Quantum Mechanics

from the context of the course
PHY 471: Quantum Mechanics

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Contents

"If you are not confused by quantum mechanics then you haven't really understood it." -Niels Bohr

0.1 The SI System

In physics it's often important to have precisely defined units for the purposes of making very accurate measurements or simply having a coherent unit system. It's possible to derive all necessary units from five measurements of **length, mass, time, current, and temperature**. The standard SI units for these properties are listed bellow:

Type	Unit	Definition
Length	Meter(m)	Length of distance light in a vacuum travels in $\frac{1}{299792458}$ seconds
Mass	Kilogram(kg)	Defined by fixing the Planck's constant $h = 6.62607015 \times 10^{-34} kg\ m^2 s^{-1}$
Time	Second(s)	Defined by fixing the ground-state hyperfine transition frequency of the caesium-133 atom, to be $9192631770 s^{-1}$
Current	Ampere(A)	Defined by fixing the charge of an electron as $1.602176634 \times 10^{-19} A \cdot s$
Temperature	Kelvin(K)	Defined by fixing the value of the Boltzmann constant k to $1.380649 \times 10^{-23} kg \cdot m^2 s^{-2} K^{-1}$

Common prefixes are listed bellow:

Prefix	Symbol	Definition
mega	M	10^6
kilo	k	10^3
milli	m	10^{-3}
micro	μ	10^{-6}
nano	n	10^{-9}
pico	p	10^{-12}
femto	f	10^{-15}

Additionally, the following are defined constants:

Symbol	Definition
$\hbar$	$\hbar = \frac{h}{2\pi} \approx 1.0546 \times 10^{-34} kg\ m^2 s^{-1}$

0.2 What's Wrong with Classical Mechanics?

Very small things behave very differently than anything big. The models in classical physics fail to describe them. When we look at things on the small scale they don't behave in a way that can be explained without inventing new math. This is what quantum mechanics hopes to explain. The classic example of this is the double slit experiment with electrons. Classically, waves traveling through a double slit will interfere with each other producing a wavy interference pattern. Again classically, fire individual particles through a double slit experiment would not be expected to produce an interference pattern. However, running this experiment with electrons produces an interference pattern. Somehow individual electrons are interfering with themselves. This would hint at the idea that electrons are waves. However if you add detectors to determine if the electron when through both slits, it will only ever pass through one and the interference is destroyed. Simply by observing the path of electrons we fundamentally changed how they behave.

0.3 Postulates of Quantum Mechanics

Towards representing these physical systems with mathematics we need to define some assumptions. Postulates are necessary statements that are assumed to be true. These postulate might not make much sense now, but it will be clear later in this book. Here are the postulates of quantum mechanics:

Postulate 1. Any quantum state can be represented with by a normalized linear combination of the basis vectors. Let $\{|1\rangle, |2\rangle, \ldots, |n\rangle\}$ be the basis vectors and let $|\psi\rangle$ be any quantum state.

$$|\psi\rangle = \psi_1 |1\rangle + \psi_2 |2\rangle + \cdots + \psi_n |n\rangle$$

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

Postulate 2. A physical observable is represented by an operator that acts on kets.

Postulate 3. The only possible result of a measurement of an observable is one of the eigenvalues a_n of the corresponding operator A.

Postulate 4. The probability obtaining the eigenvalue ϕ with eigenvector $|\phi\rangle$ from a measurement of an observable on a system in the state of $|\psi\rangle$ is given by

$$P_\phi = |\langle\phi|\psi\rangle|^2$$

Postulate 5. After a measurement of an eigenvalue ϕ with corresponding eigenvector $|\phi\rangle$, the quantum system is in the normalized projection of the original state onto the result of the measurement:

$$|\psi'\rangle = \frac{P_{|\phi\rangle} |\psi\rangle}{\langle\psi| P_{|\phi\rangle} |\psi\rangle}$$

Postulate 6. A quantum system evolves through time as described by the Schrödinger equation and the Hamiltonian operator $H(t)$ for the system.

$$i\hbar\frac{\partial}{\partial t}$$

Chapter 1

Quantum Systems and States

1.1 Stern-Gerlach Experiments

Definition 1.1. Recall from classical mechanics that **Classical Magnetic Moment** is defined using the following formula given some angular momentum $\mathbf{L}$

$$\mu = \frac{q}{2m}\mathbf{L}$$

$$\mathbf{L} = rmv$$

where r is radius, m is mass of particle, v is tangential velocity, q is charge, $\mathbf{L}$ is the angular momentum, and μ is the magnetic moment.

