The Hamiltonian operator

LHS of TDSE can be written as:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x,t)\psi = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right)\psi \equiv \widehat{H}\psi$$

where $\widehat{H}$ is called the ***Hamiltonian operator*** which is the differential operator that represents the ***total energy*** of the particle.

$$\widehat{H} \equiv -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t) = \frac{\hat{p}_x^2}{2m} + V(x,t)$$

where the ***momentum operator*** is

$$\hat{p}_x \equiv -i\hbar\frac{\partial}{\partial x}$$

Thus, shorthand for TDSE is:

$$\widehat{H}\psi = i\hbar\frac{\partial\psi}{\partial t}$$

Solving the TDSE – Challenging in general!

Suppose the potential is independent of time i.e., $V(x,t) = V(x)$ then the TDSE is:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x,t)\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi$$

The LHS involves variation of ψ with t while the RHS involves variation of ψ with x. Hence we look for a separated solution of the form:

$$\Psi(x,t) = \psi(x)T(t)$$

The TDSE becomes

$$-\frac{\hbar^2}{2m}T(t)\frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x)T(t) = i\hbar\psi(x)\frac{\partial T(t)}{\partial t}$$

Solving the TDSE –Time independent potential

Dividing both sides by ψT we find

$$-\frac{\hbar^2}{2m\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2}+V(x)=\frac{i\hbar}{T(t)}\frac{\partial T(t)}{\partial t}$$

The LHS depends only upon *x*, the RHS only on *t*.

True for all *x* and *t* so both sides must equal a constant, *E* (*E* = separation constant).

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V(x)\psi(x)=E\psi(x)$$

$$i\hbar\frac{\partial T(t)}{\partial t}=ET(t)$$

Time-independent Schrödinger equation

Solving the time equation:

$$\frac{i\hbar}{T}\frac{\partial T(t)}{\partial t} = E \Rightarrow \frac{dT}{T} = -\frac{iE}{\hbar}dt \Rightarrow T(t) = T_0 e^{-\frac{iEt}{\hbar}} = T_0 e^{-i\omega t}$$

An oscillatory solution with frequency given by $\omega = E/\hbar$.

The frequency depends on the energy, E.

To find out what the energy actually is, we must solve the spatial part of the problem...

The spatial equation is:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi = E\psi$$

This is the **time independent Schrödinger equation (TISE)** .

The TISE can often be very difficult to solve – it depends upon $V(x)$!

Eigenvalue equations

The *Schrödinger Equation* has the form of an *Eigenvalue Equation*:

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

where $\hat{H}$ is the Hamiltonian operator,

$$\hat{H} = \hat{K} + \hat{V} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

ψ is the wavefunction and is an *eigenfunction* of $\hat{H}$;

E is the total energy ($T + V$) and an *eigenvalue* of $\hat{H}$. E is just a constant!

Later in the course we will see that the eigenvalues of an operator give the possible results that can be obtained when the corresponding physical quantity is measured.

TISE for a free-particle

For a free particle $V(x) = 0$ and the TISE is:

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

The solutions are of the form:

$$\psi(x) = Ae^{ikx}$$

With energy given by

$$E = \frac{\hbar^2 k^2}{2m}$$

Thus the full solution to the full TDSE is:

$$\Psi(x,t) = \left(Ae^{ikx}\right)e^{-i\omega t}$$

Where $\omega = \frac{E}{\hbar} = \frac{\hbar k^2}{2m}$

TISE for a free-particle

Note that for negative k, the sign of the energy (and therefore, the frequency), is the same

$$\Psi(x,t) = \left(Ae^{-ikx}\right)e^{-i\omega t}$$

The solutions correspond to waves traveling in either $\pm x$ direction with:

1. An angular frequency, $\omega = E/\hbar$ (or $E = \hbar\omega$)

2. A wavevector $k = \frac{\sqrt{2mE}}{\hbar} = p/\hbar$ (or $p = \frac{h}{\lambda}$ where $\lambda = \frac{2\pi}{k} = h/\sqrt{2mE}$)

WAVE-PARTICLE DUALITY!

