Quantum Mechanics

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1 Introduction

1.1 The Wave Function

**Question:** \(|\Psi(x,t)|^2dx\) measures the probability of finding a particle in the region between \(x\) and \(x + dx\) during the time interval \(t\). The particle must have an \(x\) coordinate at time \(t\). Hence the total probability of finding the particle somewhere in space must be 1. Therefore, integrating this function from \(-\infty\) to \(\infty\) must give us 1.

**Exercise:** \(\langle x \rangle\) is given by \(\langle x \rangle = \int_{-\infty}^{\infty} x |\Psi(x,t)|^2 dx\). The integrand is odd for \(\Psi(x,0) = (\frac{m\omega}{\pi\hbar})^{1/4}e^{-m\omega x^2/2\hbar}\), which is odd, and since the interval of integration is symmetric about \(x = 0\), the integral is 0. Thus, \(\langle x \rangle = 0\).

1.2 Shrodinger’s Equation

**Question:** In classical mechanics, the standard deviation, or uncertainty of the observed value, is negligible compared to other sources of measurement error. Therefore, we can assume that the values are exact, which still results in models that are extremely consistent with observation.

**Exercise:** To find the momentum operator, we can start by finding the derivative of \(\langle x \rangle\) with respect to time.

\[
\frac{d\langle x \rangle}{dt} = \int x \frac{\partial}{\partial t} \Psi^2 dx
= \int x (\Psi^* \frac{\partial \Psi}{\partial t} + \Psi \frac{\partial \Psi^*}{\partial t}) dx
\]

From the Schrodinger equation,

\[
\frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar} V \Psi
\]

\[
\frac{\partial \Psi^*}{\partial t} = -i\frac{\hbar}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar} V \Psi^*
\]

Plugging these two into the above integral, simplify to obtain

\[
\int x \frac{i\hbar}{2m} (\Psi^* \frac{\partial^2 \Psi}{\partial x^2} - \Psi \frac{\partial^2 \Psi^*}{\partial x^2}) dx
= \int x \frac{i\hbar}{2m} \frac{\partial}{\partial x} (\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x}) dx
\]

Integrating by parts [1], \((\int x \frac{df}{dx} dx = f x |_{-\infty}^{\infty} - \int f \frac{df}{dx} dx)\)

\[
= -\frac{i\hbar}{2m} \int (\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x}) dx
\]
Integrating again, \( \int \Psi \frac{\partial \Psi}{\partial x} \, dx = \Psi|_{\infty} - \int \Psi^* \frac{\partial \Psi}{\partial x} \, dx \)
\[= -\frac{i\hbar}{m} \int (\Psi^* \frac{\partial \Psi}{\partial x}) \, dx \]

Multiplying by \( m \) on both sides gives the momentum operator on the LHS.
\[\langle p \rangle = md\langle x \rangle = -i\hbar \int \Psi^* \frac{\partial \Psi}{\partial x} \, dx = \int \Psi^* (\frac{\hbar}{i} \frac{\partial}{\partial x}) \Psi \, dx \]

From this, we conclude that \( p = \frac{\hbar}{i} \frac{\partial}{\partial x} \).

**Exercise:** \( p \) can be expressed as an operator:
\[\langle F(x, p) \rangle = \int_{-\infty}^{\infty} \Psi^* F(x, \frac{\hbar}{i} \frac{\partial}{\partial x}) \Psi \, dx = (\Psi | F(x, \frac{\hbar}{i} \frac{\partial}{\partial x}) \Psi) \]

**Exercise:** To prove that the normalization does not change, we will prove that the derivative of the area under \( |\psi|^2 \) is 0.
\[\frac{d}{dt} \int_{-\infty}^{\infty} \Psi^* \Psi \, dx \]
\[= \int_{-\infty}^{\infty} \frac{d}{dt} |\Psi|^2 \, dx = \int_{-\infty}^{\infty} \Psi^* \frac{d\Psi}{dt} + \Psi \frac{d\Psi^*}{dt} \, dx \]

From a previous exercise, this equals
\[\int \frac{i\hbar}{2m} \frac{\partial}{\partial x} (\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x}) \, dx \]
\[= \frac{i\hbar}{(2m)} (\Psi^* \frac{d\Psi}{dx} - \Psi \frac{d\Psi^*}{dx}) \bigg|_{-\infty}^{\infty} \]

However, \( \lim_{x \to \pm\infty} \Psi(x, t) = 0 \) for the normalization integral to converge, which means that the integral is 0. Therefore, \( \frac{d}{dt} \int_{-\infty}^{\infty} \Psi^* \Psi \, dx = 0 \), so it is constant, and hence stays normalized if it is normalized at any time.