It is reasonable to expect that some classical physics also applies in quantum as classical physics must emerge from quantum physics.

Definition 1.2. Electron, Protons, and Neutrons all have an **intrinsic angular momentum** called **spin** denoted $\mathbf{S}$.

Definition 1.3. Electrons, Protons, and Neutrons also have an **intrinsic magnetic moment** defined by

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

where g is the dimensionless gyroscopic ratio or g-factor with the following values:
Electron: $g_e = 2.00231930436256$
Proton: $g_p = 5.5856946893$
Neutron: $g_n = -3.82608545$

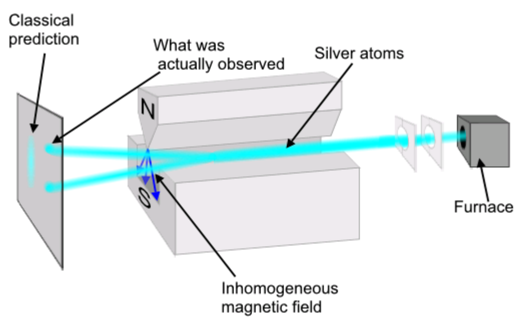


Figure 1.1: Diagram of the Stern-Gerlach experiment

The first Stern-Gerlach experiment seeks to measure the magnetic moment of the valence electron. A silver atom has 47 electrons and 47 protons. The magnetic moments depends on the inverse of mass, so we can neglect heavy protons and neutrons. Silver has an electron configuration of $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 4d^{10} 5s^1$, so the only electron that contributes to the magnetic moment is the valence electron $5s^1$. Knowing this we expect the magnetic moment of the silver atom to be

$$\mu = -g_e\frac{e}{2m_e}\mathbf{S}$$

Following the laws of electromagnetism the force in the z direction is

$$F_z = -g_e \frac{e}{2m_e} S_z \frac{\partial B_z}{\partial z}$$

The deflection of the beam is therefore a measurement of the spin of the valence electron of the silver atoms in the z-direction. Classically, we would expect the magnetic moment to be aligned in random directive and to observe a continuous range of deflection. Instead we observe two distinct magnetic moments. The magnitudes of these deflections are consistent with the spins of

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

This is called **quantization** of the electron's spin angular momentum component. The factor $\frac{1}{2}$ in the equation is why we refer to electrons as having **spin-1/2**.

Definition 1.4. quantization of a property or material is an effect that constrains the property or material to a discrete set of values.

1.1.1 Additional Stern-Gerlach Experiments

As we alluded to in the introduction the act of observing a quantum property may effect how the system behaves. By stacking multiple Stern-Gerlach experiments back to back we can observe that spin in the x direction and spin in the z direction are incompatible observables. To simplify the diagrams we will use the following simplified schematic:

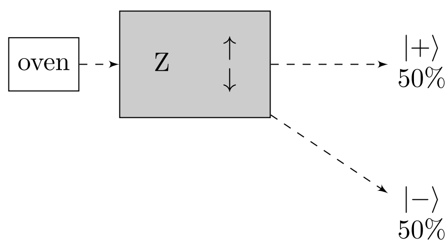


Figure 1.2: Simple schematic of the Stern-Gerlach experiment

Here we represent spin-up states with $|+\rangle$ and spin-down states with $|-\rangle$. More specifically, if a particle has a spin z-component S_z In this first example 50% of the particles are measured with spin-up and 50% of the particles are measured with spin-down. Now consider the following diagram:

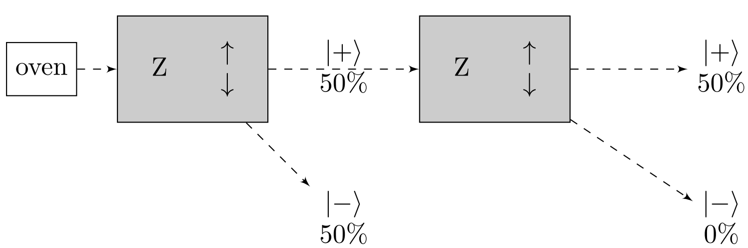


Figure 1.3: This setup measures along the z-axis twice.