Interpretation of $\Psi(x,t)$ and how to use it

As mentioned previously, the TDSE has solutions that are inherently complex $\Rightarrow \Psi(x,t)$ *cannot* be a physical wave (e.g. electromagnetic waves). Therefore, how can $\Psi(x,t)$ relate to real physical measurements on a system?

The Born Interpretation

The Probability of finding a particle in the interval dx at position x and time t is equal to

$$\Psi^*(x,t)\Psi(x,t)dx = |\Psi(x,t)|^2 dx = p(x,t)dx$$

$|\Psi(x,t)|^2$ is real as required for a probability distribution and is the probability *per unit length* (per unit area in 2D or per unit volume in 3D), namely it is a probability density.

The Born interpretation

- $\Psi(x,t)$ the ***probability amplitude***
- $|\Psi(x,t)|^2 = p(x,t)$ the ***probability density***
- $|\Psi(x,t)|^2 dx$ the ***probability***.

Normalization

Total probability of finding a particle anywhere must be 1:

$$\int_{-\infty}^{\infty} p(x,t)dx = \int_{-\infty}^{\infty} \mathit{\Psi}^*(x,t)\mathit{\Psi}(x,t)dx = 1$$

This requirement is known as the ***Normalization condition***. (This condition arises because the SE is linear in $\mathit{\Psi}$, and therefore, if $\mathit{\Psi}$ is a solution of the TDSE so is $c\mathit{\Psi}$ where c is a constant.)

Hence if an original unnormalized wavefunction is $\mathit{\Psi}_{unnorm}(x,t)$, then the normalization integral is:

$$N^2 = \int_{-\infty}^{\infty} |\Psi_{unnorm}(x,t)|^2 dx$$

And the normalized (re-scaled) wavefunction is $\Psi(x,t) = \frac{1}{N}\Psi_{unnorm}(x,t)$

Example 1:

What value of N normalizes the function $f(x)$ given below?

$$f(x) = \begin{cases} Nx(x-L) & 0 \le x \le L \\ 0 & else \end{cases}$$

$$|f(x)|^2 = N^2x^2(x-L)^2 = N^2(x^4 - 2x^3L + x^2L^2)$$

The normalization condition reads:

$$\int_{-\infty}^{\infty} |f(x)|^2 dx = \int_0^L |f(x)|^2 dx = N^2 \int_0^L \left(x^4 - 2x^3L + x^2L^2\right) dx$$

$$= N^2\left(\frac{L^5}{5} - \frac{L^5}{2} + \frac{L^5}{3}\right) = \frac{N^2L^5}{30} = 1 \Rightarrow N = \sqrt{\frac{30}{L^5}}$$

Example 2: Find the probability that a particle described by the wavefunction $g(x)$, given below, is found anywhere in the interval

$0 \leq x \leq 0.25$.

$$g(x) = \begin{cases} \sqrt{2}\sin(\pi x) & 0 \leq x \leq 1 \\ 0 & else \end{cases}$$

$$|g(x)|^2 = 2\sin^2(\pi x) = 2\,\frac{1-\cos(2\pi x)}{2} = 1-\cos(2\pi x)$$

First we verify the normalization

$$\int_{-\infty}^{\infty} |g(x)|^2 dx = \int_0^1 |g(x)|^2 dx = \int_0^1 (1-\cos(2\pi x\ ))dx$$

$$= \left(x - \frac{1}{2\pi}\sin(2\pi \mathrm{x})\right)\Big|_0^1 = 1$$

Example 2: Find the probability that a particle described by the wavefunction *g*(*x*), given below, is found anywhere in the interval