2 Mathematical Formalism and Quantum Quirks

2.1 Solving Schrodinger’s Equation

Exercise:
\[i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x) \Psi \]

Assume that the solution is separable: \( \Psi(x, t) = \psi(x)\phi(t) \), so the equation becomes
\[i\hbar \frac{\partial [\psi(x)\phi(t)]}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 [\psi(x)\phi(t)]}{\partial x^2} + V(x)\psi(x)\phi(t) \]
Simplifying the differentials,

\[ i\hbar \psi(x) \frac{d\phi(t)}{dt} = -\frac{\hbar^2}{2m} \phi(t) \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x) \phi(t) \]

Rearrange terms and divide the equation by \( \phi(t) \)

\[ -\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x) = \psi(x) \frac{i\hbar}{\phi(t)} \frac{d\phi(t)}{dt} \]

Let \( E = \frac{i\hbar}{\phi(t)} \frac{d\phi(t)}{dt} \), we have the two ordinary differential equations:

\[ -\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x) = E \psi(x) \]

\[ \frac{d\phi(t)}{dt} = -\frac{iE}{\hbar} \phi(t) \]

### 2.2 The Hamiltonian and Hermitian Operators

**Exercise:**

\[ \int (\hat{x}\phi)^* \psi dx = \int (x\phi)^* \psi = \int \phi^* x \psi dx = \int \phi^* \hat{x} \psi dx \]

Therefore, \( \hat{x} \) is hermitian. For momentum, use integration by parts and the definition of \( \hat{p} \)

\[ \int (\hat{p}\phi)^* \psi dx = \int (-i\hbar \frac{d\phi}{dx})^* \psi dx = i\hbar \int \frac{d\phi^*}{dx} \psi dx \]

\[ = i\hbar (\phi^* \psi|_{\infty}^{-\infty} - \int \phi^* \frac{d\psi}{dx} dx) \]

Wavefunctions must approach 0 as \( x \) approaches \( \pm \infty \) to satisfy the normalization condition so the above expression becomes

\[ \int -i\hbar \phi^* \frac{d\psi}{dx} dx = \int \phi^* \hat{p} \psi dx \]

\( \hat{p} \) is hermitian.

\[ \int (\hat{H}\psi)^* \phi dx \]

\[ = \int ((-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \hat{V} \hat{x})\psi)^* \phi dx \]

\[ = \int -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \phi dx + \int (V(x)\psi)^* \phi dx \]

\[ = -\frac{\hbar^2}{2m} \int \frac{d}{dx} \left( \frac{\partial \psi^*}{\partial x} \right) \phi dx + \int (V(x)\psi)^* \phi dx \]

Integration by parts:

\[ = -\frac{\hbar^2}{2m} (\psi^* \phi|_{\infty}^{-\infty} - \int \frac{\partial \phi}{\partial x} \frac{\partial \psi^*}{\partial x} dx) + \int (V(x)\psi)^* \phi dx \]

Again, wavefunctions approach 0 as \( x \) approaches \( \pm \infty \) so the first term disappears. Apply integration by parts again:

\[ = \frac{\hbar^2}{2m} (\frac{\partial \phi}{\partial x} |_{\infty}^{-\infty} - \int \psi^* \frac{\partial^2 \phi}{\partial x^2} dx) + \int (V(x)\psi)^* \phi dx \]

\[ = -\frac{\hbar^2}{2m} \int \psi^* \frac{\partial^2 \phi}{\partial x^2} dx + \int (V(x)\psi)^* \phi dx \]
Now, we manipulate the potential energy term. \( V \) is real so \( V^* = V \) and the expression becomes

\[
= -\frac{\hbar^2}{2m} \int \psi^* \frac{\partial^2}{\partial x^2} \phi dx + \int \psi^* V(x) \phi dx = -\frac{\hbar^2}{2m} \int \psi^* \frac{\partial^2}{\partial x^2} \phi dx + \int \psi^* \hat{V} \phi dx
\]

Combine terms:

\[
= \int \psi^* \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \hat{V} \right) \phi dx = \int \psi^* \hat{H} \phi dx
\]

So the Hamiltonian is Hermitian.