As expected, after the first measurement all the remaining particles are spin-z.

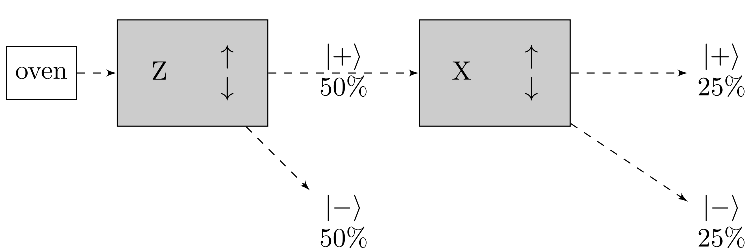


Figure 1.4: This setup measures along the z-axis followed by the x-axis.

If we instead measure along the x axis the result is random and half of the particles are measured to have spin-up or spin-down in the x direction.

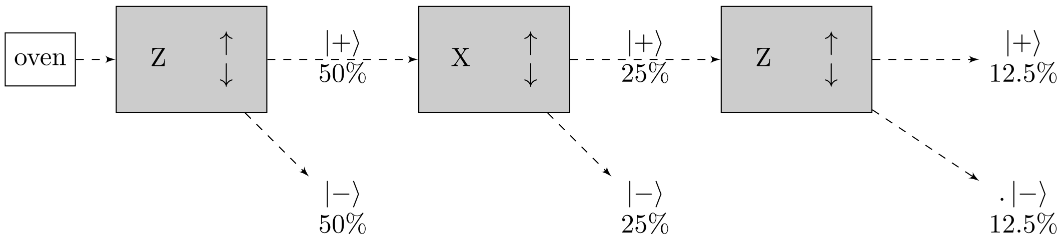


Figure 1.5: This demonstrates that Spin-z and Spin-x are incompatible observables.

After measuring in the x-direction, if we again measure in the z-direction the atoms "forget" about the earlier measurement and we observe and random spin in the z direction. Measuring the spin in the x direction destroyed the measured spin in the z direction.

Definition 1.5. **Incompatible observables** are two properties that cannot be simultaneously measured.

Definition 1.6. **Compatible observables** are two properties that can be simultaneously measured.

1.2 Quantum State Vectors

To describe quantum states such as the spin in the spin-$\frac{1}{2}$ systems that we've explored so far, we use bra-ket notation. For spin-$\frac{1}{2}$ systems we will use the basis vectors $|+\rangle$ and $|-\rangle$, where $|+\rangle$ represents the spin-up in the z-direction and $|-\rangle$ represents spin-down in the z-direction.

Definition 1.7. A **bra** is the row vector that represents the operator that measures a quantum state denoted $\langle\psi|$

Definition 1.8. A **ket** is the column vector that represents a particular quantum state denoted $|\psi\rangle$.

Definition 1.9. For any matrix/vector A the **hermitian conjugate** or **adjoint** denoted $A^\dagger$ is the conjugate transpose of A.

$$A^\dagger = (A^*)^T$$

Definition 1.10. We convert between bras and kets using the hermitian conjugate.

$$|\psi\rangle^\dagger = \langle\psi|$$

$$\langle\psi|^\dagger = |\psi\rangle$$

Corollary 1.1.

$$\langle\phi|\psi\rangle = \langle\psi|\phi\rangle$$

Definition 1.11. A **basis** is a set of quantum state vectors with the following properties:

1. **Normalization** - For every basis vector $|v\rangle$ we have $\langle v|v\rangle = 1$.
2. **Orthogonalization** - For any two basis vectors $|v\rangle$ and $|w\rangle$ where $|v\rangle \neq |w\rangle$ we have $\langle v|w\rangle = 0$.
3. **Completeness** - Any $|\psi\rangle$ can be represented as a linear combination of the bases vectors $|\psi\rangle = \psi_1 |v_1\rangle + \cdots + \psi_2 |v_n\rangle$.