$0 \leq x \leq 0.25.$

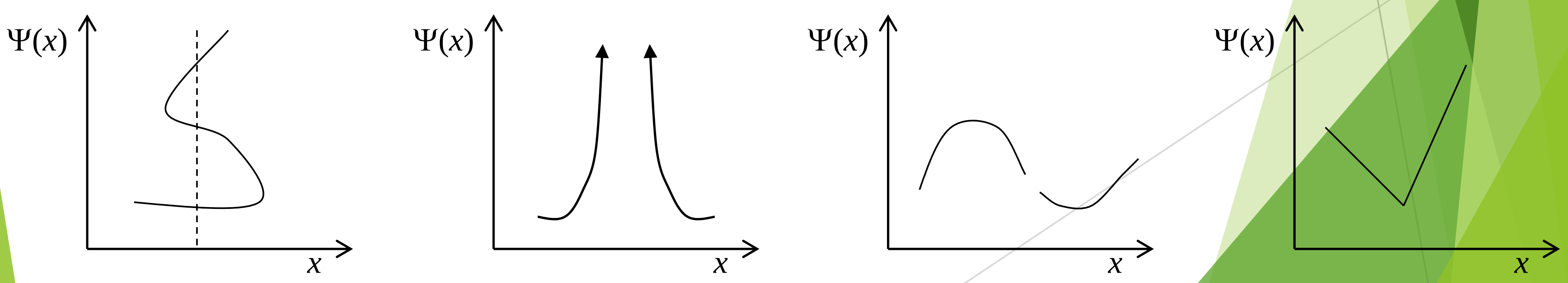
$$P(0 \leq x \leq 0.25) = \int_0^{0.25} |g(x)|^2 dx = \left(x - \frac{1}{2\pi} \sin(2\pi \mathrm{x}) \right) \Big|_0^{0.25}$$

$$= 0.25 - \frac{1}{2\pi} \sin\left(\frac{\pi}{2}\right) = 0.25 - \frac{1}{2\pi} \approx 0.0908$$

Boundary conditions for Ψ

In order for Ψ to be a solution of the Schrödinger equation representing a physically observable system, Ψ must satisfy certain constraints:

- Must be a single-valued function of x and t;
- Must be normalizable; this implies that $\Psi \to 0$ *as* $x \to \pm\infty$;
- $\psi(x)$ must be a continuous function of x;
- The *slope* of ψ must be continuous, specifically $\partial\psi(x)/\partial x$ must be continuous (except at points where the potential diverges).



Expectation values

If we know $\Psi(x, t)$ (a solution of the TDSE), then knowledge of $\Psi^*\Psi \, dx$ allows the *average* position (or any other observable) to be calculated:

$$\langle x \rangle \equiv \sum_i x_i p(x_i) \delta x$$

In the limit that $\delta x \rightarrow 0$ the summation becomes:

$$\langle x(t) \rangle = \int_{-\infty}^{\infty} x p(x) dx = \int_{-\infty}^{\infty} x \Psi^*(x,t) \Psi(\mathrm{x},\mathrm{t}) dx$$

The average is also know as the *expectation value* and is very important in quantum mechanics because in many cases precise values cannot, even in principle, be determined.

Expectation values

The expectation value is not limited to *x*, for example:

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 p(x)dx = \int_{-\infty}^{\infty} x^2 \Psi^*(x,t)\Psi(\mathrm{x},\mathrm{t})dx$$

Stationary States

We saw that even when the potential is independent of time the wavefunction still oscillates in time. The Solution to the full TDSE is:

$$\Psi(x,t) = \psi(x)T(t) = \psi(x)e^{-i\frac{E}{\hbar}t}$$

But the corresponding probability distribution is *static*:

$$p(x,t) = |\Psi(x,t)|^2 = \psi^*(x)e^{i\frac{E}{\hbar}t}\psi(x)e^{-i\frac{E}{\hbar}t} = |\psi(x)|^2$$

Therefore, a solution of the TISE which consists of a single eigenstate of the Hamiltonian (with specific energy) is known as a Stationary state.

