad S_z |-\rangle \langle -| = -\frac{\hbar}{2} |-\rangle \langle -|$$

Add the two equations together and factorize

$$\begin{aligned} S_z |+\rangle \langle +| + S_z |-\rangle \langle -| &= +\frac{\hbar}{2} |+\rangle \langle +| + -\frac{\hbar}{2} |-\rangle \langle -| \\ S_z(|+\rangle \langle +| + |-\rangle \langle -|) &= +\frac{\hbar}{2} |+\rangle \langle +| + -\frac{\hbar}{2} |-\rangle \langle -| \\ S_z &= +\frac{\hbar}{2} |+\rangle \langle +| + -\frac{\hbar}{2} |-\rangle \langle -| \end{aligned}$$

4.7 More on Matrix Notation

Kets are 2D vectors (defined by Hilbert Space for Stern Gerlach experiments), and operators must be a 2×2 matrix. Matrix elements are defined (according to rules of linear algebra) as follows:

$$S_z \xrightarrow[\text{basis}]{S_z} \begin{pmatrix} \langle +| S_z |+ \rangle & \langle +| S_z |-\rangle \\ \langle -| S_z |+ \rangle & \langle -| S_z |-\rangle \end{pmatrix} = \begin{pmatrix} \langle +| \frac{+\hbar}{2} |+ \rangle & \langle +| \frac{-\hbar}{2} |-\rangle \\ \langle -| \frac{+\hbar}{2} |+ \rangle & \langle -| \frac{-\hbar}{2} |-\rangle \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

We can check the math for our eigen-equations

$$S_z \xrightarrow[\text{basis}]{S_z} \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad |+\rangle \xrightarrow[\text{basis}]{S_z} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |-\rangle \xrightarrow[\text{basis}]{S_z} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

We want to see $S_z |+\rangle$,

$$S_z |+\rangle = +\frac{\hbar}{2} |+\rangle \xrightarrow[\text{basis}]{S_z} +\frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = +\frac{\hbar}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Note. Operators are always diagonal in their own basis and eigenvectors are always unit vectors in their own basis.

4.8 Expectation Values

Quantum Mechanics allows us to compute probabilities for outcomes of measurements. Another useful quantity is the mean average value of many repeated measurements on the same initial system. This is known as the expectation value in Quantum Mechanics. Consider observable X with i eigenvalues x_i (measured elements).

$$\text{Expectation Value } \langle x \rangle = \sum_i x_i \text{prob}(x_i)$$

For z -component of angular momentum, characterised by S_z operator with eigenvalues $\pm \frac{\hbar}{2}$,

$$\langle S_z \rangle = +\frac{\hbar}{2} \text{prob}_+ + -\frac{\hbar}{2} \text{prob}_- \quad (1)$$

Given an input state $|\Psi\rangle$,

$$\begin{aligned}\langle S_z \rangle &= +\frac{\hbar}{2} |\langle +|\Psi\rangle|^2 + \frac{-\hbar}{2} |\langle -|\Psi\rangle|^2 \\ &= +\frac{\hbar}{2} (\langle \Psi|+ \rangle \langle +|\Psi\rangle) + \frac{-\hbar}{2} (\langle \Psi|- \rangle \langle -|\Psi\rangle) \\ &= \langle \Psi | \underbrace{\left(+\frac{\hbar}{2} |+\rangle \langle +| + \frac{-\hbar}{2} |- \rangle \langle -| \right)}_{\text{spectral decomposition for } S_z} | \Psi \rangle\end{aligned}$$

Then,

$$\langle S_z \rangle = \langle \Psi | S_z | \Psi \rangle \quad (2)$$

The expression (2) is completely general: given an operator Λ representing a Quantum Mechanical observable with eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$, and eigenkets $|\lambda_1\rangle, |\lambda_2\rangle, \dots, |\lambda_n\rangle$ then Λ can be expressed as

$$\Lambda = \sum_{i=1}^n \lambda_i |\lambda_i\rangle \langle \lambda_i| \quad \text{spectral decomposition}$$

If a measurement of Λ is made on an arbitrary input state $|+\rangle$, the expectation value of many repeated identical measurements will be

$$\langle \Lambda \rangle = \langle \Psi | \Lambda | \Psi \rangle \quad \text{Expectation value}$$

Definition 4.7 (trace). We are going to introduce a linear operation that assigns a number to each matrix.

$$\text{Tr} \{ |1\rangle \langle 2| \} = \langle 2|1\rangle$$

Example 4.6.

$$|1\rangle = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \quad |2\rangle = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \quad \langle 2|1\rangle = \begin{pmatrix} b_1^* & b_2^* \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = a_1 b_1^* + a_2 b_2^*$$

Also

$$|1\rangle \langle 2| = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \begin{pmatrix} b_1^* & b_2^* \end{pmatrix} = \begin{pmatrix} a_1 b_1^* & a_1 b_2^* \\ a_2 b_1^* & a_2 b_2^* \end{pmatrix}$$

so

$$\text{Tr} \{ |1\rangle \langle 2| \} = a_1 b_1^* + a_2 b_2^*$$

Consider an arbitrary operator X and completeness relation for a set of basis kets

$$|+\rangle \langle +| + |-\rangle \langle -| = \mathbb{1}$$

then

$$\begin{aligned}\text{Tr} \{ X \} &= \text{Tr} \{ \mathbb{1} X \} = \text{Tr} \{ |+\rangle \langle +| + |-\rangle \langle -| X \} \\ &= \text{Tr} \{ |+\rangle (|+\rangle \langle X) + |-\rangle (|-\rangle \langle X) \} \\ &= \text{Tr} \{ |+\rangle (|+\rangle \langle X) \} + \text{Tr} \{ |-\rangle (|-\rangle \langle X) \} \\ &= \langle +| X |+ \rangle + \langle -| X |-\rangle\end{aligned}$$

which is the sum of the diagonal elements of X when written in co-ordinate representation with respect to basis $|+\rangle$

and $|-\rangle$.

$$X = \begin{pmatrix} \langle +| X |+ \rangle & \langle +| X |-\rangle \\ \langle -| X |+ \rangle & \langle -| X |-\rangle \end{pmatrix}$$

Properties of Trace

- (i) $\text{Tr}\{X + Y\} = \text{Tr}\{X\} + \text{Tr}\{Y\}$
- (ii) $\text{Tr}\{\lambda X\} = \lambda \text{Tr}\{X\}$
- (iii) $\text{Tr}\{XY\} = \text{Tr}\{YX\}$
- (iv) $\text{Tr}\{XYZ\} = \text{Tr}\{YZX\} = \text{Tr}\{ZXY\}$

In regard to the expectation value for a Quantum Mechanical measurement for operator X and input state Ψ ,

$$\langle X \rangle = \langle \Psi | X | \Psi \rangle = \langle \Psi | (X | \Psi \rangle) = \text{Tr}\{(X | \Psi \rangle) \langle \Psi |\} = \text{Tr}\{X | \Psi \rangle \langle \Psi |\}$$

Separate the properties of measured system (atoms) from Observable X .

4.9 Stastical Operator / Density Matrix

Mixed state or Pure State (superposition state)?

So far we have discussed sources (input states) that are composed of a single type of atom - this may be a superposition state (pure state) like

$$|\Psi\rangle = a|+\rangle + b|-\rangle \quad \text{e.g.,} \quad |+\rangle_x = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}|-\rangle$$

How do we describe a source that is, say, a 50% mixture of atoms in $|+\rangle$ state and 50% in $|-\rangle$ state - at first glance this may appear similar to $|+\rangle_x$, but think about S_x .

Consider a mixture of $P_1|+\rangle_x$ atoms and $P_2|+\rangle_z$ atoms, ($P_1 + P_2 = 1$) and an arbitrary Stern Gerlach measurement S_n . The overall expectation value $\langle S_n \rangle$ is the weighted sum of individual expectation values.

$$\langle S_n \rangle = P_1 \langle S_n \rangle_x + P_2 \langle S_n \rangle_z$$

with

$$\langle S_n \rangle_x = {}_x \langle + | S_n | + \rangle_x = \text{Tr}\{S_n | + \rangle_x {}_x \langle + |\}$$

and

$$\langle S_n \rangle_z = {}_z \langle + | S_n | + \rangle_z = \text{Tr}\{S_n | + \rangle_z {}_z \langle + |\}$$

Thus

$$\begin{aligned} \langle S_n \rangle &= P_1 \text{Tr}\{S_n | + \rangle_x {}_x \langle + |\} + P_2 \text{Tr}\{S_n | + \rangle_z {}_z \langle + |\} \\ &= \text{Tr} \left\{ S_n \underbrace{({}_x \langle + | + {}_z \langle + |)}_{\text{Statistical Operator}} \right\} \end{aligned}$$

Definition 4.8 (Statistical Operator (Density Matrix)).

$$\rho = P_1 |+\rangle_x \langle +| + P_2 |+\rangle_z \langle +|$$

the weighted sum of outer products of source atoms.

$$\langle S_n \rangle = \text{Tr} \{S_n \rho\}$$

In general,

$$\rho = \sum_i P_i |x_i\rangle \langle x_i| \quad \text{with } \sum_i P_i = 1$$

If there is only one type of atom, it is a pure state (e.g., $|\Psi\rangle$) and the statistical operator is $\rho = |\Psi\rangle \langle \Psi|$.

Example 4.7. (i) Use spectral decomposition and the expressions for $|+\rangle_x$, $|-\rangle_x$ in co-ordinate representation with respect to the S_z basis to find S_x as a matrix, also in the S_z basis.

The spectral decomposition for S_x is

$$S_x = +\frac{\hbar}{2} |+\rangle_x \langle +| + -\frac{\hbar}{2} |-\rangle_x \langle -|$$

and

$$|+\rangle_x \xrightarrow[\text{basis}]{S_z} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad |-\rangle_x \xrightarrow[\text{basis}]{S_z} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

then

$$\begin{aligned} S_z &\xrightarrow[\text{basis}]{S_z} \frac{+\hbar}{2} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \frac{1}{\sqrt{2}} (1 \ 1) + \frac{-\hbar}{2} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \frac{1}{\sqrt{2}} (1 \ -1) \\ &= \frac{+\hbar}{2} \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{-\hbar}{2} \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \\ &= \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{aligned}$$

(ii) A source of atoms is prepared as 20% $|+\rangle$ and 80% $|-\rangle_y$ and a measurement of the x -component of angular momentum is performed. What is the expectation value for this experiment?

$$\langle S_x \rangle = \text{Tr} \{S_x \rho\}$$

and

$$\rho = \sum_i P_i |\lambda_i\rangle \langle \lambda_i| = \frac{20}{100} |+\rangle \langle -| + \frac{80}{100} |-\rangle_y \langle -|$$

which in the z -basis is

$$\begin{aligned} \rho &\xrightarrow[\text{basis}]{S_z} \frac{20}{100} \begin{pmatrix} 1 \\ 0 \end{pmatrix} (1 \ 0) + \frac{80}{100} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} \frac{1}{\sqrt{2}} (1 \ i) \\ &= \frac{1}{5} \begin{pmatrix} 3 & 2i \\ -2i & 2 \end{pmatrix} \end{aligned}$$

So,

$$\langle S_x \rangle = \text{Tr} \left\{ \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{1}{5} \begin{pmatrix} 3 & 2i \\ -2i & 2 \end{pmatrix} \right\} = \frac{\hbar}{10} \text{Tr} \left\{ \begin{pmatrix} 2i & 3 \\ 2 & -2i \end{pmatrix} \right\} = 0$$

4.10 Projection Operators and Measurements

Definition 4.9 (Postulate 5). After a measurement of 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 (or kets) corresponding to the result of the measurement:

$$|\Psi'\rangle = \frac{P_n |\Psi\rangle}{\sqrt{\langle\Psi| P_n |\Psi\rangle}}$$

We have seen projection operators before, for example

$$|\Psi\rangle = \langle +|\Psi\rangle |+\rangle + \langle -|\Psi\rangle |-\rangle = \underbrace{\left(\begin{array}{c} |+ \rangle \langle +| \\ \text{projection} \end{array} \right)}_{\text{projection}} |\Psi\rangle + \underbrace{\left(\begin{array}{c} |-\rangle \langle -| \\ \text{projection} \end{array} \right)}_{\text{projection}} |\Psi\rangle$$

In this case, these are projection operators for $|+\rangle$ and $|-\rangle$ states respectively. Applying the projection operator is analogous to taking components of geometric vectors. It produces a new state that is aligned along the eigenstate, with magnitude equal to the probability amplitude for the state to be in that eigenstate.

$$P_+ = |+\rangle \langle +| \xrightarrow[\text{basis}]{S_z} \begin{pmatrix} 1 \\ 0 \end{pmatrix} (1 \ 0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$P_- = |-\rangle \langle -| \xrightarrow[\text{basis}]{S_z} \begin{pmatrix} 0 \\ 1 \end{pmatrix} (0 \ 1) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$P_+ |\Psi\rangle = |+\rangle \langle +|\Psi\rangle = \langle +|\Psi\rangle |+\rangle$$

$$P_- |\Psi\rangle = |-\rangle \langle -|\Psi\rangle = \langle -|\Psi\rangle |-\rangle$$

where $|+\rangle$ and $|-\rangle$ are eigenstates, and $(\langle +|\Psi\rangle)$ and $(\langle -|\Psi\rangle)$ are probability amplitudes.