Definition 1.12. The **z-spin-$\frac{1}{2}$ basis** represented with the basis vectors $|+\rangle$ and $|-\rangle$ represents the quantum state with the spin up or down respectively in the z-direction. We will write all **spin-$\frac{1}{2}$** quantum states with this basis.

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

Definition 1.13. Under these definitions we can define a bases for the X and Y directions. It must be orthogonal to the z direction so we chose the following values:

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

$$|+\rangle_Y = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}, |-\rangle_Y = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$$

Now consider postulate 1, we can understand the Stern-Gerlach experiments mathematically. Consider the two following example from earlier.

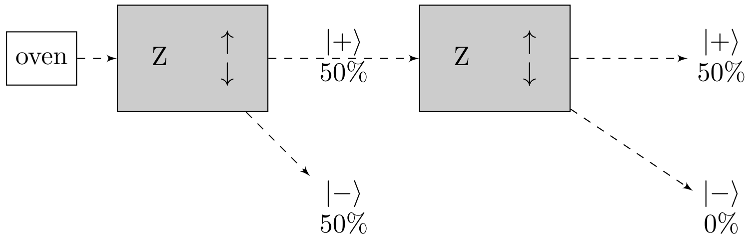


Figure 1.6: This setup measures along the z-axis twice.

The first Stern-Gerlach will serve to purpose of preparing the quantum states for the following Stern-Gerlach. So to calculate the probability of $|+\rangle$ in the z-direction we find that

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

As expected, 100% of the particles that make it to the second detector are measured as $|+\rangle$.

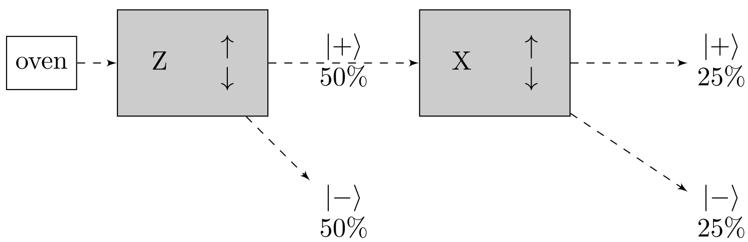


Figure 1.7: This setup measures along the z-axis followed by the x-axis.

Again the first detector on serves the purpose of preparing the state for the second detector. To calculate the probability of $|+\rangle_X$ we have

$$P = |{}_X\langle + | + \rangle|^2 = \left| \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right|^2 = \frac{1}{2}$$

So the probability of measuring spin up in the x-direction is 50%.

1.3 General Quantum Systems

Up until this point, we've been working in the Spin-$\frac{1}{2}$ quantum system with only two basis vectors. More generally we can represent a quantum system with more that two basis vectors. A quantum system can have any number of basis vectors.

Definition 1.14. A **General Quantum System** is a set of quantum states represented using a set of basis states.

$$|\psi\rangle = v_1 |v_1\rangle + v_2 |v_2\rangle + \cdots + v_n |v_n\rangle$$

Example. The spin-1 system is another quantum system similar to the spin-$\frac{1}{2}$ system. It has three basis vectors representing spin up $|+\rangle$, spin down $|-\rangle$, and no spin $|0\rangle$. In spin-1 systems we observe a spin values of $S_z = \hbar, 0, -\hbar$.

$$|\psi\rangle = a|+\rangle + b|0\rangle + c|-\rangle$$

where the basis vectors are for spin in the z direction are:

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

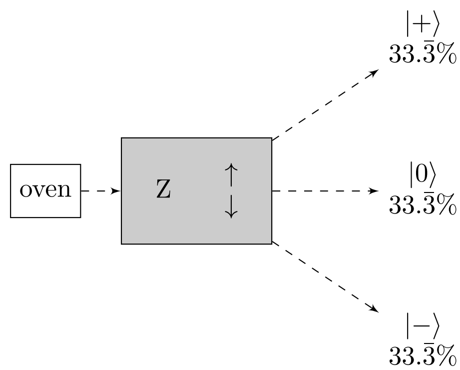


Figure 1.8: Diagram of a spin-1 observable

Chapter 2

Operators and Observables

Definition 2.1. An **operator** is a complex matrix that represents an operation that acts on a ket to produce a new ket.

$$A\left|\phi\right\rangle = \left|\varphi\right\rangle$$

The use of Dirac notation allow for the elements of the matrix to be denoted using the basis vectors of a quantum system.