What other information can you get from ψ? (and how!)

We have seen how we can use the probability density function, $\psi^*\psi$, to calculate the average position of a particle. What happens if we want to calculate the *average energy* or *momentum ?*

These observables are represented by the following differential operators:

$$\hat{H} = \frac{\hat{\vec{p}}^{\,2}}{2m} + V(x) \quad \text{and} \quad \hat{\vec{p}} = -i\hbar\nabla \quad \text{with} \quad \nabla \equiv \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$$

Do the operators work on $\psi^*\psi$, or on ψ, or on ψ^* alone?

What other information can you get from ψ? (and how!)

Take TISE for an eigenfunction of the Hamiltonian, multiply from the left by ψ^* and integrate (ψ is normalized).

$$\hat{H}\psi_n = E_n\psi_n$$

$$\int_{-\infty}^{\infty} \psi_n^* \hat{H}\psi_n dx = \int_{-\infty}^{\infty} \psi_n^* E_n \psi_n dx = E_n$$

This suggests that in order to calculate the *average value* of the physical quantity associated with a QM operator we carry out the following integration:

$$\langle \hat{q} \rangle = \int_{-\infty}^{\infty} \psi^* \, \hat{q}\psi dx$$

Note that sometimes the limits of the integration are not specified and it implies that the integration is from $-\infty$ to ∞.

Momentum and energy expectation values

The expectation value of *momentum* involves the representation of momentum as a quantum mechanical operator:

$$\langle p_x \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\widehat{p_x}\Psi(x,t)dx = \int_{-\infty}^{\infty} \Psi^*(x,t)\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi(x,t)dx \quad \textit{where we used} \quad \widehat{p_x} \equiv \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$\widehat{p_x}$ is the operator for the *x* component of momentum.

Example: Derive an expression for the average energy of a free particle.

$$E = \frac{p^2}{2m} \Longrightarrow \langle E \rangle = \frac{\langle p^2 \rangle}{2m}$$

Since $V = 0$ the expectation value for energy for a particle moving in one dimension is

$$\langle E \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\Psi(x,t)dx$$

Our definition of the expectation value is one of the postulates of QM.

The Heisenberg Uncertainty Principle

We saw earlier that the energy of a free particle with momentum p_0 can be written as

$$E_0 = \frac{p_0^2}{2m} = \frac{\hbar^2 k_0^2}{2m} = \hbar\omega(k_0)$$

And its wavefunction can be written as $\psi(x,t) = A_0 e^{i(k_0 x - \omega(k_0)t)}$

Considering the fact that we interpret the square of the wavefunction as the probability density we find

$$p(x,t) = |\psi(x,t)|^2 = |A_0|^2$$

Namely, the probability density is independent of the position. We have the same probability to find the particle at any location! which implies we have no knowledge about the position. However, the momentum is precisely defined.

The Heisenberg Uncertainty Principle

The Heisenberg uncertainty principle states that, in any **simultaneous measurement** of the position and the momentum of a particle,

$$\Delta x \cdot \Delta p \geq \hbar/2$$

where Δx is the uncertainty in the measurement of a particular coordinate x, and Δp is the uncertainty in the measurement of the corresponding momentum.