Now Postulate 5 lets us determine the output state using the projection operator.

$$|\Psi'\rangle = \frac{P_\Psi |\Psi\rangle}{\sqrt{\langle\Psi| P_\Psi |\Psi\rangle}}$$

where

$$\begin{aligned} P_\Psi &= |\Psi'\rangle \langle \Psi'| \\ \sqrt{\langle\Psi| P_\Psi' |\Psi\rangle} &= \sqrt{\langle\Psi| \Psi'\rangle \langle \Psi'| \Psi\rangle} \\ &= \sqrt{|\langle\Psi| \Psi'\rangle|^2} = \text{probability amplitude} \end{aligned}$$

Now, the expectation value for the projection operator is

$$\begin{aligned}
 \langle P_+ \rangle &= \langle \Psi | P_+ | \Psi \rangle \\
 &= \langle \Psi | + \rangle \langle + | \Psi \rangle \\
 &= | \langle + | \Psi \rangle |^2 \\
 &= prob_+
 \end{aligned}$$

4.11 Spin Components in Arbitrary Directions

For spin components in arbitrary directions, we are going to use as our operator a linear combination of the operators S_z, S_x, S_y . First we express an arbitrary vector \hat{n} (for field gradient direction) in terms of polar co-ordinates. We'll use θ as the polar angle (angle between \hat{n} and the z axis), ϕ as the azimuthal angle (angle between \hat{n} and the x axis), and then

$$\hat{n} = \hat{i} \sin \theta \cos \phi + \hat{j} \sin \theta \sin \phi + \hat{k} \cos \theta$$

where $\hat{i}, \hat{j}, \hat{k}$ are unit vectors in direction x, y, z respectively.

Then the operator for spin component along direction \hat{n} is obtained by projecting spin vector operator $S = (S_x, S_y, S_z)$ on \hat{n} unit vector. Then,

$$\text{operator } S_n = S \cdot \hat{n} = S_x \sin \theta \cos \phi + S_y \sin \theta \sin \phi + S_z \cos \theta$$

in matrix form with respect to the S_z basis

$$\begin{aligned}
 S_n &\xrightarrow[\text{basis}]{S_z} \frac{\hbar}{2} \left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \sin \theta \cos \phi + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \sin \theta \sin \phi + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cos \theta \right] \\
 &= \frac{\hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta \cos \phi - i \sin \theta \sin \phi \\ \sin \theta \cos \phi + i \sin \theta \sin \phi & -\cos \theta \end{pmatrix} \\
 &= \frac{\hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta e^{-i\theta} \\ \sin \theta e^{i\theta} & -\cos \theta \end{pmatrix}
 \end{aligned}$$

This can be diagonalised to find eigenvalues and eigenvectors,

$$\text{Eigenvalues} = \pm \frac{\hbar}{2}$$

$$\begin{aligned}
 \text{Eigenvectors} &= |+\rangle_n = \cos \frac{\theta}{2} |+\rangle + \sin \frac{\theta}{2} e^{i\phi} |-\rangle \xrightarrow[\text{basis}]{S_z} \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} e^{i\phi} \end{pmatrix} \\
 &= |-\rangle_n = \sin \frac{\theta}{2} |+\rangle - \cos \frac{\theta}{2} e^{i\phi} |-\rangle \xrightarrow[\text{basis}]{S_z} \begin{pmatrix} \sin \frac{\theta}{2} \\ -\cos \frac{\theta}{2} e^{i\phi} \end{pmatrix}
 \end{aligned}$$

We can check that this is consistent using spectral decomposition:

$$S_n = \frac{+\hbar}{2} |+\rangle_n n \langle +| + \frac{-\hbar}{2} |-\rangle_n n \langle -|$$

Example 4.8. Consider an input state with $\theta = \frac{2\pi}{3}$ and $\phi = \frac{\pi}{4}$, and we want to take an X measurement. Then, in general we have

$$Prob = |\langle \text{out} | \text{in} \rangle|^2$$

and in this case

$$\begin{aligned} |\text{in}\rangle &= |+\rangle_n = \cos \frac{\theta}{2} |+\rangle + \sin \frac{\theta}{2} e^{i\phi} |-\rangle = \cos \frac{\pi}{3} |+\rangle + \sin \frac{\pi}{3} e^{i\frac{\pi}{4}} |-\rangle \\ &= \frac{1}{2} |+\rangle + \frac{\sqrt{3}}{2} e^{i\frac{\pi}{4}} |-\rangle \end{aligned}$$

For Prob_{+x} , $|\text{out}\rangle = |+\rangle_x = \frac{1}{\sqrt{2}} |+\rangle + \frac{1}{\sqrt{2}} |-\rangle$,

$$\begin{aligned} \text{Prob}_{+x} &= |_x \langle +| +\rangle_n|^2 = \left| \left(\frac{1}{\sqrt{2}} \langle +| + \frac{1}{\sqrt{2}} \langle -| \right) \left(\frac{1}{2} |+\rangle + \frac{\sqrt{3}}{2} e^{i\frac{\pi}{4}} |-\rangle \right) \right|^2 \\ &= \left| \frac{1}{\sqrt{2}} \left(\frac{1}{2} \langle +| + \frac{\sqrt{3}}{2} e^{i\frac{\pi}{4}} \langle +| - \frac{1}{2} \langle -| + \frac{\sqrt{3}}{2} e^{i\frac{\pi}{4}} \langle -| - \right) \right|^2 \\ &= \left| \frac{1}{2\sqrt{2}} \left(1 + \sqrt{3} e^{i\frac{\pi}{4}} \right) \right|^2 \\ &= \frac{1}{8} \left(1 + \sqrt{3} e^{i\frac{\pi}{4}} \right) \left(1 + \sqrt{3} e^{-i\frac{\pi}{4}} \right) \\ &= 0.806 \end{aligned}$$

Then of course $\text{prob}_{-x} = 1 - 0.806 = 0.194$. Next for the expectation value we could do it any of these ways

- (i) use weighted sum of products of eigenvalues $\frac{\pm\hbar}{2}$ and probabilities
- (ii) $\langle S_x \rangle = {}_n \langle +| S_x |+\rangle_n$
- (iii) $\langle S_x \rangle = \text{Tr} \{ S_x |+\rangle_n {}_n \langle +| \}$
- (iv) use projection operator (expectation value) to compute probabilities and perform weighted sum as in (i)

4.12 Commuting Observables

Looking at the Stern Gerlach Experiment number 3, we see that simultaneous knowledge of a spin-component in more than one direction is not possible. How do we mathematically characterize the incompatible nature of certain observables? We use the **commutator**.

Definition 4.10 (commutator).

$$[A, B] = AB - BA$$

The difference in the products of the two operators taken in alternate orders. For $[A, B] = 0$, we know that $AB = BA$ so the operators (or observables) commute and the order of operation does not matter.

Consider the effect of commutation on eigen-equations. For operator A , with eigenvalues a and eigenkets $|a\rangle$,

$$A |a\rangle = a |a\rangle$$

then for a second operator B ,

$$BA |a\rangle = Ba |a\rangle = aB |a\rangle$$

If $[A, B] = 0$ then $AB = BA$ which implies

$$BA |a\rangle = A(B |a\rangle) = a(B |a\rangle)$$

Hence BA is an eigenket of A with eigenvalue a , so $B|a\rangle$ is a scalar multiple of $|a\rangle$, say $b|a\rangle$ and therefore

$$B|a\rangle = b|a\rangle$$

So, A and B share common eigenkets $|a\rangle$. Therefore the general statement is that

Theorem 4.1. Commuting operators (observables) share common eigenkets, eigenstates, and eigenvectors.

The consequence for measurement is shown in page 29 of the textbook. So, Commuting observables preserve the state information, and eigenvalues (a_1, b_1) of the operators can be known simultaneously. So with non-commuting operators it means we have incompatible observables which cannot be shown simultaneously.

From experiment 3,

$$[S_z, S_x] \xrightarrow[\text{basis}]{S_z} \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = -i\hbar \cdot \frac{\hbar}{2} \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} = +i\hbar S_y$$

4.13 Uncertainty in Measurement of Observables

- The outcome of measurements is probabilistic.
- Compute "ideal" probabilities to which experimental results converge.

Expectation value is the average of repeated identical measurements but sees nothing about the distribution of results. Information on distribution requires variance or standard deviation. In Quantum Mechanics we call this the uncertainty,

Definition 4.11 (uncertainty).

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

where $\langle A \rangle^2$ is the square of the expectation value for observable A and $\langle A^2 \rangle$ is the expectation value of $A^2 = AA$.

Definition 4.12 (Uncertainty Principle). Connects the possibility or not of having simultaneous knowledge of two Quantum Mechanical observables to the product of their respective uncertainties in their measurement through the commutation relation.

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

Example 4.9. For observables S_x and S_y , where $[S_x, S_y] = i\hbar S_z$,

$$\begin{aligned} \Delta S_x \Delta S_y &\geq \frac{1}{2} |\langle [S_x, S_y] \rangle| \\ &= \frac{1}{2} |\langle i\hbar S_z \rangle| \\ &= \frac{\hbar}{2} |\langle S_z \rangle| \end{aligned}$$

If $|+\rangle$ is used as the input state for a Z-SG measurement, then

$$\underbrace{\langle S_z \rangle}_{\text{always deflected up}} = \frac{+\hbar}{2}, \quad \underbrace{\Delta S_z = 0}_{\text{always get same result}}$$

The uncertainty principle then continues to say

$$\Delta S_x \Delta S_y \geq \frac{\hbar}{2} |\langle S_z \rangle| \geq \left(\frac{\hbar}{2}\right)^2 \neq 0$$

This implies that

$$\Delta S_x \neq 0 \quad \text{and} \quad \Delta S_y \neq 0$$

That is, if we know S_z with certainty ($\Delta S_z = 0$), then we have non-zero uncertainty in S_x and S_y . This is entirely consistent with the concept of incompatible observables.

For observables that do commute, then $[A, B] = 0$ and $\Delta A \Delta B \geq 0$, so uncertainties can be simultaneously zero and we can have simultaneous knowledge of observables A and B .

5 Quantum Dynamics

We'll study how quantum systems evolve in time including details on the Schrödinger Equation, the Hamiltonian operator and energy eigenstates, the Time independent Hamiltonian, and some Examples.