**Exercise:** Let \( \hat{A} \) be a Hermitian operator and \( a \) one of its eigenvalues.

\[
\hat{A} \psi = a \psi
\]

\[
\int_{-\infty}^{\infty} (\hat{A} \psi)^* \psi dx = \int_{-\infty}^{\infty} (a \psi)^* \psi dx = a \int_{-\infty}^{\infty} \psi^* \psi dx
\]

Use the Hermiticity property:

\[
\int_{-\infty}^{\infty} (\hat{A} \psi)^* \psi dx = \int_{-\infty}^{\infty} \psi^* \hat{A} \psi dx = \int_{-\infty}^{\infty} \psi^* a \psi dx = a \int_{-\infty}^{\infty} \psi^* \psi dx
\]

Subtract the two equivalent expressions:

\[
(a^* - a) \int_{-\infty}^{\infty} \psi^* \psi dx = (a^* - a) \int_{-\infty}^{\infty} |\psi|^2 dx = 0
\]

Since \( \psi \) cannot be zero everywhere, \( a^* - a \) must equal 0, so \( a \), the eigenvalue, has no non-real component and must be real.

**Exercise:** Let \( \phi, \psi \) be eigenfunctions of \( \hat{A} \) with distinct eigenvalues \( a, b \) (also real, as proven previously). Take their inner product and use the Hermiticity of \( \hat{A} \):

\[
\int \phi^* \hat{A} \psi dx = \left( \int (\hat{A} \phi)^* \psi dx \right)
\]

Using the definition of eigenvalues:

\[
\int \phi^* b \psi dx = \left( \int (a \phi)^* \psi dx \right)
\]

\[
b \int \phi^* \psi dx = a \int \phi^* \psi dx
\]

\[
(b - a) \int \phi^* \psi dx = 0
\]

\( a \) and \( b \) are given to be distinct so \( b - a \neq 0 \), therefore \( \int \phi^* \psi dx = 0 = \langle \phi | \psi \rangle \), the inner product is 0, and the eigenfunctions are orthogonal.

**Question:** The coefficient of one of the wave functions can be found by taking the inner product of that function and the entire state function. Thinking of the wavefunction as a vector, we can find the "component" of the vector in each direction by taking a "dot product" between the unit vector \( \psi_n \) in that direction and the wavefunction.

**Exercise:** Write the wavefunction as a sum and use the inner product distributive property:

\[
\langle \psi(x, 0) | \psi_i \rangle = \sum_n c_n \langle \psi_n | \psi_i \rangle = \sum_n c_n (\psi_n | \psi_i) 
\]

All \( \psi_n \) are given to be normal so all \( c_n \langle \psi_n | \psi_i \rangle = 0 \) for \( i \neq j \) and the only nonzero term in the sum is \( c_i \langle \psi_i | \psi_i \rangle = c_i \). (Length of \( \psi_i \) is 1 because it is a unit vector). Therefore,

\[
\langle \psi_n(x) | \psi(x, 0) \rangle = c_n
\]
Exercise:
\[ \int \psi^* \psi \, dx = 1 \]
by (2). Plugging in the linear combination representation of \( \psi \),
\[ \int \left( \sum_n c_n \psi_n \right)^* \sum_n c_n \psi_n \, dx = 1 \]
This is equivalent to
\[ \int \sum_n (c_n \psi_n^*) c_n \psi_n \, dx = 1 \]
because all other pairs of the form \( \int (c_i \psi_i)^* c_j \psi_j \, dx \) will equal 0 due to the orthogonality of the eigenfunctions.
\[ \int \sum_n c_n^2 \psi_n^* \psi_n \, dx = \sum_n (c_n^2 \int \psi_n^* \psi_n \, dx) = \sum_n c_n^2 = 1 \]
because \( \int \psi_n^* \psi_n = 1 \) for all \( n \) (orthonormality is given).