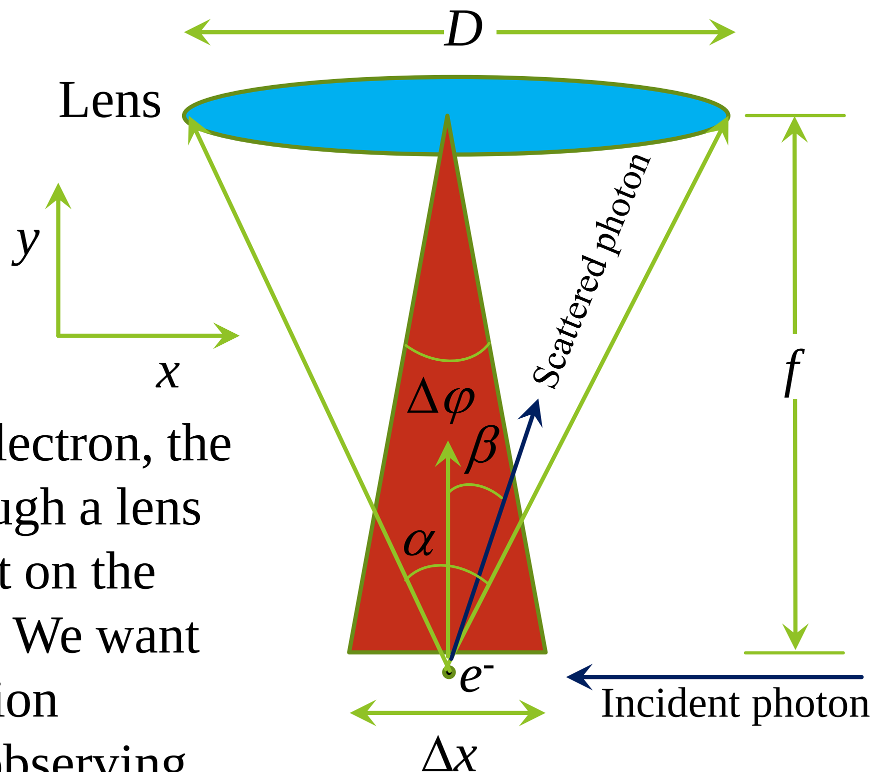
Since 1927, there have been many attempts to invent methods by which this principle could be violated, but none has succeeded. Let us examine a simple thought experiment to see how these uncertainties actually occur.

Heisenberg Microscope

Imagine that we are able to use a microscope to measure the position of an electron, and that we can detect a single photon scattered from the electron.

Photographic plate or CCD

From the geometry, $\tan(\alpha/2) = D/(2f)$



Electron position (Δx)

After striking the electron, the photon passes through a lens and produces a spot on the photographic plate. We want to deduce the position of the electron by observing the position of the spot on the plate.

Conservation of momentum yields

$$\vec{p}_{photon} = \frac{h}{\lambda}\left(\sin\beta\,\hat{x} + \cos\beta\,\hat{y}\right)$$

(scattered photon)

From optics, the minimum angular resolving power is

$$\Delta\varphi \approx \frac{\lambda}{D}$$

$$\textit{then} \quad \Delta x \approx f\,\Delta\varphi \approx \frac{f\lambda}{D},$$

which is the uncertainty in the position of the electron.

The Heisenberg Uncertainty Principle

From the geometry, $\tan\left(\frac{\alpha}{2}\right) = \frac{D}{2f}$, assuming that the angle α is small we can write $\alpha \approx D/f$.

For the scattered photon, the momentum is given by

$$\vec{p}_{photon} = p_x\,\hat{x} + p_y\,\hat{y} = \frac{h}{\lambda}(sin\beta\hat{x} + cos\beta\,\hat{y})$$

with p_x lying in the range:

$$-\frac{h}{\lambda}\sin\left(\frac{\alpha}{2}\right) \le p_x \le \frac{h}{\lambda}\sin\left(\frac{\alpha}{2}\right) \qquad since\ \beta \le \alpha/2$$

Using the small angle approximation

$$-\frac{h}{\lambda}\frac{\alpha}{2} \le p_x \le \frac{h}{\lambda}\frac{\alpha}{2} \qquad or -\frac{h}{\lambda}\frac{D}{2f} \le p_x \le \frac{h}{\lambda}\frac{D}{2f}$$

The Heisenberg Uncertainty Principle

Consequently, $\Delta p_x = hD/(f\lambda)$ and $\Delta x \approx f\lambda/D$ which results in

$$\Delta p_x \cdot \Delta x \approx h$$

which is independent of the size and focal length of the lens (D) and wavelength of the photon (λ).