5.1 Time Dependence in Quantum Mechanics

Definition 5.1 (Postulate 6). The time evolution of a quantum system is determined by the Hamiltonian or total energy operator $H(t)$ through the Schrödinger equation

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = H(t) |\Psi(t)\rangle$$

How does a quantum state (ket) evolve with time? Time dependence is governed by the Schrödinger Equation (see postulate 6). $H(t)$ is a new operator called the Hamiltonian Operator. It is an observable corresponding to the **total** energy of the system. It is also a Hermitian operator, which means some important things for us:

- Its eigenvalues are real
- Eigenvectors form a complete basis set

Eigenvalues are allowed energies of the system, and **may be discrete or continuous**. Eigenstates are the energy eigenstates of the system. If the allowed energy states are $|E_n\rangle$ corresponding to allowed energy eigenvalues E_n , Then

$$H |E_n\rangle = E_n |E_n\rangle$$

Where H is a Hamiltonian operator, $|E_n\rangle$ is the energy eigenket, and E_n the energy eigenvalue. Given a Hamiltonian, it can be diagonalised to find the eigenvalues and eigenvectors.

Energy eigenstates form a complete basis, and any arbitrary state can be constructed as a linear combination of them

$$|\Psi\rangle = \sum_n c_n |E_n\rangle \quad \text{with } c_n = \langle E_n | \Psi \rangle$$

and

$$\langle E_k | E_n \rangle = \delta_{kn} = \begin{cases} 0 & \text{if } k \neq n \\ 1 & \text{if } k = n \end{cases}$$

The Time Independent Hamiltonian is then

$$H(t) = H(0) = H$$

Since H is time independent, then eigenvalues and eigenkets must be time independent too (think spectral decomposition).

Time evolution of the quantum state $|\Psi(t)\rangle$ is governed by time independent coefficients of an expansion in the energy basis

$$|\Psi(t)\rangle = \sum_n c_n(t) |E_n\rangle$$

The goal is to find an expression for the $c_n(t)$'s. We're going to substitute the expansion in the energy basis into the Schrödinger Equation

$$\begin{aligned} i\hbar \frac{d}{dt} |\Psi(t)\rangle &= H(t) |\Psi(t)\rangle \\ i\hbar \frac{d}{dt} \left(\sum_n c_n(t) |E_n\rangle \right) &= H \sum_n c_n(t) |E_n\rangle \\ i\hbar \sum_n \frac{dc_n(t)}{dt} |E_n\rangle &= \sum_n c_n(t) E_n |E_n\rangle \end{aligned}$$

now we'll multiply on the left by the bra of the particular eigenstate $|E_k\rangle$

$$\begin{aligned} \langle E_k | i\hbar \sum_n \frac{dc_n(t)}{dt} |E_n\rangle &= \langle E_k | \sum_n c_n(t) E_n |E_n\rangle \\ i\hbar \sum_n \frac{dc_n(t)}{dt} \langle E_k | E_n \rangle &= \sum_n c_n(t) E_n \langle E_k | E_n \rangle \\ i\hbar \frac{dc_k(t)}{dt} &= c_k(t) E_k \end{aligned}$$

This picks out the single eigenstate when $k = n$, and $\langle E_k | E_n \rangle = 1$

$$\begin{aligned} i\hbar \frac{dc_k(t)}{dt} &= c_k(t) E_k \\ \frac{dc_k(t)}{dt} &= \frac{-iE_k}{\hbar} c_k(t) \end{aligned}$$

So a general solution is that

$$c_k(t) = c_k(0) \exp \left\{ \frac{-iE_k}{\hbar} t \right\}$$

Each coefficient in the linear expansion for $|\Psi(t)\rangle$ has the same form of complex exponential, with exponent proportional to the eigenvalue associated with energy eigenket

$$|\Psi(t)\rangle = \sum_n c_n(0) \exp \left\{ \frac{-iE_n}{\hbar} t \right\}$$

We can deduce the consequences for computing probabilities depending on what form the arbitrary state $|\Psi(t)\rangle$

takes.

- (1) $|\Psi(0)\rangle$ is an energy eigenstate $\implies |\Psi(0)\rangle = |E_1\rangle$. At time t ($t > 0$), the quantum state is described by the ket:

$$|\Psi(t)\rangle = \exp\left\{\frac{-iE_1}{\hbar}t\right\}|E_1\rangle$$

Consider measuring observable A , the probability of measuring eigenvalue a_i , corresponding to eigenstate $|a_i\rangle$ is given then by

$$\begin{aligned} prob_{a_i} &= |\langle \text{out} | \text{in} \rangle|^2 \\ &= |\langle a_i | \Psi(t) \rangle|^2 \\ &= \left| \langle a_i | \exp\left\{\frac{-iE_1}{\hbar}t\right\} | E_1 \rangle \right|^2 \\ &= |\langle a_i | E_1 \rangle|^2 \end{aligned}$$

So the probability is time independent, and the energy eigenstates are termed **stationary states**. If a system starts in that state it will continue to be in that state.

- (2) Suppose that our input state is a linear combination of energy eigenstates,

$$|\text{in}\rangle = |\Psi(0)\rangle = c_1 |E_1\rangle + c_2 |E_2\rangle$$

At some time $t > 0$, the quantum state is described by

$$|\Psi(t)\rangle = c_1 \exp\frac{-iE_1}{\hbar}t |E_1\rangle + c_2 \exp\frac{-iE_2}{\hbar}t |E_2\rangle$$

- (i) Consider measuring the energy of the system at some time t . The only possible outcomes are E_1 or E_2 (others may exist but $pr = 0$). This input state would yield E_1 with probability:

$$\begin{aligned} prob_{E_1} &= |\langle \text{out} | \text{in} \rangle|^2 \\ &= |\langle E_1 | \Psi(t) \rangle|^2 \\ &= \left| \langle E_1 | \left(c_1 \exp\frac{-iE_1}{\hbar}t |E_1\rangle + c_2 \exp\frac{-iE_2}{\hbar}t |E_2\rangle \right) \right|^2 \\ &= |c_1|^2 \end{aligned}$$

- (ii) Consider measuring a different observable A , using $|\Psi(t)\rangle$ as $|\text{in}\rangle$

- * If A commutes with the Hamiltonian ($[A, H] = 0$), then A and H share common eigenstates. The probabilities for outcomes of A will proceed as in (2)(i) and will be time independent.
- * If A does **not** commute with H ($[A, H] \neq 0$) then eigenstates of A can be written as a linear combination of energy eigenstates of H . For example, an eigenstate of A

$$|a_1\rangle = \alpha_1 |E_1\rangle + \alpha_2 |E_2\rangle$$

The probability for measuring a_1 ,

$$\begin{aligned}
 prob_{a_1} &= |\langle \text{out} | \text{in} \rangle|^2 = |\langle a_1 | \Psi(t) \rangle|^2 \\
 &= \left| (\alpha_1^* \langle E_1 | + \alpha_2^* \langle E_2 |) \left(c_1 \exp \frac{-iE_1}{\hbar} t |E_1\rangle + c_2 \exp \frac{-iE_2}{\hbar} t |E_2\rangle \right) \right|^2 \\
 &= \left| \alpha_1^* c_1 \exp \frac{-iE_1}{\hbar} t + \alpha_2^* c_2 \exp \frac{-iE_2}{\hbar} t \right|^2 \\
 &= \left| \exp \frac{-iE_1}{\hbar} t \right|^2 \left| \alpha_1^* c_1 + \alpha_2^* c_2 \exp \frac{-i(E_2 - E_1)}{\hbar} t \right|^2 \\
 &= |\alpha_1|^2 |c_1|^2 + |\alpha_2|^2 |c_2|^2 + 2\Re \left(\alpha_1 c_1^* \alpha_2^* c_2 \exp \frac{-i(E_1 - E_2)}{\hbar} t \right)
 \end{aligned}$$

Time dependence is determined by the difference in energy of two energy eigenstates in the superposition for $|\Psi(t)\rangle$. The probability oscillates with a frequency

$$\omega_{21} = \frac{E_2 - E_1}{\hbar} \quad \text{Bohr Frequency} \quad E = \hbar\omega$$

Example 5.1. The time evolution of a spin state in a constant magnetic field (Spin Precession).

Classically, we established that the potential energy for a magnetic dipole moment in a magnetic field depends on their relative orientation, such that:

$$PE = E = -\vec{\mu} \cdot \vec{B}$$

Consider only intrinsic magnetic dipole moment (spin):

$$\vec{\mu} = \vec{\mu}_s = g \frac{q}{2m} \vec{S} \approx \frac{-e}{m_e} \vec{S} \quad (\text{for electron})$$

So, $E = \frac{e}{m_e} \vec{S} \cdot \vec{B}$. The Hamiltonian operator is then generated by analogy:

$$H = \frac{e}{m_e} \vec{S} \cdot \vec{B} \quad \text{where } \vec{S} = S_x + S_y + S_z$$

and operators of spin observables as before. Consider a magnetic field along the x -direction

$$\vec{B} = B_0 \hat{x} \implies H = \frac{eB_0}{m_e} S_x = \omega_0 S_x$$

where $\omega_0 = \frac{eB}{m_e}$ is angular frequency. What are the eigenstates and eigenvalues of our time independent Hamiltonian? Clearly H is proportional to S_x so H and S_x commute, so they share common eigenstates; also the eigenvalues are eigenvalues of S_x multiplied by ω_0 ,

$$\text{eigenvalues} = \pm \frac{\hbar\omega_0}{2} \quad (\text{note these are energies})$$

We could also compute in the z -basis,

$$H = \omega_0 S_x = \frac{\hbar\omega_0}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \implies |+\rangle_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |-\rangle_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

The eigenequations are then

$$H |+\rangle_x = \frac{\hbar\omega_0}{2} |+\rangle_x, \quad H |-\rangle_x = \frac{-\hbar\omega_0}{2} |-\rangle_x$$

Consider time evolved states and probabilities for different source states.

- (i) Consider the initial state to be an eigenstate of Hamiltonian (e.g., $|\Psi(0)\rangle = |+\rangle_x$). The time dependent state is then

$$\begin{aligned} |\Psi(t)\rangle &= \exp \frac{-i \left(+\frac{\hbar\omega_0}{2} t \right)}{\hbar} |+\rangle_x \\ &= \exp \frac{-i\omega_0 t}{2} |+\rangle_x \end{aligned}$$

The overall phase does **not** affect probabilities. For example,

$$\begin{aligned} \text{prob}(|+\rangle) &= |\langle \text{out} | \text{in} \rangle|^2 \\ &= |\langle + | \Psi(t) \rangle|^2 \\ &= \left| \langle + | \exp \frac{-i\omega_0 t}{2} |+\rangle_x \right|^2 \end{aligned}$$

We can then compute this in abstract notation: $|+\rangle_x = \frac{1}{\sqrt{2}} |+\rangle + \frac{1}{\sqrt{2}} |-\rangle$

$$\text{prob}(|+\rangle) = \frac{1}{2} \left| \langle + | \exp \frac{-i\omega_0 t}{2} (|+ \rangle + |-\rangle) \right|^2 = \frac{1}{2} \left| \exp \frac{-i\omega_0 t}{2} \right|^2 = \frac{1}{2} \quad (\text{time independent})$$

- (ii) Consider the initial state that is not an eigenstate of H , $|\Psi(0)\rangle = |+\rangle_y$. We need to express this in terms of energy eigenstates

$$|+\rangle_y = \alpha |+\rangle_x + \beta |-\rangle_x$$

So,

$$\begin{aligned} \alpha &= {}_x \langle + | + \rangle_y \xrightarrow[\text{basis}]{S_z} \frac{1}{\sqrt{2}} (1 \ 1) \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} = \frac{1+i}{2} \\ \beta &= {}_x \langle - | + \rangle_y \xrightarrow[\text{basis}]{S_z} \frac{1}{\sqrt{2}} (1 \ -1) \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} = \frac{1-i}{2} \end{aligned}$$

Then

$$\begin{aligned} |\Psi(0)\rangle &= |+\rangle_y = \frac{1}{2} ((1+i) |+\rangle_x + (1-i) |-\rangle_x) \\ |\Psi(t)\rangle &= \frac{1}{2} \left(\exp \frac{-i\omega_0 t}{2} (1+i) |+\rangle_x + \exp \frac{+i\omega_0 t}{2} (1-i) |-\rangle_x \right) \end{aligned}$$

What about probabilities?