Proposition 2.1. For an operator $\hat{A}$ in a quantum system with n basis vectors $\{\left|1\right\rangle, \left|2\right\rangle, \ldots, \left|n\right\rangle\}$. The ith row and jth column entry of the matrix representation of $\hat{A}$ can be written as

$$\hat{A}_{ij} = \left\langle i\right|\hat{A}\left|j\right\rangle$$

Definition 2.2. An operator $\hat{A}$ is **hermitian** if

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

Using postulate 2 and 3, we can write the operator for spin in the z-direction. The possible results are $\pm\frac{\hbar}{2}$ and the eigenvectors are the spin-up and spin-down states in the z-direction.

Proposition 2.2. The operator for spin-1/2 in the z-direction can be derived from the following properties

$$S_z\left|+\right\rangle = \frac{\hbar}{2}\left|+\right\rangle$$

$$S_z\left|-\right\rangle = \frac{\hbar}{2}\left|-\right\rangle$$

Therefore, the matrix representation of the spin-1/2 in the z-direction is

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

Similarly, for the x-direction and y-directions we can derive the following matrices.

Proposition 2.3. The operator for spin-1/2 in the x-direction can be derived from the following properties

$$S_x\left|+\right\rangle_x = \frac{\hbar}{2}\left|+\right\rangle_x$$

$$S_x\left|-\right\rangle_x = \frac{\hbar}{2}\left|-\right\rangle_x$$

Therefore, the matrix representation of the spin-1/2 in the x-direction is

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

Proposition 2.4. The operator for spin-1/2 in the y-direction can be derived from the following properties

$$S_y\left|+\right\rangle_y = \frac{\hbar}{2}\left|+\right\rangle_y$$

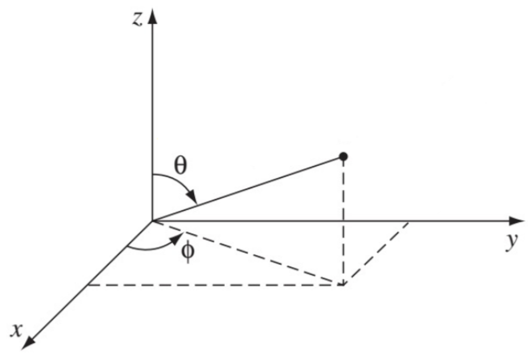
$$S_y\left|-\right\rangle_y = \frac{\hbar}{2}\left|-\right\rangle_y$$

Therefore, the matrix representation of the spin-1/2 in the y-direction is

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

Now that we have the operators for the spin components along all three axes, we can construct the general operator for spin-$\frac{1}{2}$ systems. We will represent the direction of this operator in spherical coordinates describing the vector $\hat{\mathbf{n}}$ with

$$\hat{\mathbf{n}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$



To find the operator associated with measuring in this spin direction we simply project this the spin operators for the three axes onto this unit vector.

$$S_n = S_x \sin\theta\cos\phi + S_y \sin\theta\sin\phi + S_z \cos\theta$$

Proposition 2.5. The operator for measuring spin-$\frac{1}{2}$ at an arbitrary direction (ϕ, θ) is given by

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

Diagonalizing this matrix yields use the values for spin up and spin down in this arbitrary direction:

$$|+\rangle_n = \cos\frac{\theta}{2}|+\rangle + \sin\frac{\theta}{2}e^{i\phi}|-\rangle$$

$$|-\rangle_n = \sin\frac{\theta}{2}|+\rangle - \cos\frac{\theta}{2}e^{i\phi}|-\rangle$$

2.1 Projection Operators

Definition 2.3. A **projection operator** projects a quantum state to another quantum state. The projection operator for a vector $|\phi\rangle$ is given by

$$P_\phi = |\phi\rangle\langle\phi|$$

Example. Consider a quantum state $|\psi\rangle$ in a spin-$\frac{1}{2}$ system, and the projection operator P_+ for the spin up state $|+\rangle$. If $|\psi\rangle = a|+\rangle + b|-\rangle$, then we have

$$P_+|\psi\rangle = |+\rangle\langle+|\psi\rangle = a|+\rangle$$

Proposition 2.6. The projection operator for spin-1/2 up in the z-direction can be derived fro m the following