Notice that a small (large) wavelength leads to a large (small) Δp_x and small (large) Δx.

The exact expression that we use for the Heisenberg uncertainty principle is $\Delta x \cdot \Delta p \geq \hbar/2$ and can be derived using straightforward methods in quantum mechanics.

Wave packet

One way to get a localized particle is to consider a wave packet. As we saw earlier the Shcrödinger equation is linear and any linear combination of solutions is also a solution.

$$\psi(x,t) = \int_{-\infty}^{\infty} \frac{1}{2\pi} e^{ikx} \tilde{\psi}(k,t) dk$$

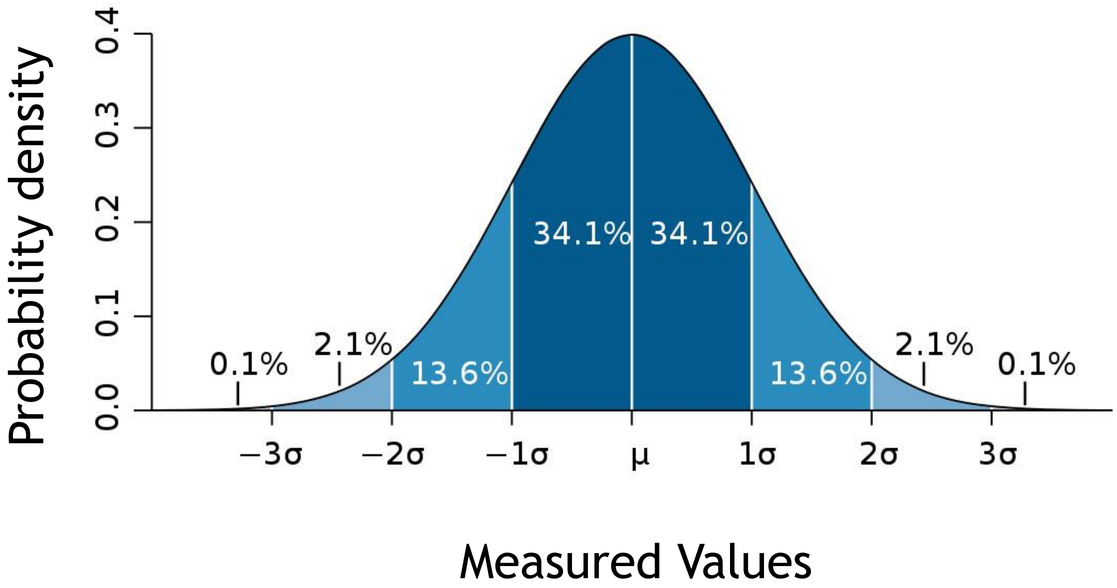
The wave packet is a linear combination of waves.

Many things closely follow a Normal or Gaussian Distribution in Nature:

For example:

- Heights of people
- Weights of elephants
- Marks (grades) on a test
- Random errors in many types of measurements in nature

We say the data is "normally distributed“ when there are random variations about a mean, average, or expectation value (μ). σ is the standard deviation. σ^2 is the variance.



$$P(x) = \frac{\exp\left[-(x-\mu)^2 / 2\sigma^2\right]}{\sigma\sqrt{2\pi}}$$

$$\int_{-\infty}^{\infty} P(x)dx = 1$$

The Heisenberg Uncertainty Principle using Gaussian wave packets

We consider a Gaussian wave packet

$$\tilde{\psi}(k) = \left(2\pi a^2\right)^{1/4} e^{-\frac{a^2}{4}(k-k_0)^2}$$

We can use Parseval's theorem to check for normalization

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} \left|\tilde{\psi}(k)\right|^2 dk = \int_{-\infty}^{\infty} |\psi(x)|^2 dx \qquad Parseval's\ theorem$$