(a) Consider a probability for an energy eigenstate, e.g., $|+\rangle_x$

$$\begin{aligned} \text{prob}(|+\rangle_x) &= |\langle \text{out} | \text{in} \rangle|^2 \\ &= |_x \langle + | \Psi(t) \rangle|^2 \\ &= \left| \frac{1}{2} \exp \frac{-i\omega_0 t}{2} (1+i) \right|^2 \quad (\text{because of orthonormal properties of } |\pm\rangle_x) \\ &= \frac{1}{2} \end{aligned}$$

(b) Consider the probability for an eigenstate that doesn't commute with H , for example an eigenstate of $S_z, |+\rangle$.

$$\begin{aligned} \text{prob}(|+ \rangle) &= |\langle \text{out} | \text{in} \rangle|^2 \\ &= |\langle + | \Psi(t) \rangle|^2 \\ &= \left| \langle + | \left(\frac{1}{2} \left(\exp \frac{-i\omega_0 t}{2} (1+i) |+\rangle_x + \exp \frac{+i\omega_0 t}{2} (1-i) |-\rangle_x \right) \right) \right|^2 \\ &= \left| (1 \ 0) \left(\frac{1}{2} \exp \frac{-i\omega_0 t}{2} (1+i) \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{1}{2} \exp \frac{+i\omega_0 t}{2} (1-i) \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \right) \right|^2 \\ &= \left| \frac{1}{2\sqrt{2}} \left(\exp \frac{-i\omega_0 t}{2} (1+i) + \exp \frac{+i\omega_0 t}{2} (1-i) \right) \right|^2 \\ &= \frac{1}{2} - \frac{1}{2} \sin(\omega_0 t) \quad (\text{time dependent in range } 0 - 1) \end{aligned}$$

Check $t = 0$, $|\text{in}\rangle = |+\rangle_y, |\text{out}\rangle = |+\rangle$, so the probability is $\frac{1}{2}$.

What about expectation values?

$$\begin{aligned} \langle S_x \rangle &= \langle \Psi(t) | S_x | \Psi(t) \rangle \\ &= \frac{1}{2} \left(\exp \frac{+i\omega_0 t}{2} (1-i)_x \langle + | + \exp \frac{-i\omega_0 t}{2} (1+i)_x \langle - | \right) S_x \frac{1}{2} \left(\exp \frac{-i\omega_0 t}{2} (1+i) |+\rangle_x + \exp \frac{+i\omega_0 t}{2} (1-i) |-\rangle_x \right) \end{aligned}$$

This is horrific so we use eigenequations,

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

$$\langle S_x \rangle = \frac{1}{4} \left((1+i)(1-i) \frac{\hbar}{2} + (1+i)(1-i) \left(-\frac{\hbar}{2} \right) \right) = 0$$

Then for S_y ,

$$\begin{aligned} \langle S_y \rangle &= \langle \Psi(t) | S_y | \Psi(t) \rangle \quad (\text{use co-ordinate representation}) \\ &= \frac{\hbar}{2} \cos(\omega_0 t) \end{aligned}$$

likewise for S_z , $\langle S_z \rangle = \frac{\hbar}{2} \sin(\omega_0 t)$. Checking consistency at $t = 0$, we see $|\Psi(0)\rangle = |+\rangle_y$, and

$$\underbrace{\langle S_x \rangle = 0}_{\text{equal prob } \pm \frac{\hbar}{2}} \quad \underbrace{\langle S_y \rangle = +\frac{\hbar}{2}}_{\text{all } +\frac{\hbar}{2}} \quad \underbrace{\langle S_z \rangle = 0}_{\text{equal prob } \pm \frac{\hbar}{2}}$$

Can assembling vector for expectation value of total spin

$$\langle S \rangle = \begin{pmatrix} \langle S_x \rangle & , & \langle S_y \rangle, \langle S_z \rangle \\ \text{time indep} & & \text{time depen} \end{pmatrix}$$

Time dependence is consistent with $\langle S \rangle$ precessing about $\vec{B} = B_0 \hat{x}$ in the yz -plane. This is consistent with our classical expectation for a spin dipole moment precessing about the field direction.

6 Continuous Observables in Quantum Mechanics

6.1 Transition to Infinite Dimensions

An example of an observable that has a continuum of possible outcomes would be the position of an atom (1 dimension for mathematical simplicity). We're going to characterize the quantum state associated with the position observable by a position ket and an associated bra

$$|x\rangle \equiv \text{"atom is at position } x\text{"}$$

$$\langle x| \equiv |x\rangle^\dagger$$

These are known as **position eigenstates**. They require an infinite number of such kets (and bras) to allow for atoms existing anywhere on the x -axis. The theoretical idealization that a particle is at position x (singularity on the x -axis) is not realistic, this is because there is a question of precision and spatial extent of a real particle. However, the realistic situation is that a physical position (i.e., one that occurs in reality) is a superposition of theoretically ideal position eigenstates.

Now we wish to build up an analogous formalism for continuous eigenstates to that which we have for discrete systems (e.g., Stern-Gerlach)

- (1) Expressing arbitrary state as a linear combination of basis states. In Finite Dimensions with basis $|a_k\rangle$, then

$$|\Psi\rangle = \sum_x |a\rangle_k k \langle a|\Psi\rangle = \sum_k \Psi_k |a_k\rangle$$

where $|a\rangle_k$ is a basis state and $k \langle a|\Psi\rangle = \Psi_k$ are the probability amplitude. Similarly if we express $|\Psi\rangle$ as a vector in co-ordinate representation with respect to the ordered basis $|a_k\rangle$

$$|\Psi\rangle \xrightarrow[\text{basis}]{|a_k\rangle} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_n \end{pmatrix} \quad \text{with } \Psi_k = \langle a_k|\Psi\rangle$$

In **infinite dimensions** (position basis) then we write

$$|\Psi\rangle = \int dx |x\rangle \langle x|\Psi\rangle = \int dx |x\rangle \Psi(x)$$

with **position wave function** $\Psi(x) = \langle x|\Psi\rangle$. Note that $\langle x|\Psi\rangle$ is not a number as it was in the finite case, it is now a function over all possible values of x ; a continuous function of probability amplitude for finding a particle in state $|\Psi\rangle$ at position x . The integrals are taken over the entire space unless otherwise noted.

- (2) **Probabilities.** In order to use coefficients of linear expansions to compute probabilities the position kets must be normalized. Consider the special case of $|\Psi\rangle = |x'\rangle$ (position eigenstate), then

$$|\Psi\rangle = |x'\rangle = \int dx |x\rangle \langle x|x'\rangle$$

This only makes sense if $\langle x|x'\rangle = \delta(x - x')$ (Dirac-delta function).

Definition 6.1 (Dirac-delta function). This is the continuous analogue of the kronecker delta function (δ_{mn}) from considering orthonormal properties of discrete kets. Its operation definition is

$$\int dx' \delta(x - x') f(x') = f(x)$$

with properties

$$\begin{aligned} \int dx' \delta(x - x') &= 1 && \text{(special case that } f(x') = 1\text{)} \\ \delta(x - x') &= 0 && \text{for all } x \neq x' \\ \delta(x - x') &= \infty && \text{for } x = x' \end{aligned}$$

(but really only makes sense in the context of integration)

However, now it appears that when $x = x'$, then $\langle x|x'\rangle = \delta(x - x')$ is infinite, and so our probability amplitude would apparently be infinite too. However, as already stated, the idea or concept of an exact position is not realistic. So, $\langle x|x'\rangle$ is not related to any physical observable quantity.

The correct stance to take is to consider our position over some region of space (a linear superposition of position eigenstates), so the Dirac-delta function is integrated and results will be finite.

For normalisation we require that $\langle \Psi|\Psi\rangle = 1$

$$\begin{aligned} \langle \Psi|\Psi\rangle &= \int \int dx dx' \langle \Psi|x\rangle \langle x|x'\rangle \langle x'|\Psi\rangle \\ &= \int \int dx' dx \langle \Psi|x\rangle \delta(x - x') \langle x'|\Psi\rangle \\ &= \int dx \langle \Psi|x\rangle \langle x|\Psi\rangle \\ &= \int dx |\langle x|\Psi\rangle|^2 \end{aligned}$$

If the state $|\Psi\rangle$ is normalised, then

$$\langle \Psi | \Psi \rangle = \int dx |\langle x | \Psi \rangle|^2 = 1$$

Also, since $\Psi(x) = \langle x | \Psi \rangle$ is the position wave function (a continuous function of probability amplitudes for all x)

$$\langle \Psi | \Psi \rangle = \int dx \Psi^*(x) \Psi(x) = \int dx |\Psi(x)|^2 = 1$$

It's then natural to identify $dx |\Psi(x)|^2 = dx |\langle x | \Psi \rangle|^2$ with probability that the particle will be bound between x and $x + dx$. Now, the normalisation condition ensured that the probability to find the particle somewhere on the x -axis ($-\infty \leftrightarrow \infty$) is 1.

Then, the probability of finding the particle between $x = a$ and $x = b$ is

$$prob(a < x < b) = \int_a^b |\langle x | \Psi \rangle|^2 dx = \int_a^b \Psi^*(x) \Psi(x) dx$$

(3) The completeness relation in finite dimensions is

$$\sum_k |a_k\rangle \langle a_k| = \mathbb{1}$$

and in infinite dimensions (continuous) it is

$$\int dx |x\rangle \langle x| = 1$$

(4) The inner product is defined in finite dimensions as

$$\langle \phi | \Psi \rangle \longrightarrow \sum_x \langle \phi | a_k \rangle \langle a_k | \Psi \rangle = \sum_k \phi_k^* \Psi_k$$

where $\phi_k = \langle a_k | \phi \rangle$ and $\Psi_k = \langle a_k | \Psi \rangle$. Then, in infinite dimensions the inner product is defined like

$$\langle \phi | \Psi \rangle \longrightarrow \int dx \langle \phi | x \rangle \langle x | \Psi \rangle = \int dx (\phi(x))^* \Psi(x)$$

with $\phi(x) = \langle x | \phi \rangle$ and $\Psi(x) = \langle x | \Psi \rangle$.

(5) The **expectation value** is the mean value of many repeated experiments on identical states. For observable \hat{A} and input state $|\Psi\rangle$,

$$\langle \hat{A} \rangle = \langle \Psi | \hat{A} | \Psi \rangle$$

In the position basis, it yields a continuous spectrum of results.

Now to summarize the transition from finite dimensional expectation values to infinite dimensions,

$$\begin{aligned}
|\Psi\rangle &\longrightarrow \Psi(x) \\
\langle\Psi| &\longrightarrow \Psi^*(x) \\
\hat{A} &\longrightarrow A(X) \\
\langle\hat{A}\rangle &\longrightarrow \int dx \Psi^*(x) A(x) \Psi(x)
\end{aligned}$$

(6) The position operator, \hat{x}

$$\text{position basis } \hat{x} \longrightarrow x \text{ multiply by scalar } x$$

The Eigenvalue equation is

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

Therefore the expectation value can be written like

$$\langle\hat{x}\rangle = \langle\Psi|\hat{x}|\Psi\rangle \longrightarrow \int dx \Psi^*(x) x \Psi(x)$$

We can explore this value more formally:

$$\langle\hat{x}\rangle = \langle\Psi|\hat{x}|\Psi\rangle$$

Now we need to express $|x\rangle$ in the position basis, so

$$\begin{aligned}
|\Psi\rangle &\longrightarrow \int dx |x\rangle \langle x|\Psi\rangle \\
\implies \langle\hat{x}\rangle &= \int dx \langle\Psi|\hat{x}|x\rangle \langle x|\Psi\rangle
\end{aligned}$$

Now we use the eigenvalue equation for \hat{x} and we get

$$\begin{aligned}
\langle\hat{x}\rangle &= \int dx \langle\Psi|x|x\rangle \langle x|\Psi\rangle \\
&= \int dx \langle\Psi|x\rangle x \langle x|\Psi\rangle \\
&= \int dx \Psi^*(x) x \Psi(x)
\end{aligned}$$

Also by the same arguments, we see that

$$\langle\hat{x}^2\rangle = \int dx \Psi^*(x) x^2 \Psi(x) \text{ useful for computing uncertainties}$$

Even more generally,

$$\langle f(\hat{x}) \rangle = \int dx \Psi^*(x) f(x) \Psi(x) \quad \text{for } f \text{ a function}$$

Another operator of interest is the **momentum operator**, \hat{p} . In the position basis we note that

$$\hat{p} \longrightarrow -i\hbar \frac{d}{dx} \quad (\text{advanced derivation through consideration of spatial translations})$$

The expectation value for this operator is then $\langle \hat{p} \rangle = \langle \Psi | \hat{p} | \Psi \rangle$ for an input state $|\Psi\rangle$ and then written in the position basis it is

$$\langle \hat{p} \rangle = \int dx \Psi^*(x) \left(-i\hbar \frac{d}{dx} \right) \Psi(x)$$

where we have a spatial derivative of the wavefunction and so order is important. So we require an explicit form of the wavefunction.