Exercise: Use (16):
\[ 1 = (|c1|)^2 + (|c2|)^2 = (|2N/t|^2 + |Ne^{i\pi/2}|)^2 \]
\[ 1 = 4N^2 + N^2 \]
\[ N = 1/\sqrt{5} \]
\[ \langle H \rangle = \sum |c_n|^2 E_n = (|2N/t|^2 E_1) + (|Ne^{i\pi/2}|^2 E_2) = \frac{-4E_1}{5} - \frac{E_2}{5} \]

Exercise: \( V = 0 \) everywhere the particle can be.
\[ \frac{-\hbar^2 \partial^2 \psi}{2m \partial x^2} = E\psi \]
Solutions to this differential equation can be written in the form [3]:
\[ \psi(x) = A \cos(\sqrt{\frac{2mE}{\hbar^2}} x) + B \sin(\sqrt{\frac{2mE}{\hbar^2}} x) \]
\( \psi(0) = \psi(L) = 0 \) because the probability of finding the particle outside the interval should be 0. Therefore, \( A = 0 \) (the cosine term will always be nonzero at \( x = 0 \) if \( A \neq 0 \). In addition, \( \sqrt{\frac{2mE}{\hbar^2}} L = n\pi \) (\( n \) is an integer) for the sine term to be 0 at right edge of the interval. Solving for \( E \), we find the possible eigenenergies,
\[ E_n = \frac{n^2 \pi^2}{2mL^2} \]
Next, the eigenfunctions need to be normalized. Substituting \( E_n \),
\[ \psi_n = B \sin(\frac{n\pi x}{L}) \]
\[ \int_0^L |\psi_n|^2 \, dx = \frac{B^2 L}{2} = 1 \]
Therefore, \( B = \sqrt{\frac{2}{L}} \) and the eigenfunctions are
\[ \psi_n = \sqrt{\frac{2}{L}} \sin(\frac{n\pi x}{L}) \]
**Exercise:** Normalize:

\[ \int_0^L (N \sin^3 \left( \frac{\pi x}{L} \right))^2 dx = \frac{5LN^2}{16} = 1 \]

\[ N = \frac{4}{\sqrt{5L}} \]

Write the wavefunction as the superposition of eigenfunctions:

\[ N \sin^3 \left( \frac{\pi x}{L} \right) = \frac{1}{\sqrt{5L}} \left( 3 \sin \left( \frac{\pi x}{L} \right) - \sin \left( \frac{3\pi x}{L} \right) \right) \]

To find \( \psi(x, t) \), add time dependence to each eigenfunction after calculating the eigenenergies

\[ E_n = \frac{\hbar^2 \pi^2}{2mL^2} n^2 \]

\[ \psi(x, t) = c_1 \psi_1 e^{-iE_1 t/\hbar} + c_3 \psi_3 e^{-iE_3 t/\hbar} \]

\[ = \frac{1}{\sqrt{5L}} \left( 3 \sin \left( \frac{\pi x}{L} \right) e^{-\frac{\hbar \pi^2 t}{2mL^2}} - \sin \left( \frac{3\pi x}{L} \right) e^{-\frac{9\hbar \pi^2 t}{2mL^2}} \right) \]

\[ \langle x \rangle = \int x |\psi|^2 dx = \int x \psi^* \psi dx \]

\[ = \int_0^L x - 6 \sin \left( \frac{3\pi x}{L} \right) \sin \left( \frac{\pi x}{L} \right) \cos \left( \frac{(E_1 - E_3)t}{\hbar} \right) + 9 \sin^2 \left( \frac{3\pi x}{L} \right) + \sin^2 \left( \frac{\pi x}{L} \right) \frac{5L}{dx} \]

The last two terms evaluate to \( |c_i|^2 \langle x_i \rangle \) and the cosine term evaluates to 0 according to Mathematica. Both \( \psi_1 \) and \( \psi_3 \) have \( \langle x \rangle = \frac{L}{2} \) because they are symmetric about the center of the interval, so

\[ \langle x \rangle = \frac{L}{2} \]

\[ \langle E \rangle = |c_1|^2 E_1 + |c_3|^2 E_3 \]

Calculate \( c_i \) from the normalized eigenfunctions.

\[ c_1 = \frac{3}{\sqrt{10}}, \quad c_3 = \frac{-1}{\sqrt{10}} \]

\[ \langle E \rangle = \frac{9 \hbar^2 \pi^2}{10 \cdot 2mL^2} e^{-\frac{\hbar \pi^2 t}{2mL^2}} + \frac{1}{10 \cdot 2mL^2} e^{-\frac{9\hbar \pi^2 t}{2mL^2}} \]

**Exercise and Question:** Solve time independent equation first:

\[ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E \psi \]

\[ \frac{\partial^2 \psi}{\partial x^2} = -\frac{2mE}{\hbar^2} \psi \]