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

$$\hat{P}_+|\psi\rangle = a|+\rangle$$

Therefore, the projection operator for spin-1/2 up in the z-direction is

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

Similarly, for spin-1/2 down in the z-direction we have

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

$$\hat{P}_-|\psi\rangle = b|-\rangle$$

Therefore, the projection operator for spin-1/2 down in the z-direction is

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

Theorem 2.1. These projection operators can be used to write the probability of a particular measurement. Recall, from postulate 4 that the probability of measuring a quantum state $|\phi\rangle$ is given by

$$P(|\phi\rangle) = |\langle\phi|psi\rangle|^2$$

We can rewrite this in terms of the projection operator for $|\phi\rangle$:

$$P(|\phi\rangle) = \langle\psi|\hat{P}_\phi|\psi\rangle$$

We now have the notation necessary to understand postulate 5. So, after a measurement of an eigenvalue ϕ with corresponding eigenvector $|\phi\rangle$, the quantum system is in the normalized projection of the original state onto the result of the measurement:

$$|\psi'\rangle = \frac{P_{|\phi\rangle}|\psi\rangle}{\langle\psi|P_{|\phi\rangle}|\psi\rangle}$$

2.2 Measurement

Since all possible measurements are represented by a hermitian operator we can prove a few useful properties of measurements.

Proposition 2.7. The eigenvalues of a hermitian operator are real.

Proof. Let $|a_n\rangle$ be eigenstates of a hermitian operator $\hat{A}$, with eigenvalues a_n. For any $|\varphi\rangle$ we have

$$\langle\varphi|a_n\rangle = \langle a_n|\varphi\rangle^*$$

Now, let $|\varphi\rangle = \hat{A}|a_n\rangle$ we have

$$\langle\varphi| = \langle a_n|\hat{A}^\dagger = \langle a_n|\hat{A}$$
$$\langle a_n|\hat{A}|a_n\rangle = \langle a_n|\hat{A}|a_n\rangle^*$$
$$a_n = a_n^*$$

□

Proposition 2.8. The eigenvectors of a hermitian operator with different eigenvalues are orthogonal. That is for two eigenvectors $|a\rangle$ and $|b\rangle$ with eigenvalues $a \neq b$ we have

$$\langle a|b\rangle = 0$$

Proposition 2.9. Eigenstates of an hermitian operator form a basis for a complete Hilbert space.

We know from the Stern-Gerlach experiments that measurements in quantum mechanics are statistical. This section will discuss how to calculate common statistical quantities such as average value and standard deviation for measurements.

Example. Measuring $\hat{S}_z$ we have two possible results $\pm\frac{\hbar}{2}$ with probabilities determined by postulate 4. So the average value is given by

$$\langle\hat{S}_z\rangle = \frac{\hbar}{2}|\langle+|\psi\rangle|^2 - \frac{\hbar}{2}|\langle-|\psi\rangle|^2$$

Definition 2.4. The **average value** or **expected value** of a measurement with operator $\hat{A}$ denoted $\langle\hat{A}\rangle$ is given by

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

For the standard deviation there is a similar derivation from standard statistics:

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

Definition 2.5. The **standard deviation** of a measurement with operator $\hat{A}$ denoted $\Delta\hat{A}$ is given by

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

2.3 The Uncertainty Principle

As determined in the Stern-Gerlach examples, two observations can be incompatible observables. Incompatible observables cannot be simultaniously measured. We can represent this property mathematically by defining a commutator of both matrices.

Definition 2.6. The **commutator** of two operators A, B denoted $[A, B]$ is given by

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

When the commutator is zero, the operators are commutative with each other. Otherwise, the operators represent incompatible observables that cannot be simultaniously measured. This property my be familiar to you as the uncertainty principle.

Proposition 2.10. If the operators representing two observables A, B have a zero commutator that is $[A, B] = 0$, then the observables are compatible observables.

Proposition 2.11. If the operators representing two observables A, B have a zero commutator that is $[A, B] = 0$, then the observables share eigenstates.

Theorem 2.2. **The Uncertainty Principle** states that the minimum product of the standard deviation of two observables is determined by the commutator of the operators representing the observables.

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

2.4 S^2 Operator

Another indication