Now we can consider **the Hamiltonian Operator**, \hat{H} . It is a total energy observable where total energy is equal to the sum of the potential energy and the kinetic energy, and the potential energy depends on position $V(\hat{x})$, a function of the position operator. The kinetic energy then depends on speed : $\frac{\hat{p}^2}{2m}$, a function of the momentum operator. The total energy given by the hamiltonian operator is then

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

in the position basis then it looks like

$$H = V(\hat{x}) + \frac{\hat{p}^2}{2m} \longrightarrow V(x) + \frac{1}{2m} \left(-i\hbar \frac{d}{dx} \right)^2$$

The energy eigenvalue equation is

$$\hat{H} |E_i\rangle = E_i |E_i\rangle$$

Now if we express it in the position basis: $|E_i\rangle \longrightarrow \phi_{E_i}(x)$ we have the energy eigenfunction as a wavefunction in the position basis. The energy eigen equation in the position basis is then

$$\left[V(x) + \frac{1}{2m} \left(-i\hbar \frac{d}{dx} \right)^2 \right] \phi_{E_i}(x) = E_i \phi_{E_i}(x)$$

Second order differential equation, often called "time independent Schrödinger equation" (TISE)

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \phi_{E_i}(x) + V(x) \phi_{E_i}(x) = E_i \phi_{E_i}(x)$$

Now we consider the eigenstate ($\phi_{E_i}(x)$) and eigenvalues (E_i) of the Hamiltonian operator for different potential energy functions $V(x)$.

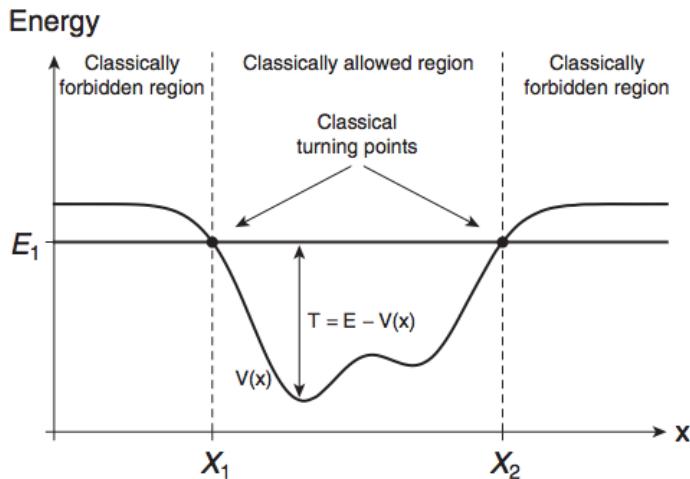


Figure 6.1: A generic potential energy well.

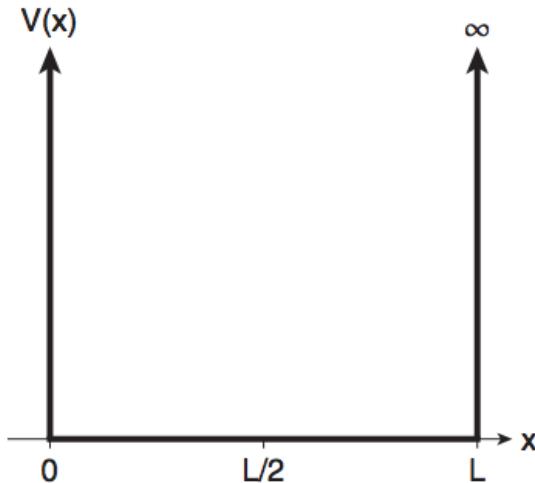


Figure 6.2: Infinite square potential energy well.

6.2 Infinite Square Well Potential

This is an approximation as the limiting case for a charged particle between two charged plates. So,

$$V(x) = \begin{cases} 0 & 0 \leq x \leq L \\ \infty & \text{otherwise} \end{cases}$$

Outside the well (classically forbidden for all possible energies), we have that

$$V(x) = \infty$$

We express the wavefunction (energy eigenstate) as $\Psi(x) = \phi_{E_i}(x)$ and so

$$\Psi(x) = 0$$

is the probability of finding the particle outside of the box ($x < 0$ or $x > L$), because the potential is infinite. **Inside the well** now we have $V(x) = 0$ so looking again at the time independent Schrödinger equation,

$$-\frac{\hbar^2}{2m} \frac{d^2\Psi(x)}{dx^2} = E\Psi(x)$$

which we can rewrite as

$$\frac{d^2\Psi(x)}{dx^2} = -k^2\Psi(x) \quad \text{with } k = \frac{\sqrt{2mE}}{\hbar}$$

Since $E > 0$, so k is real and so k^2 is positive. Here, we have a general solution

$$\Psi(x) = c_1 \exp\{ikx\} + c_2 \exp\{-ikx\}$$

Since complex exponentials can be rewritten as oscillatory functions. Now, constants c_1 and c_2 are fixed by boundary conditions. Ordinarily these are $\Psi(x)$ is continuous and $\frac{d\Psi(x)}{dx}$ is continuous. Ensure that energy remains finite and the Schrödinger Equation can be solved.

In this case, because $V(x) = \infty$ and $\Psi(x) = 0$, the latter condition may be relaxed (i.e., derivative need not be continuous). Thus continuity for $\Psi(x)$ requires that $\Psi(0) = \Psi(L) = 0$, so we have matching solutions inside and outside the potential well. So,

$$\begin{aligned} \Psi(0) &\implies c_1 + c_2 = 0 \implies c_1 = -c_2 \\ &\implies \Psi(x) = c_1 (\exp\{+ikx\} - \exp\{-ikx\}) \\ &\implies \Psi(x) = A \sin(kx) \qquad \qquad \qquad [\text{Euler } e^{i\alpha} = (\cos \alpha + i \sin \alpha)] \end{aligned}$$

The other side of the well, given

$$\Psi(L) = 0 \implies A \sin(kL) = 0 \implies kL = n\pi$$

Hence the values of k are restricted to a set of discrete values.

$$k_n = \frac{n\pi}{L} \quad n = 1, 2, 3, 4, \dots$$

The solution to the time independent Schrödinger equation for $0 \leq x \leq L$ is then

$$\Psi_n(x) = A_n \sin\left(\frac{n\pi x}{L}\right) \quad \text{energy eigenfunctions (wavefunctions) in position basis}$$

Furthermore, since $k^2 = \frac{2mE}{\hbar^2}$ and $k_n = \frac{n\pi}{L}$ for $n = 1, 2, 3, \dots$. Then,

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2 \hbar^2}{8mL^2} \quad \text{energy eigenvalues.}$$

Probability Density

Integrate over a finite region of the x -axis to get the probability that it is to be in that region. The wavefunction (energy eigenfunction) must be normalised. Find A_n such that

$$\int_{-\infty}^{\infty} dx \Psi_n^*(x) \Psi_n(x) = 1 \quad \left(A_n = \sqrt{\frac{2}{L}} \right)$$

If we compare this with the classical expectation, then we would have a classical particle bouncing around in a box that has equal probability to be found anywhere. Not so far in Quantum Mechanics when n is small, but as n gets very large, changes in the probability become extremely small on the spatial scale and the classical result is approximated (**correspondence principle**).

Zero Point Energy

Energy is quantised in n (quantum number), but $n = 0$ is not a "physical" solution, so the lowest eigenstate is $n = 1$ (ground state). The first energy eigenvalue $E_1 = \frac{\pi^2 \hbar^2}{2mL^2}$ is zero point energy. There are some purely Quantum Mechanical effect:

- Stops Helium from solidifying
- Can be large enough to disrupt crystalline or magnetic order (quantum phase transition)

Completeness and Orthonormality

The set of solutions of the time independent Schrödinger equation form a complete set in the sense that any arbitrary wavefunction may be written as a linear combination of the $\Psi_n(x)$ (Fourier Series).

The $\Psi_n(x)$ are orthonormal

$$\int_{-\infty}^{\infty} \Psi_n^*(x) \Psi_m(x) dx = \delta_{mn} = \begin{cases} 0 & \text{if } m \neq n \\ 1 & \text{if } m = n \end{cases}$$

Symmetry

The potential energy function is symmetric about its center line, $x = \frac{L}{2}$. The eigenfunctions $\Psi_n(x)$ are alternatively odd and even functions as n is increased.

These are very general properties of any solutions to a symmetric potential energy function (see finite potential well, harmonic oscillator).

Example 6.1. Consider a particle in the ground state of an infinite square well potential. Find the expectation value for a measurement of position, and the probability that a measurement of position would find the particle in the first third of the well.

We want to work in the position basis, so

$$|E_1\rangle \xrightarrow[\text{basis}]{\text{position}} \Psi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right) \quad (0 < x < L)$$

then,

$$\langle \hat{x} \rangle = \langle E_1 | \hat{x} | E_1 \rangle = \int_{-\infty}^{\infty} dx \Psi_1^*(x) x \Psi_1(x) = \frac{2}{L} dx \int_0^L x \sin^2\left(\frac{\pi x}{L}\right)$$

and finally the probability,

$$prob\left(0 < x < \frac{L}{3}\right) = \int_0^{\frac{L}{3}} \Psi_1^*(x) \Psi_1(x) dx = \frac{2}{L} \int_0^{\frac{L}{3}} \sin^2\left(\frac{\pi x}{L}\right) dx = 0.195$$

6.3 Harmonic Oscillator Potential

The harmonic oscillator potential $V(x) = \frac{1}{2}kx^2$ for spring constant $k = m\omega^2$ and $\omega = \sqrt{\frac{k}{m}}$. This is distinct from the earlier piecewise functions because it is continuous. Since $V(x)$ is a quadratic function, we can split up the regions for which it has meaning into three; region II being the rectangular region bounded by the line $y = E$ and $y = 0$ and bounded on the left and right by the x for which $y = E$. Region I is to the left of this, and region III to the right. So, for region II (classically allowed),

$$\frac{d^2\psi}{dx^2} = -k^2\psi \quad k = \frac{\sqrt{2m(E - V(x))}}{\hbar}$$

Let $V(x) = V_0$,

Classically we have that $E > V_0$, so k is real, and so k^2 is positive. This means that a general solution in this case is a complex exponential (oscillatory functions, wavelength determined by k).

Classically forbidden, $E < V_0$, which means k is imaginary, k^2 is negative, and so our general solution is a real exponential (diverging or decreasing with x).

We can use physical arguments based on required properties of $\Psi(x)$ as probability amplitude to discard "unphysical" terms in the general solution.