Take \( k = \sqrt{2mE}/\hbar \), solution to this can be written as

\[ \psi(x) = Ae^{ikx} + Be^{-ikx} \]

Adding the time dependence:

\[ \psi(x, t) = Ae^{ikx - \frac{ik^2\hbar t}{2m}} + Be^{-ikx + \frac{ik^2\hbar t}{2m}} \]

The integral \( \int |\psi|^2 dx \) diverges so the wavefunction cannot be normalized. This means that there is no definite "energy" associated with a free particle and it cannot be represented by a single wavefunction.
2.3 The Harmonic Oscillator

Exercise:

\[ [x, p] \psi = xp\psi - px\psi = -x \hbar \frac{d\psi}{dx} + \hbar \frac{d}{dx} (x\psi) \]

\[ = -\hbar \left( \frac{d\psi}{dx} - \left(x \frac{d\psi}{dx} + \psi\right) \right) = -\hbar (-\psi) = i\hbar \psi \]

Therefore, \([x, p] = i\hbar\]

**Exercise:** First, we show the distributive property of the commutator:

\[ [A, B + C] = A(B + C) - (B + C)A = AB + AC - BA - CA = [A, B] + [A, C] \]

Also,

\[ [cA, dB] = cAdB - dBcA = cdAB - cdBA = cd(AB - BA) = cd[A, b] \]

We can thus evaluate the commutator

\[ [a_+, a_-] = \frac{1}{2\hbar \omega} (-[ip, ip] + [-ip, m\omega x] + [m\omega x, ip] + [m\omega x, m\omega x]) \]

The commutator of a function with itself (or a constant multiple) is 0 so the commutator becomes

\[ \frac{1}{2\hbar \omega} (m\omega h + m\omega h) = 1 \]

Therefore, \(a_- a_+ = a_+ a_- - 1\) and \(H = \hbar \omega (a_- a_+ - \frac{1}{2}) = \hbar \omega (a_+ a_- + \frac{1}{2})\)

**Exercise:**

\[ H(a_+ \psi) = \hbar \omega (a_+ a_- + \frac{1}{2}) (a_+ \psi) = \hbar \omega (a_+ a_- a_+ + \frac{1}{2} a_+) \psi = \hbar \omega a_+ (a_- a_+ + \frac{1}{2}) \psi \]

\[ = \hbar \omega a_+ \left( \frac{H}{\hbar \omega} + \frac{1}{2} \frac{1}{2} \right) \psi = \hbar \omega a_+ (H + \hbar \omega) \psi = a_+ (E + \hbar \omega) \psi = (E + \hbar \omega) (a_+ \psi) \]

**Question:** The ground state energy is very small and unnoticeable classically, where it is assumed to be 0. In quantum mechanics, however, harmonic oscillators cannot have exactly zero energy.

**Exercise:** Given the eigenfunction \(\psi_n\), we find the constant factor \(c\) of the eigenfunction with the raising operator applied. This \(c\) must satisfy the normalization condition.

\[ \psi_{n+1} = c(a_+ \psi_n) \]

\[ 1 = \int |\psi_{n+1}|^2 dx = c^2 \int |a_+ \psi_n|^2 dx = c^2 \int (a_+ \psi_n)^*(a_+ \psi) dx \]

As \(a_+\) and \(a_-\) are hermitian conjugates [4] \((\langle \psi^* | a_+ \phi \rangle = \langle (a_- \psi) | \phi \rangle \) and vice versa\), this equals

\[ c^2 \int (a_+^\dagger a_+ \psi_n)^* \psi_n dx = c^2 \int (a_- a_+ \psi_n)^* \psi_n dx \]

From (25),

\[ c^2 \int \left( \frac{E_n}{\hbar \omega} + \frac{1}{2} \right) \psi_n^* \psi_n dx \]

and from (31),

\[ c^2 \int \left( (n + \frac{1}{2}) + \frac{1}{2} \right) \psi_n^* \psi_n dx = c^2 (n + 1) \int |\psi_n|^2 dx = c^2 (n + 1) \]

because \(\psi_n\) is also assumed to be normalized. Thus, \(c = \frac{1}{\sqrt{n+1}}\)

If \(\psi_{n+1} = \frac{1}{\sqrt{n+1}} a_+ \psi_n\) then, in general, \(\psi_n = \frac{1}{\sqrt{n!}} (a_+)^n \psi_0\)
Exercise: It is easy to verify that 
\[ x = \sqrt{\frac{\hbar}{2m\omega}}(a_+ + a_-) \]