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} \left|\left(2\pi a^2\right)^{\frac{1}{4}} e^{-\frac{a^2}{4}(k-k_0)^2}\right|^2 dk = \frac{1}{2\pi}\int_{-\infty}^{\infty} \left(2\pi a^2\right)^{\frac{1}{2}} e^{-\frac{a^2}{2}(k-k_0)^2} dk$$

$$= 1$$

By inverting the Fourier transform of the wavefunction we find

$$\psi(x) = \left(\frac{2}{\pi a^2}\right)^{\frac{1}{4}} e^{ik_0 x} e^{-\frac{x^2}{a^2}}$$

The Heisenberg Uncertainty Principle using Gaussian wave packets

$$Var(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left|\tilde{\psi}(k)\right|^2 \Delta k^2 dk = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left(2\pi a^2\right)^{\frac{1}{2}} e^{-\frac{a^2}{2}(\Delta k)^2}\Delta k^2 dk = \frac{1}{a^2}$$

$$Var(x) \;= \int_{-\infty}^{\infty}|\psi(x)|^2 \Delta x^2 dx = \int_{-\infty}^{\infty}\left(\frac{2}{\pi a^2}\right)^{\frac{1}{2}} e^{-2\frac{x^2}{a^2}} x^2 dx = \frac{a^2}{4}$$

$$\Delta k = \sqrt{Var(k)} = \frac{1}{a}; \Delta x = \sqrt{Var(x)} = a/2$$

$$p = \hbar k \rightarrow \Delta p = \hbar \Delta k = \hbar / a$$

$$\Delta p \Delta x = \frac{\hbar}{2}$$

which agrees with the Heisenberg uncertainty principle $\Delta x \cdot \Delta p \geq \hbar/2$.

The Heisenberg Uncertainty Principle using Gaussian wave packets

An alternative derivation of the momentum uncertainty is by considering the momentum operator.

$$Var(p) = \langle p^2 \rangle - \langle p \rangle^2$$

$$\psi(x) = \left(\frac{2}{\pi a^2}\right)^{\frac{1}{4}} e^{ik_0 x} e^{-\frac{x^2}{a^2}} \rightarrow \frac{\partial}{\partial x}\psi(x) = \left(ik_0 - \frac{2x}{a^2}\right)\psi(x)$$

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^*(x) \frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x)dx = \hbar k_0$$

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} \psi^*(x) \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 \psi(x)dx = \hbar^2 k_0^2 - \frac{4\hbar^2}{a^4}\langle x^2 \rangle + \frac{2\hbar^2}{a^2} = \hbar^2 k_0^2 + \frac{\hbar^2}{a^2}$$

$$\psi(x) = \left(\frac{2}{\pi a^2}\right)^{\frac{1}{4}} e^{ik_0 x} e^{-\frac{x^2}{a^2}} \rightarrow \frac{\partial^2}{\partial x^2}\psi(x) = \left(-k_0^2 - \frac{2x}{a^2}\left(ik_0 - \frac{2x}{a^2}\right) - \frac{2}{a^2}\right)\psi(x)$$

$$Var(p) = \langle p^2 \rangle - \langle p \rangle^2 = \frac{\hbar^2}{a^2} \rightarrow \Delta p = \frac{\hbar}{a}$$

Commutation Relations

If two observables, A and B, have linear operators associated with them, the commutator is defined by,

$$[\hat{A},\hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$$

The commutator is a composite operator and must be treated as such when operating on any function.

$$[\hat{A},\hat{B}]\psi \equiv (\hat{A}\hat{B} - \hat{B}\hat{A})\psi = \hat{A}\hat{B}\psi - \hat{B}\hat{A}\psi$$