6.4 Harmonic Oscillator - Algebraic Method

The potential energy $V(x) = \frac{1}{2}m\omega^2x^2$, and we know that the time independent Schrödinger equation (energy eigenvalue equation) states,

$$\hat{H} |\psi\rangle = E |\psi\rangle$$

The Hamiltonian is also,

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) = \frac{1}{2m} [\hat{p}^2 + (m\omega\hat{x})^2]$$

This is the sum of the two squared operators, which can be factorized. For numbers, it is straightforward

$$v^2 + u^2 = (v + iu)(v - iu)$$

For operators, order is important because they may not commute.

However, consider

$$\hat{a}_{\pm} = \frac{1}{\sqrt{2\hbar m\omega}} (\mp i\hat{p} + m\omega\hat{x})$$

The product of the two can be computed,

$$\begin{aligned}\hat{a}_-\hat{a}_+ &= \frac{1}{2\hbar m\omega} (i\hat{p} + m\omega\hat{x}) (-i\hat{p} + m\omega\hat{x}) \\ &= \frac{1}{2\hbar m\omega} (\hat{p}^2 + (m\omega\hat{x})^2 - im\omega(\hat{x}\hat{p} - \hat{p}\hat{x}))\end{aligned}$$

Where the latter term is the commutator $[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x}$.

To find the commutator, move to the position basis and apply it to the wavefunction.

$$\begin{aligned}[\hat{x}, \hat{p}] |\psi\rangle &\longrightarrow \left[x, (-i\hbar) \frac{d}{dx} \right] \psi(x) \\ &= x(-i\hbar) \frac{d}{dx} \psi(x) - (-i\hbar) \frac{d}{dx} (x\psi(x)) \\ &= -i\hbar \left(x \frac{d\psi(x)}{dx} - x \frac{d\psi(x)}{dx} - \psi(x) \right) \\ &= i\hbar\psi(x)\end{aligned}$$

Thus the commutator relationship for \hat{x} and \hat{p} is

$$[\hat{x}, \hat{p}] = i\hbar$$

Substitute this into the product of factoring operators,

$$\begin{aligned}\hat{a}_-\hat{a}_+ &= \frac{1}{2\hbar m\omega} (\hat{p}^2 + (m\omega\hat{x})^2) - \frac{i}{2\hbar} [\hat{x}, \hat{p}] \\ &= \frac{1}{2\hbar m\omega} (\hat{p}^2 + (m\omega\hat{x})^2) - \frac{i}{2\hbar} (i\hbar) \\ &= \frac{1}{\hbar\omega} \hat{H} + \frac{1}{2}\end{aligned}\tag{1}$$

Similarly,

$$\hat{a}_+\hat{a}_- = \frac{1}{\hbar\omega} \hat{H} - \frac{1}{2}\tag{2}$$

Using (1) and (2),

$$\hat{H} = \hbar\omega \left(\hat{a}_+\hat{a}_- + \frac{1}{2} \right) = \hbar\omega \left(\hat{a}_-\hat{a}_+ - \frac{1}{2} \right)$$

Substitute with the time independent Schrödinger equations,

$$\hbar\omega \left(\hat{a}_\pm \hat{a}_\mp \pm \frac{1}{2} \right) |\psi\rangle = E |\psi\rangle$$

Also,

$$[\hat{a}_-, \hat{a}_+] = \hat{a}_- \hat{a}_+ - \hat{a}_+ \hat{a}_- = 1$$

Now we can use operator manipulation to show that if $|\psi\rangle$ is an eigenstate of the Hamiltonian for the Harmonic Oscillator with energy eigenvalue E , then $\hat{a}_+ |\psi\rangle$ is also an eigenstate with energy eigenvalue $E + \hbar\omega$.

$$\begin{aligned} \hat{H}(\hat{a}_+ |\psi\rangle) &= \hbar\omega \left(\hat{a}_+ \hat{a}_- + \frac{1}{2} \right) (\hat{a}_+ |\psi\rangle) \\ &= \hbar\omega \left(\hat{a}_+ \hat{a}_- \hat{a}_+ + \frac{1}{2} \hat{a}_+ \right) |\psi\rangle \\ &= \hbar\omega \hat{a}_+ \left(\hat{a}_- \hat{a}_+ + \frac{1}{2} \right) |\psi\rangle && \text{use commutator} \\ &= \hat{a}_+ \hbar\omega \left(\hat{a}_+ \hat{a}_- + 1 + \frac{1}{2} \right) |\psi\rangle && \text{use Hamiltonian} \\ &= \hat{a}_+ (\hat{H} + \hbar\omega + \hbar\omega) |\psi\rangle \\ &= \hat{a}_+ (E + \hbar\omega) |\psi\rangle \\ &= (E + \hbar\omega) \hat{a}_+ |\psi\rangle \end{aligned}$$

The same method can be used to show that $(\hat{a}_- |\psi\rangle)$ is the eigenstate with energy $E - \hbar\omega$.

We call these \hat{a}_\pm **ladder operators**, once we have one solution we can obtain all others by applying \hat{a}_+ and or \hat{a}_- .

Definition 6.2 (Lowest Energy Eigenstate). We require that repeated application of the lowering operator \hat{a}_- , will eventually result in zero, this is the **ladder termination condition**.

That is, at the lowest rung,

$$\hat{a}_- |\psi_0\rangle = 0$$

is the lowest energy eigenstate.

Expressing this equation in the position basis,

$$\frac{1}{2\hbar m\omega} \left(-\hbar \frac{d}{dx} + m\omega x \right) \psi_0(x) = 0 \implies \frac{d\psi_0(x)}{dx} = -\frac{m\omega}{\hbar} x \psi_0(x)$$

We can solve this equation by integrating,

$$\begin{aligned} \int \frac{1}{\psi_0(x)} d\psi_0(x) &= -\frac{m\omega}{\hbar} \int x dx \implies \ln(\psi_0(x)) = -\frac{-m\omega}{2\hbar} x^2 + A' \\ \implies \psi_0(x) &= A \exp \left\{ -\frac{m\omega}{2\hbar} x^2 \right\} \end{aligned}$$

We find A by normalizing,

$$A^2 \int_{-\infty}^{\infty} \exp \left\{ -\frac{m\omega}{\hbar} x^2 \right\} dx \implies A = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}}$$

So,

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left\{-\frac{m\omega}{2\hbar}x^2\right\} \quad (|\psi_0\rangle \text{ in position basis})$$

What about the corresponding energy eigenvalues? The time independent Schrödinger equation is,

$$\hbar\omega \left(\hat{a}_+ \hat{a}_- + \frac{1}{2} \right) |\psi_0\rangle = E_0 |\psi_0\rangle$$

Then expanding the operator,

$$\begin{aligned} \hbar\omega \hat{a}_+ \hat{a}_- |\psi_0\rangle + \frac{\hbar\omega}{2} |\psi_0\rangle &= E_0 |\psi_0\rangle \\ &= \frac{\hbar\omega}{2} |\psi_0\rangle \\ &= E_0 |\psi_0\rangle \end{aligned}$$

So,

$$\frac{\hbar\omega}{2} = E_0 \quad \text{ground state energy}$$

Since we know the lowest energy eigenvalue and eigenstate, all others are computed using the raising operator \hat{a}_+

$$\begin{aligned} \psi_n(x) &= A_n (\hat{a}_+)^n \psi_0(x) \quad \text{with } E_n = \left(n + \frac{1}{2}\right) \hbar\omega \\ \text{and } \psi_0(x) &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left\{-\frac{m\omega}{2\hbar}x^2\right\}, \quad E_0 = \frac{1}{2}\hbar\omega \\ \hat{a}_+ &\longrightarrow \frac{1}{\sqrt{2\hbar m\omega}} \left(-i(-i\hbar) \frac{d}{dx} + m\omega x \right) \end{aligned}$$

Now, let's explore the Time Dependent Wavefunction

$$\Psi_n(x, t) = \exp\left\{\frac{-iE_n}{\hbar}t\right\} \psi_n(x) \quad \text{consequence of } \psi_n(x) \text{ being an Energy eigenstate}$$

Here are some properties of Eigenstates of H.O. Potential,

1. Penetration into classically forbidden region
 - Non-zero probability that if a measurement of position is made, it maybe found in a classically forbidden region ($V(x) > E_n$)
 - Ultimately leads to quantum mechanical tunnelling
2. Note energy of ground state is $n = 0$ (c.f., $n = 1$ for infinite potential well). Separation in energy between adjacent states is equal (c.f., $\delta E \propto n^2$ for infinite potential well)
3. Low quantum numbers implies high probability for finding the particle in the centre of the well. Classically, we expect the highest probability when moving most slowly, so the edges of the well Classical expectation is recorded for $n \rightarrow \text{large}$ (see e.g., $n = 100$)
4. As for solutions to the infinite potential well, eigenstates of the H.O. potential have the following generic properties:

- (i) Symmetry \rightarrow they are alternately odd and even
- (ii) Orthonormality \rightarrow Eigenstates are orthonormal and normalized
- (iii) Completeness - any arbitrary state may be expressed as a linear combination of them.

6.5 Time Dependence for Continuous Observables

Eigenstates for time independent Hamiltonians are a simple generation of time dependant states.

$$|E_n(0)\rangle \longrightarrow \psi_n(x) \quad \text{wavefunction in position basis}$$

$$|E_n(t)\rangle \longrightarrow \Psi(x, t) = \exp\left\{\frac{-iE_n}{\hbar}t\right\}\psi_n(x)$$

Eigenstates of such Hamiltonians are stationary states, so the probabilities and expectation values are time independent. Consider making a measurement of observable A with eigenstates $|a_i\rangle$ on energy eigenstate $|E_n(t)\rangle$,

$$\text{prob}(a_i) = |\langle \text{out} | \text{in} \rangle|^2 = |\langle a_i | E_n(t) \rangle|^2$$

In the position basis,

$$|a_i\rangle \longrightarrow a_i(x)$$

$$|E_n(t)\rangle \longrightarrow \psi_n(x) \exp\left\{\frac{-iE_n}{\hbar}t\right\}$$

So,

$$\begin{aligned} \text{prob}(a_i) &= \left| \int dx a_i^*(x) \psi_n(x) \exp\left\{\frac{-iE_n}{\hbar}t\right\} \right|^2 \\ &= \left| \exp\left\{\frac{-iE_n}{\hbar}t\right\} \right|^2 \exp\left\{ \int dx a_i^*(x) \psi_n(x) \right\} \\ &= \left| \int dx a_i^* \psi_n(x) \right|^2 \quad \text{time independent} \end{aligned}$$

For arbitrary states that are linear combinations of energy eigenstates

$$|\alpha\rangle = \sum_n c_n |E_n\rangle \longrightarrow \sum_n c_n \psi_n(x) \quad \text{linear combination of position energy eigenfunctions}$$

$$c_n = \langle E_n | \alpha \rangle \longrightarrow \int dx \psi_n^*(x) \alpha(x)$$

If $|\alpha\rangle = |\alpha(0)\rangle$ (initial state), the state at time t is given by

$$\alpha(t) = \sum_n c_n \exp\left\{\frac{-iE_n}{\hbar}t\right\} |E_n\rangle \longrightarrow \sum_n c_n \exp\left\{\frac{-iE_n}{\hbar}t\right\} \psi_n(x)$$

$$c_n = \langle E_n | \alpha(0) \rangle \longrightarrow \int dx \psi_n^*(x) \alpha(x, 0)$$

Time dependence for probabilities and expectation values, for example

$$|\alpha(0)\rangle = c_1 |E_1\rangle + c_2 |E_2\rangle \quad c_1 = \langle E_1 | \alpha(0) \rangle, c_2 = \langle E_2 | \alpha(0) \rangle$$

So,

$$|\alpha(t)\rangle = c_1 \exp\left\{\frac{-iE_1}{\hbar}t\right\} |E_1\rangle + c_2 \exp\left\{\frac{-iE_2}{\hbar}t\right\} |E_2\rangle$$

In the position basis, $|\alpha(t)\rangle = \alpha(x, t)$ (time independent wavefunction in a position basis), so

$$c_1 \exp\left\{\frac{-iE_1}{\hbar}t\right\} \psi_1(x) + c_2 \exp\left\{\frac{-iE_2}{\hbar}t\right\} \psi_2(x)$$

with

$$c_1 = \int dx \psi_1^*(x) \alpha(x, 0) \quad c_2 = \int dx \psi_2^*(x) \alpha(x, 0)$$

- (i) If observable is Hamiltonian, then the probabilities and expectations will be time independent. (use eigenvalue equations to compute where possible)
- (ii) If observable commutes with the Hamiltonian, then the probabilities and expectation values will be time independent.
- (iii) If observable does not commute, then the probabilities and expectation values will be time independent.