Let 
\[ \beta = (a_+ + a_-) \]
\[ \langle x^4 \rangle = \frac{\hbar^2}{4m^2\omega^2} < \beta^4 > = \frac{\hbar^2}{4m^2\omega^2} \int \psi_n^* \beta^4 \psi_n dx \]

There are \( 2^4 = 16 \) terms but we only keep the ones with \( 2a_+ \) and \( 2a_- \) because the others will all be orthogonal to \( \psi_n \) and add 0 to the integral.

\[ < x^4 > = \frac{\hbar^2}{4m^2\omega^2} < a_+^2a_-^2 + a_+a_-a_+a_- + a_+a_-a_+ + a_+a_-a_+ + a_+a_-a_+ + a_+a_-a_+ + a_+a_- > \]

From above, \( a_+\psi_n = \sqrt{n+1}\psi_{n+1} \) and \( a_-\psi_n = \sqrt{n}\psi_{n-1} \). Expanding everything out, we obtain
\[ \langle x^4 \rangle = \frac{\hbar^2}{4m^2\omega^2} < n(n-1) + n^2 + n(n+1) + (n+1)^2 + n(n+1) + (n+1)(n+2) > = \frac{\hbar^2}{4m^2\omega^2}(6n^2 + 6n + 3) \]

To answer the question, \( \langle x^4 \rangle = \frac{\hbar^2}{m^2\omega^2} \frac{34203}{4} \)

Exercise: From definition of potential energy:
\[ V = \frac{1}{2} m\omega^2 x^2 \]
\[ \langle V \rangle = \frac{1}{2} m\omega^2 \langle x^2 \rangle \]

With a similar methodology to the previous problem, write \( x \) in terms of \( a_+ \) and \( a_- \), removing orthogonal terms.
\[ \langle V \rangle = \frac{\hbar\omega}{4} a_+ + a_+ a_- = \frac{\hbar\omega}{4} (n + 1) + n = \frac{\hbar\omega}{4} (2n + 1) \]

Kinetic energy can be expressed in terms of the hamiltonian and potential energy:
\[ \langle T \rangle = \langle H \rangle - \langle V \rangle = \hbar\omega((n+1) - \frac{1}{2}) - \frac{\hbar\omega}{4} (2n + 1) = \frac{\hbar\omega}{4} (2n + 1) \]

Therefore we conclude that \( \langle T \rangle = \langle V \rangle \). This is analogous to the virial theorem, which states that the average kinetic energy of a system is equal to the average total potential energy [5].

2.4 The Commutator

Question: \( \hat{H} \) is hermitian so \( \langle \hat{H}\psi | \hat{O}\psi \rangle = \langle \psi | \hat{H} \hat{O}\psi \rangle \)

Exercise:
\[ \frac{d}{dt} \langle x \rangle = \frac{i}{\hbar} \langle [\hat{H}, \hat{x}] \rangle + \langle \frac{d\hat{x}}{dt} \rangle \]
\( \hat{x} \) does not depend on time so its time derivative is 0.
\[ [\hat{H}, \hat{x}] = [\hat{T}, \hat{x}] + [\hat{V}, \hat{x}] \]
\[ [\hat{V}, \hat{x}] = \hat{V} \hat{x} \psi - \hat{x} \hat{V} \psi = \hat{V} x \psi - \hat{x} V \psi = V x \psi - x V \psi = 0 \]
\[ [\hat{T}, \hat{x}] = \left[ \frac{\hat{p}^2}{2m}, \hat{x} \right] \]
We will use one of the properties of commutators:

\[
[\hat{A}, \hat{B} \hat{C}] = \hat{A}\hat{B}\hat{C} - \hat{B}\hat{C}\hat{A} = \hat{B}(\hat{A}\hat{C} - \hat{C}\hat{A}) + (\hat{A}\hat{B} - \hat{B}\hat{A})\hat{C} = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}
\]

\[
[x, \hat{p}^2] = \hat{p}[x, \hat{p}] + [x, \hat{p}]\hat{p}
\]

Substiting for \(\hat{p}\) and the commutator calculated previously:

\[
= -i\hbar \frac{\partial}{\partial x} (\hat{p}\hbar) + (-i\hbar \frac{\partial}{\partial x})(\hat{p}\hbar) = 2\hbar^2 \frac{\partial}{\partial x}
\]