If ψ is an eigenfunction, with eigenvalues a and b for observables A and B respectively, and if the operators commute then

$$\hat{A}\psi = a\psi \quad and \qquad \hat{B}\psi = b\psi$$

Therefore,

$$[\hat{A},\hat{B}]\psi = \hat{A}\hat{B}\psi - \hat{B}\hat{A}\psi = \hat{A}b\psi - \hat{B}a\psi = ab\psi - ba\psi = 0$$

In this case, the observables A and B can be measured simultaneously with infinite precision, i.e., uncertainties $\Delta A = 0$ and $\Delta B = 0$, simultaneously. ψ is then said to be the simultaneous eigenfunction of A and B.

When observables commute, measurements of A and B do not cause any change of state (i.e., initial and final states are the same before and after the measurement).

Suppose we measure A to get value a. We then measure B to get the value b. We measure A again and still get the same value a. Clearly the state (ψ) of the system is not destroyed and so we are able to measure A and B simultaneously with infinite precision. However, if

$$[\hat{A}, \hat{B}] \neq 0$$

then the operators do not commute and the two observables cannot be measured simultaneously, resulting in an uncertainty principle relation.

The most relevant example is for momentum and position:

$$[\hat{x},\hat{p}_x]\psi = (\hat{x}\hat{p}_x - \hat{p}_x\hat{x})\psi = x\frac{\hbar}{i}\frac{\partial}{\partial x}\psi - \frac{\hbar}{i}\frac{\partial}{\partial x}(x\psi)$$

$$= x\frac{\hbar}{i}\frac{\partial}{\partial x}\psi - \frac{\hbar}{i}\left(x\frac{\partial}{\partial x}\psi + \psi\frac{\partial}{\partial x}x\right) = i\hbar\psi$$

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

which is consistent with the
Heisenberg uncertainty principle.

The uncertainty relation can be generalized as follows for any two observables *A* and *B* (*Robertson uncertainty relation*) :

$$If \quad \left[\hat{A},\hat{B}\right] = i\hat{C} \quad then \qquad \Delta A\cdot\Delta B \ge \frac{1}{2}\left|\left\langle\left[\hat{A},\hat{B}\right]\right\rangle\right|$$

Example: $\Delta x\cdot\Delta p \ge \frac{1}{2}\left|\left\langle\left[\hat{x},\hat{p}\right]\right\rangle\right| = \frac{1}{2}\left|\left\langle i\hbar\right\rangle\right| \quad \Rightarrow \quad \Delta x\cdot\Delta p \ge \frac{\hbar}{2}$

More generally, $\left[\hat{r}_i,\hat{p}_j\right] = i\hbar\delta_{ij}$ where the Kronecker delta is $\delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \ne j \end{cases}$

Summary

TDSE:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V(x,t)\Psi=i\hbar\frac{\partial\Psi}{\partial t}$$

Born interpretation:

$$\Psi^*(x,t)\Psi(x,t)dx=\left|\Psi(x,t)\right|^2dx=P(x,t)dx$$

Normalization:

$$\int_{-\infty}^{\infty}P(x)dx=\int_{-\infty}^{\infty}\left|\Psi(x,t)\right|^2dx=1$$

TISE:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V(x)\psi=E\psi \quad \text{or} \quad \hat{H}\psi=E\psi$$

$$\Psi(x,t)=\psi(x)\,T(t)=\psi(x)e^{-iEt/\hbar}$$

Conditions on ψ: single-valued, continuous, normalizable, continuous first derivative.

Expectation value of operator Ω: $\int_{-\infty}^{\infty}\Psi^*(x,t)\hat{\Omega}\Psi(x,t)dx$

The Heisenberg uncertainty principle: $\Delta x\cdot\Delta p\geq\hbar/2$

Additional References

1. *The Quantum Theory of Atoms and Molecules*, Grant Ritchie, University of Oxford
2. *Introduction to Modern Physics*, John D. McGervey
3. The lecture notes linked on the course webpage.