Example 6.2. Consider a particle in an infinite potential well with an initial wavefunction that is:

$$|\alpha(0)\rangle = 3|E_1\rangle + 2|E_3\rangle$$

where $|E_n\rangle$ is an eigenstate of the Hamiltonian

- i. Normalize the initial state

$$\langle \alpha(0) | \alpha(0) \rangle = 1 = A^2 [3 \langle E_1 | + 2 \langle E_3 |] [3 |E_1\rangle + 2 |E_3\rangle]$$

provided $|E_1\rangle$ and $|E_3\rangle$ are orthonormal, which they are as they're eigenstates of an infinite potential well, then

$$1 = |A|^2(9 + 4) \implies A = \frac{1}{\sqrt{13}} \quad \text{choose to be real and positive}$$

- ii. Find the expectation values for position and energy

$$\begin{aligned} \langle \hat{x} \rangle &= \langle \alpha(0) | \hat{x} | \alpha(0) \rangle \\ &= \left[\frac{3}{\sqrt{13}} \langle E_1 | + \frac{2}{\sqrt{13}} \langle E_3 | \right] \hat{x} \left[\frac{3}{\sqrt{13}} |E_1\rangle + \frac{2}{\sqrt{13}} |E_3\rangle \right] \end{aligned}$$

We don't know how \hat{x} acts on $|E_n\rangle$ (it is not an eigenstate of \hat{x}), therefore we move to the position basis.

$$\langle \alpha(0) | \hat{x} | \alpha(0) \rangle = \int_{-\infty}^{\infty} dx \left[\frac{3}{\sqrt{13}} \psi_1^*(x) + \frac{2}{\sqrt{13}} \psi_3^*(x) \right] x \left[\frac{3}{\sqrt{13}} \psi_1(x) + \frac{2}{\sqrt{13}} \psi_3(x) \right]$$

Energy eigenstates in the position basis:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad n = 1, 2, 3, \dots \quad 0 \leq x \leq L$$

See page 144 of the textbook for full math details. There are two types of integral.

$$\frac{2}{L} \int_0^L dx \sin^2\left(\frac{n\pi x}{L}\right) x = \frac{L}{2} \quad [\text{diagonal terms, } n \text{ is same}]$$

$$\frac{2}{L} \int_0^L dx \sin^2\left(\frac{n\pi x}{L}\right) x \sin\left(\frac{m\pi x}{L}\right) = \begin{cases} 0 & \text{if } m+n \text{ is even} \\ \frac{-16L}{9\pi^3} & \text{if } m+n \text{ is odd} \end{cases}$$

So,

$$\begin{aligned} \langle \hat{x} \rangle &= \frac{9}{13} \int_0^L dx \psi_1^*(x) x \psi_1(x) + \frac{6}{13} \int_0^L dx \psi_1^*(x) x \psi_3(x) + \frac{6}{13} \int_0^L dx \psi_3^*(x) x \psi_1(x) + \frac{4}{13} \int_0^L dx \psi_3^*(x) x \psi_3(x) \\ &= \frac{L}{2} \end{aligned}$$

Next, the expectation value for energy is

$$\begin{aligned} \langle \hat{H} \rangle &= \langle \alpha(0) | \hat{H} | \alpha(0) \rangle \\ &= \left(\frac{3}{\sqrt{13}} \langle E_1 | + \frac{2}{\sqrt{13}} \right) \hat{H} \left(\frac{3}{\sqrt{13}} |E_1\rangle + \frac{2}{\sqrt{13}} |E_3\rangle \right) \\ &= \frac{9}{\sqrt{13}} \langle E_1 | \hat{H} | E_1 \rangle + \frac{6}{\sqrt{13}} \langle E_1 | \hat{H} | E_3 \rangle + \frac{6}{\sqrt{13}} \langle E_3 | \hat{H} | E_1 \rangle + \frac{4}{\sqrt{13}} \langle E_3 | \hat{H} | E_3 \rangle \quad (\text{use energy eigen equation}) \\ &= \frac{9}{\sqrt{13}} E_1 \langle E_1 | E_1 \rangle + \frac{6}{\sqrt{13}} E_3 \langle E_1 | E_3 \rangle + \frac{6}{\sqrt{13}} E_1 \langle E_3 | E_1 \rangle + \frac{4}{\sqrt{13}} E_3 \langle E_3 | E_3 \rangle \\ &= \frac{1}{13} (9E_1 + 4E_3) \end{aligned}$$

Now,

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \implies \langle \hat{H} \rangle = \left(\frac{9 \times 1}{13} + \frac{4 \times 9}{13} \right) \frac{\pi^2 \hbar^2}{2mL^2} = \frac{45}{13} \frac{\pi^2 \hbar^2}{2mL^2}$$

The solution could have also been obtained by

$$\langle \hat{E} \rangle = \sum_n E_n \times \text{prob}(E_n)$$

iii. Find the wavefunction at a later time t .

Since $|\alpha(0)\rangle$ is written as a linear combination of energy eigenstates then,

$$|\alpha(t)\rangle = \frac{3}{\sqrt{13}} \exp\left\{\frac{-iE_1}{\hbar}t\right\} |E_1\rangle + \frac{2}{\sqrt{13}} \exp\left\{\frac{-iE_2}{\hbar}t\right\} |E_2\rangle$$

iv. Find the time dependence of the expectation value for position and energy.

$$\begin{aligned}
\langle \hat{x} \rangle &= \langle \alpha(t) | x | \hat{\alpha}(t) \rangle \\
&= \left(\frac{3}{\sqrt{13}} \exp \left\{ \frac{+iE_1}{\hbar} t \right\} \langle E_1 | + \frac{2}{\sqrt{13}} \exp \left\{ \frac{+iE_3}{\hbar} t \right\} \langle E_3 | \right) \hat{x} \left(\frac{3}{\sqrt{13}} \exp \left\{ \frac{-iE_1}{\hbar} t \right\} | E_1 \rangle + \frac{2}{\sqrt{13}} \exp \left\{ \frac{-iE_3}{\hbar} t \right\} | E_3 \rangle \right) \\
&= \frac{9}{13} \langle E_1 | \hat{x} | E_1 \rangle + \frac{4}{13} \langle E_3 | \hat{x} | E_3 \rangle + \frac{6}{13} \exp \left\{ \frac{-i(E_1 - E_3)}{\hbar} t \right\} \langle E_3 | \hat{x} | E_1 \rangle + \frac{6}{13} \exp \left\{ \frac{-i(E_3 - E_1)}{\hbar} t \right\} \langle E_1 | \hat{x} | E_3 \rangle
\end{aligned}$$

We need to switch to the position basis to evaluate the inner products. Same integrals as earlier.

$$\langle \hat{x} \rangle = \frac{9}{13} \frac{L}{2} + \frac{4}{13} \frac{L}{2} = \frac{L}{2} \quad \text{as before}$$

time dependence has disappeared because of the nature of integrals for $\langle E_n | \hat{x} | E_m \rangle$ with $m+n$ being even, **not** because of orthogonality. In general, we expect to see time dependence because $[\hat{x}, \hat{H}] \neq 0$.

7 Free Particle

To consider a free particle in Quantum Mechanics, we solve the time independent Schrödinger equation for $V(x) = 0$

$$\frac{d^2\psi_E(x)}{dx^2} = \frac{-2mE}{\hbar^2} \psi_E(x) = -k^2 \psi_E(x) \quad k = \frac{\sqrt{2mE}}{\hbar}$$

again since $E > 0$, k is REAL and so k^2 is positive. The general solution is then

$$\psi_E(x) = A \exp \{+ikx\} + B \exp \{-ikx\}$$

No boundary conditions to apply means that solutions exist for all k (and E), this means that $\psi_E(x)$ and E for a continuous spectrum of eigenfunctions and eigenvalues respectively.

Mathematically, the system is underconstrained with only normalisation (if possible) to get A, B and E . How one proceeds depends on what problem is being solved.

1. Physical interpretation

Consider the full time dependent eigenfunction

$$\Psi_E(x, t) = \psi_E(x) \exp \left\{ \frac{-iE}{\hbar} t \right\}$$

then using $E = \hbar\omega$,

$$\Psi_E(x, t) = A \exp \{i(kx - \omega t)\} + B \exp \{-i(kx + \omega t)\}$$

and expand $\psi_E(x)$. If we compare this to a classical expression for a travelling wave, we see that $\Psi_E(x, t)$ is a linear superposition of a plane wave travelling in the positive x direction and plane wave travelling in the negative x direction.

8 Tutorials

8.1 Tutorial 1

1. Given two vectors

$$\vec{a} = \begin{pmatrix} 1 \\ 2 \\ 4 \end{pmatrix}, \quad \vec{b} = \begin{pmatrix} 6 \\ 4 \\ 1 \end{pmatrix}$$

- (a) Compute the inner product $\vec{a}^T \vec{b}$

$$1 \cdot 6 + 2 \cdot 4 + 4 \cdot 1 = 12$$

- (b) Compute the outer product $\vec{a} \vec{b}^T$

$$6 \cdot 1 + 4 \cdot 2 + 1 \cdot 4 = 12$$

2. Given two matrices

$$A = \begin{pmatrix} 1 & 9 \\ 4 & 3 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 2 \\ 5 & 6 \end{pmatrix}$$

- (a) Compute the product AB

$$\begin{pmatrix} 1 \cdot 0 + 9 \cdot 5 & 1 \cdot 2 + 9 \cdot 6 \\ 4 \cdot 0 + 3 \cdot 5 & 4 \cdot 2 + 3 \cdot 6 \end{pmatrix} = \begin{pmatrix} 45 & 56 \\ 15 & 20 \end{pmatrix}$$

- (b) Do these matrices commute?

Let's check

$$\begin{pmatrix} 0 \cdot 1 + 2 \cdot 4 & 0 \cdot 9 + 2 \cdot 3 \\ 5 \cdot 1 + 6 \cdot 4 & 5 \cdot 9 + 6 \cdot 3 \end{pmatrix} = \begin{pmatrix} 8 & 6 \\ 29 & 63 \end{pmatrix}$$

No.

3. Given the matrix

$$C = \begin{pmatrix} 7 & 2 \\ 2 & 4 \end{pmatrix}$$

- (a) Compute the eigenvalues of C . The characteristic polynomial is

$$C(\lambda) = \det(C - \lambda I) = \det \begin{pmatrix} 7 - \lambda & 2 \\ 2 & 4 - \lambda \end{pmatrix} = (7 - \lambda)(4 - \lambda) - 4 = 24 - 11\lambda + \lambda^2 \implies \lambda = 8, 3$$

- (b) Compute the eigenvectors of C

$$C - 8I = \begin{pmatrix} -1 & 2 \\ 2 & -4 \end{pmatrix} \equiv \begin{pmatrix} -1 & 2 \\ 0 & 0 \end{pmatrix} \implies \vec{v} = t \begin{pmatrix} 2 \\ 1 \end{pmatrix} \quad s, t \in \mathbb{R}$$

$$C - 3I = \begin{pmatrix} 4 & 2 \\ 2 & 1 \end{pmatrix} \equiv \begin{pmatrix} 0 & 0 \\ 2 & 1 \end{pmatrix} \implies \vec{v} = t \begin{pmatrix} -1 \\ 2 \end{pmatrix} \quad s, t \in \mathbb{R}$$

- (c) Are the eigenvectors orthogonal?