Therefore, \([\hat{T}, \hat{x}] = -\frac{\hbar^2}{m} \frac{\partial}{\partial x} = -\frac{i\hbar}{m} \hat{p}\) and, plugging into the first equation,

\[
\frac{d}{dt} \langle x \rangle = \langle \frac{\hat{p}}{m} \rangle = \langle \hat{p} \rangle \frac{m}{m}
\]

, confirming the previous conjecture.

\[
\frac{d}{dt} \langle p \rangle = \frac{i}{\hbar} ([\hat{H}, \hat{p}]) + \langle \frac{d\hat{p}}{dt} \rangle
\]

Again, \(\hat{p}\) doesn’t depend on time so \(\frac{d\hat{p}}{dt} = 0\).

\[
[\hat{T}, \hat{p}] = [\hat{T}, \hat{p}] + [\hat{V}, \hat{p}]
\]

\[
[T, p] \psi = Tp\psi - pT\psi = (-\frac{\hbar^2}{2m} \frac{d^2}{dx^2})(-i\hbar \frac{d}{dx})\psi - (-i\hbar \frac{d}{dx})(-\frac{\hbar^2}{2m} \frac{d^2}{dx} \psi)
\]

\[
= i\hbar^3 \frac{d}{2m dx^3} \psi - i\hbar^3 \frac{d^3}{2m dx^3} \psi = 0
\]

\[
[V, \hat{p}] = Vp\psi - pV\psi = V \frac{\hbar}{i} \frac{d}{dx} \psi - (\frac{\hbar}{i}) \frac{d}{dx} (V \psi) = V \frac{\hbar}{i} \frac{d}{dx} \psi - (\frac{\hbar}{i})(V \frac{d}{dx} \psi + \psi \frac{d}{dx} V)
\]

\[
= i\hbar \frac{dV}{dx} \psi
\]

\[
[V, \hat{p}] = i\hbar \frac{dV}{dx} \psi
\]

so

\[
\frac{d}{dt} \langle p \rangle = \frac{i}{\hbar} (\langle i\hbar \frac{dV}{dx} \rangle) = -\langle V'(x) \rangle
\]

**Exercise:** \(\hat{O} - \langle O \rangle\) is hermitian because \(\hat{O}\) is given to be an observable and is thus hermitian. Then

\[
\sigma^2_{\hat{O}} = \langle (O - \langle O \rangle)^2 \rangle = \int \psi^*(O - \langle O \rangle)^2 \psi dx = \int ((O - \langle O \rangle)\psi)^*(O - \langle O \rangle)\psi dx = \langle (O - \langle O \rangle)\psi | (O - \langle O \rangle)\psi \rangle
\]

Let \(\hat{a} = O_1 - \langle O_2 \rangle\) and \(\hat{b} = O_2 - \langle O_2 \rangle\) and apply Cauchy-Schwarz [6]

\[
\sigma^2_{\hat{O}_1, \hat{O}_2} = \langle a\psi | a\psi \rangle \langle b\psi | b\psi \rangle \geq |\langle a\psi | b\psi \rangle|^2
\]

Let \(z = \langle a\psi | b\psi \rangle\). By the axioms of inner products [7], \(z^\ast = \langle b\psi | a\psi \rangle\). Applying the hermiticity of \(a\) and \(b\) again,

\[
z - z^\ast = \int (a\psi)^* b\psi dx - \int (b\psi)^* a\psi dx = \int \psi^* ab\psi dx - \int \psi^* ba\psi dx = (\langle ab \rangle - \langle ba \rangle)\psi = \langle [a, b] \rangle \psi
\]

From the definition of the commutator, this equals \(\langle [a, b] \rangle = \langle [O_1 - \langle O_1 \rangle, O_2 - \langle O_2 \rangle] \rangle = \langle [O_1, O_2] \rangle\). Then

\[
\sigma^2_{\hat{O}_1, \hat{O}_2} \geq |\langle a\psi | b\psi \rangle|^2 \geq (\frac{1}{2\hbar^2} (z - z^\ast))^2 = \frac{1}{2\hbar^2} \langle [O_1, O_2] \rangle^2
\]
# 3 Experimental Foundations: Stern-Gerlach Experiment

## 3.1 Motivation

In the 1920s, Bohr’s model of the atom, with quantized electron energy states, was the leading model. The Stern-Gerlach experiment attempted to confirm the quantization of the direction of electron angular momentum vectors. [8] Because orbiting charged particles create a magnetic moment that depends on their orbital angular momentum, using a magnetic field to deflect atoms would be able to measure angular momentum determine if its direction was quantized. However, this experiment instead confirmed the existence of quantized electron spin and can be used to demonstrate the uncertainty principle.