Yes.

- (d) Normalize the eigenvectors.

$$\left(\frac{2}{\sqrt{5}}, \frac{1}{\sqrt{5}} \right), \left(\frac{-1}{\sqrt{5}}, \frac{2}{\sqrt{5}} \right)$$

4. Given the complex number

$$z = 3 + 3i$$

(a) Compute the complex conjugate of z (denoted \bar{z})

$$\bar{z} = 3 - 3i$$

(b) Compute the norm of z (denoted $|z|$)

$$|z| = \sqrt{z \cdot \bar{z}} = \sqrt{18}$$

(c) Express z as $z = re^{i\theta}$.

$$z = (\sqrt{18})e^{i\arctan(\frac{3}{3})} = \sqrt{18}e^{\frac{\pi i}{2}}$$

(d) Express z as $z = r(\cos\theta + i \sin\theta)$

$$z = \sqrt{18} \left(\cos \frac{\pi}{2} + i \sin \frac{\pi}{2} \right)$$

8.2 Tutorial 2

Tutorial 2 concerns coin flipping, the SPINS program, and connections to Quantum Theory. We played games.

8.3 Tutorial 3

We are given a matrix $M_2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, so first we find the eigenvalues:

$$(1 - \lambda)(-1 - \lambda) = 0 \implies \lambda = \pm 1$$

Then for $\lambda_1 = 1$ we get

$$\begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & -2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \implies \vec{v}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

and $\lambda_2 = -1$ which corresponds to $\vec{v}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. Now we want to determine if this matrix is a reflection and if so on what line; well actually this is pretty straightforward because you can see that for any vector, $M_2 \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} x_1 \\ -x_2 \end{pmatrix}$ which means it is a vertical reflection (over the x -axis).

Also a little bit on Group Theory.

8.4 Tutorial 4

On the theory of ideal finite-dimensional Quantum Mechanics and for an application, a Numerical QST Exercise.
Axioms for Finite-Dimensional Quantum Mechanics

- Axiom 0. Systems Exist
- Axiom 1. For each preparation device \mathcal{P} , there is an associated $|\Psi\rangle \in \mathbb{C}^d : \langle \Psi | \Psi \rangle = 1$.
- Axiom 2. For each transformation channel \mathcal{T} , there is an associated $u \in U(\mathbb{C}^d), |\Psi\rangle \rightarrow u|\Psi\rangle$

- Axiom 3. For each measurement device \mathcal{M} , there is an associated Hermitian A with eigenvalues λ_r and eigenkets $|\xi_r\rangle$ such that for input $|\phi\rangle$,

$$pr(\lambda_r) = |\langle\phi|\xi_r\rangle|^2$$

This is The Born Rule.

Note. $uu^\top = \mathbb{1}$ implies unitary, and $A = A^\top$ implies hermitian.

Example 8.1. Suppose that we have some preparation device with four possible states $\Psi_1, \Psi_2, \Psi_3, \Psi_4$, then we can describe Ψ_1 as

$$|\Psi_1\rangle = a|+z\rangle + be^{i\theta}|-z\rangle$$

for $a, b \in \mathbb{R}_+$, and $\theta \in [0, 2\pi]$. Then,

$$pr(+z) = |\langle\Psi|+z\rangle|^2 = a^2$$

and remember that $a^2 + b^2 = 1$. Also,

$$\begin{aligned} pr(+x) &= |\langle\Psi|+x\rangle|^2 \\ &= \left| \left(a\langle+z| + be^{-i\theta}\langle-z| \right) \left(\frac{|+z\rangle + |-z\rangle}{\sqrt{2}} \right) \right|^2 \\ &= \frac{1}{2} |a + be^{-i\theta}|^2 \\ &= \frac{1}{2} (a^2 + b^2 + ab(e^{-i\theta} + e^{i\theta})) \\ pr(+x) &= \frac{1}{2}(1 + 2ab\cos\theta) \end{aligned}$$

Using this framework we can find a_r, b_r , and θ_r from experimental results (finding $pr(+x), pr(+y), pr(+z)$ for each Ψ_r)

Example 8.2. Prove that $|\langle\Psi|\phi\rangle|^2 = |\langle\tau|\phi\rangle|^2$ where $|\tau\rangle = e^{i\theta}|\Psi\rangle$, for $|\Psi\rangle, |\phi\rangle \in \mathbb{C}^d$.

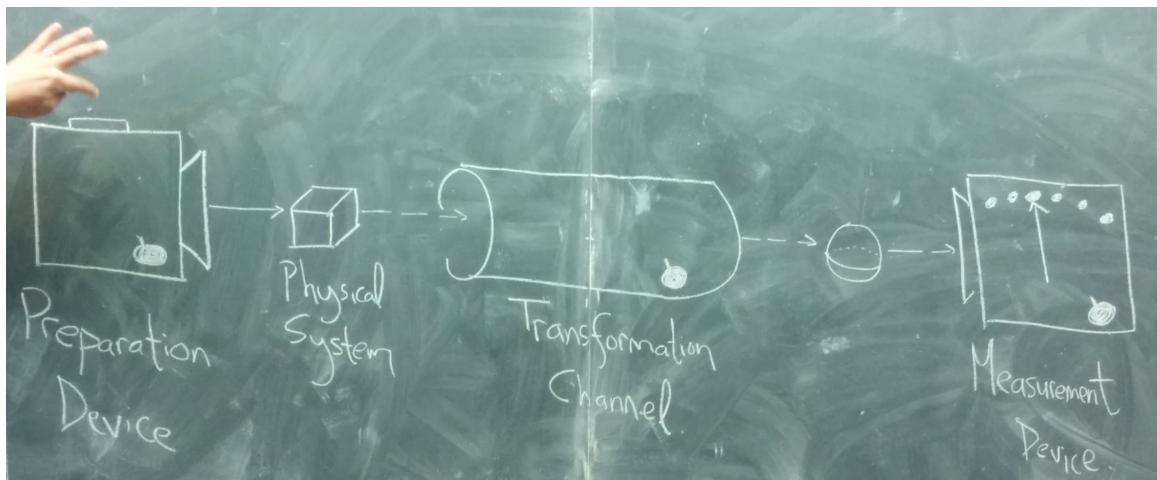


Figure 8.1: "Any physical experiment, classical, quantum, or other, can be viewed as the type of experiment described here." - L. Hardy (2001)

$$\begin{aligned} |\langle \tau | \phi \rangle|^2 &= |e^{-i\theta}|^2 |\langle \Psi | \phi \rangle|^2 \\ &= |\langle \Psi | \phi \rangle|^2 \\ \langle \tau | \phi \rangle &= \langle \Psi | \phi \rangle \end{aligned}$$

8.5 Tutorial 5

Remember the axioms.

- Axiom 0. Systems Exist
- Axiom 1. For each preparation device \mathcal{P} , there is an associated $|\Psi\rangle \in \mathbb{C}^d : \langle \Psi | \Psi \rangle = 1$.
- Axiom 2. For each transformation channel \mathcal{T} , there is an associated $u \in U(\mathbb{C}^d), |\Psi\rangle \rightarrow u|\Psi\rangle$
- Axiom 3. For each measurement device \mathcal{M} , there is an associated Hermitian $A = A^\dagger$

Theorem 8.1. Let $A \in \mathcal{M}_d(\mathbb{C}) : AA^\dagger = A^\dagger A$, then $\exists \lambda_1, \dots, \lambda_m \in \mathbb{C}, m \leq d$. Then,

$$\pi_1, \dots, \pi_m \in \mathcal{M}_d(\mathbb{C}) : \forall r \in \{1, \dots, m\}, \pi_r^2 = \pi_r \wedge \forall r \neq s, \pi_r \pi_s = 0.$$

So,

$$A = \sum_{r=1}^m \lambda_r \pi_r$$

where λ_r is a unique eigenvalue of A and π_r is an eigenprojector where

$$\pi_r = \sum_{s=1}^{\text{mult}(\lambda_r)} |\xi_{rs}\rangle \langle \xi_{rs}|$$

for eigenvectors associated with λ_r .

So a slight generalization to Axiom 3 is

Axiom 3. For each \mathcal{M} , there is an associated $A = A^\dagger$ such that

$$pr(\lambda_r) = \sum_{s=1}^{\text{mult}(\lambda_r)} |\langle \Psi | \xi_{rs} \rangle|^2$$

For input $|\Psi\rangle, |\Psi\rangle \xrightarrow{\frac{\pi_r|\Psi\rangle}{\langle\Psi|\pi_r|\Psi\rangle}}$ when outcome λ_r is registered.

There we go. My question is, is this just a special case of the unitary axiom?

$$\langle u\Psi | u\phi \rangle = \langle \Psi | u^\dagger u | \phi \rangle = \langle \Psi | \phi \rangle$$

Let $|\Psi_1\rangle = |+_z\rangle$ and $|\Psi_2\rangle = |-_z\rangle$ and $\langle \Psi_1 | \Psi_2 \rangle = 0$ and then

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad x \text{ measurement}$$

Suppose a $+_x$ outcome, then

$$|\Psi_1\rangle \rightarrow |+x\rangle, \quad |\Psi_2\rangle \rightarrow |+x\rangle \quad \langle +x|+x\rangle = 1$$

Let's do an example. Consider the situation in the figure at the bottom:

Find the values mentioned on the board at the different parts of the experiment. I'm not going to do it but essentially all you need to do is apply the function in the transformation to the input state to get the first one, then given the + outcome occurs the new state just tacks off the - component and is then normalized. Next, do the transformation again and normalize and getting the probability after that is just the same old way of getting probabilities from states. For more of a challenge instead of just measuring twice, say we are measuring n times. This leads to the Quantum Zeno effect because we'll notice that as we keep observing the state of system over the course of the experiment, we nullify the experiment.

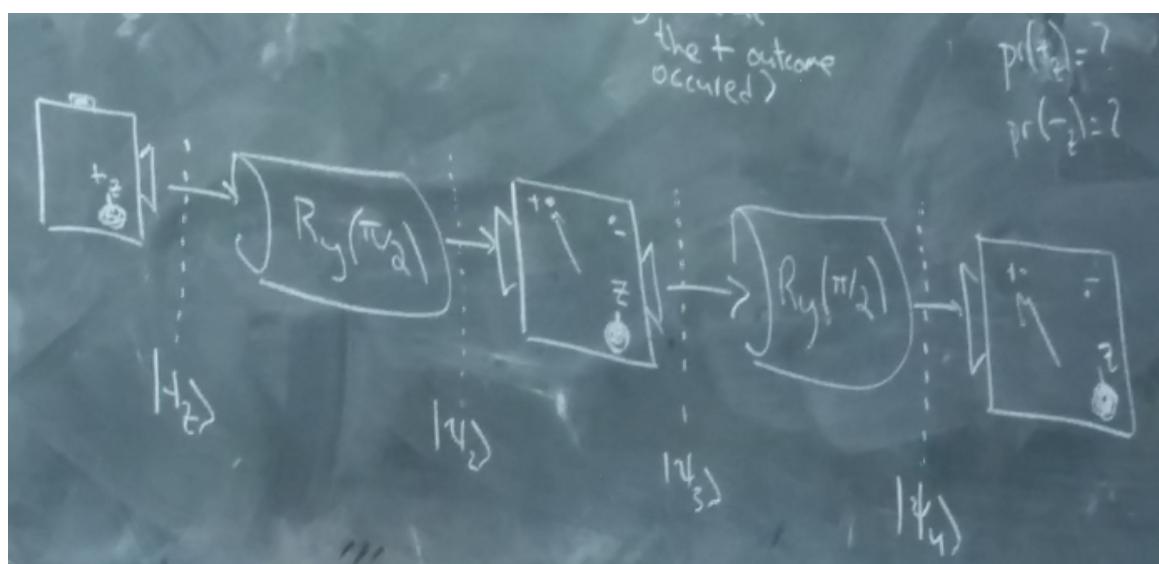


Figure 8.2: Example