## 3.2 Experimental Setup

A beam of silver atoms (produced by vaporizing silver in an oven) was sent through a non-uniform magnetic field perpendicular to their velocity, landing on a detection plate. The distribution of atoms on the plate was then measured. The potential of the magnetic moment is given by [9]

\[ U = -\vec{\mu} \cdot \vec{B} = -\mu_z B \]

Thus, the force on the atom would be

\[ F = -\frac{\partial U}{\partial z} = \mu_z \frac{\partial B}{\partial z} \]

and the position of atoms on the screen would correspond to the atom’s magnetic moment component in the direction of the magnetic field. If the magnetic moment was quantized, a discrete number of spots would be observed instead of a continuous spectrum.

## 3.3 Results

The observations confirmed the prediction of quantization: there was a concentration of atoms at two points. Unfortunately, there was a problem with the Bohr-Sommerfeld theory. If the angular momentum quantum number, \( L \), of the silver electrons were 0, then no deflection should be expected. If \( L = 1 \), as assumed, there should have been three spots, one corresponding to the zero angular momentum state. To account for this, spin of the electrons was proposed. This was consistent with the observations and further experiments with hydrogen atoms. Each component of spin \( S \) was observed to be quantized with possible values \( \pm \frac{1}{2} \hbar \).

## 3.4 Extensions and Implications

A further experiment involves multiple Stern-Gerlach devices with their magnetic fields in different orientations placed in series. These act as filters because they split the input beam into two beams based on spin: \( S_n = \frac{1}{2} \hbar \) and \( S_n = -\frac{1}{2} \hbar \) (\( n \) is the direction of the magnetic field). If only one output beam is sent to the next device, then the spin of that beam should be exactly known. When three devices, one choosing for \( S_x = \frac{1}{2} \hbar \), the next \( S_y = \frac{1}{2} \hbar \), and the final one \( S_x = \frac{1}{2} \hbar \), are placed in series, an unexpected result occurs. The output of the third device contains particles of both possible values for spin in the \( x \), even though the first device had already determined its value. This suggests that the second device’s measurement of \( S_y \) changed the value of \( S_x \), and that measuring the two values exactly simultaneously is impossible.

An explanation can be obtained from the uncertainty principle [2]. If the two beams can be measured accurately enough to be distinguishable, then the \( S_x \) value would become random. The magnetic field applies a force

\[ F_x = -\mu_x \frac{\partial B}{\partial x} \]

and also rotates the magnetic moment at a rate of

\[ \omega = \frac{\mu_x B}{\hbar} \]
To make this the same for all atoms, we could try to make sure that all particles experience exactly the same $B$ field and the precession rate would be accounted for. However, if the uncertainty principle is true, then there must be some uncertainty in position:

$$\Delta p_x \Delta x \approx \hbar$$

$$m \Delta v_x \Delta x \approx \hbar$$

The total uncertainty of the size of each beam as the particle moves through the machine is

$$\delta x = \Delta v_x t \approx \frac{\hbar t}{m \Delta x}$$

The distance between the beams as they are pulled apart by the force is given by

$$d = 2 \cdot \frac{\mu_x}{m} \frac{\Delta B}{\partial x} t^2 \approx \mu_x \frac{x}{m} \frac{\partial B}{\partial x} t^2$$

If the uncertainty in beam size is too large compared to the distance between the two beams, then they would be indistinguishable and $S_x$ would not be measured precisely. Therefore

$$d >> \delta x$$

$$\frac{\Delta x}{h} \frac{\partial B}{\partial x} t >> 1$$

Assuming that $\frac{\partial B}{\partial x}$ is constant,

$$\Delta \omega = \frac{\mu_x \Delta B}{h} = \frac{\mu_x}{h} \frac{\partial B}{\partial x} \Delta x >> \frac{1}{t}$$

Therefore, the total rotation angle uncertainty, $\Delta \omega t$, is very large and makes the measurement of the spin $S_x$ random. This is consistent with the results of the experiment. This experiment demonstrates both the quantization of angular momentum and the uncertainty in measurement predicted by quantum theory.

References