PH 101: Physics I

Module 3: Introduction to Quantum Mechanics

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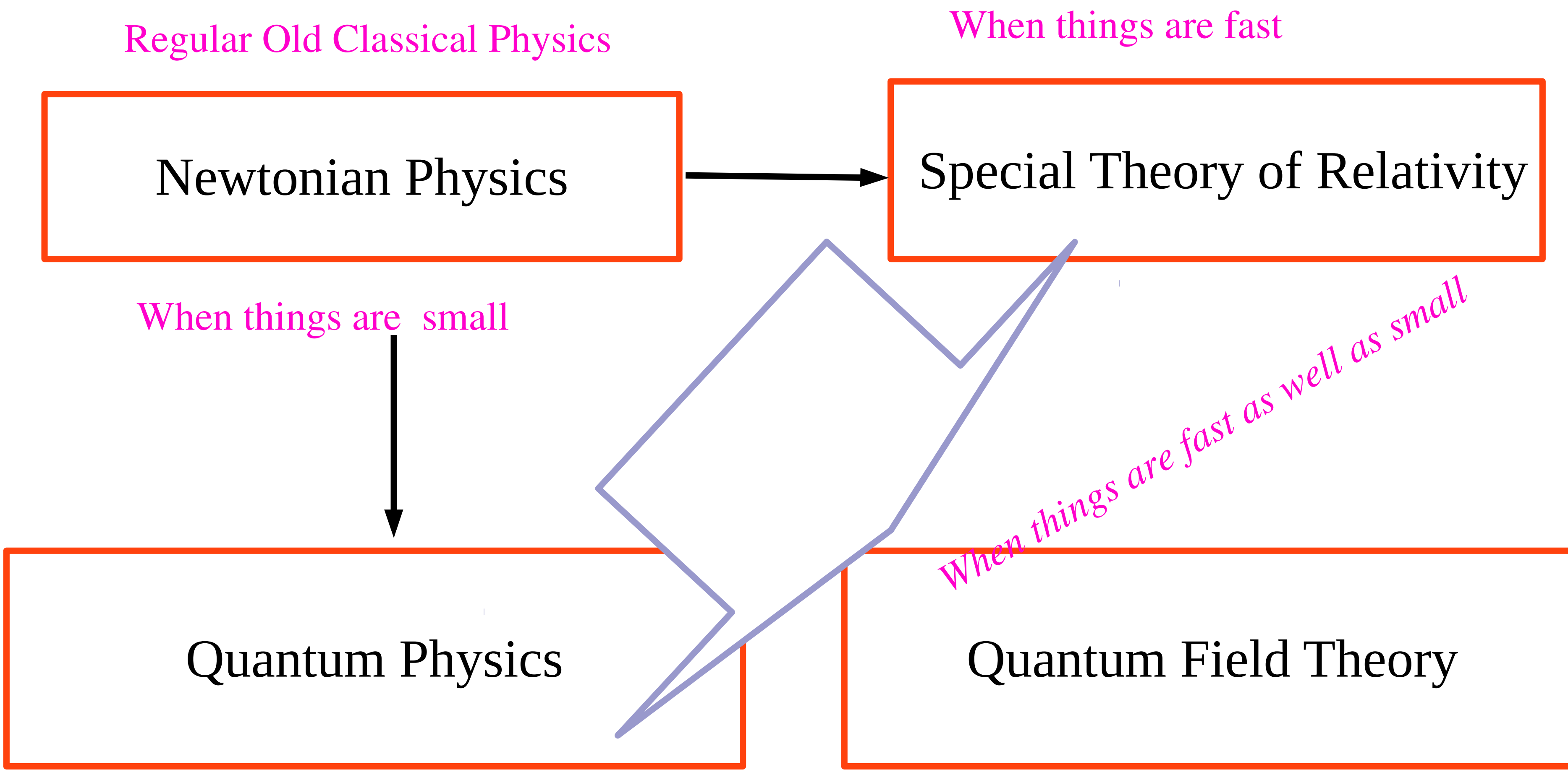
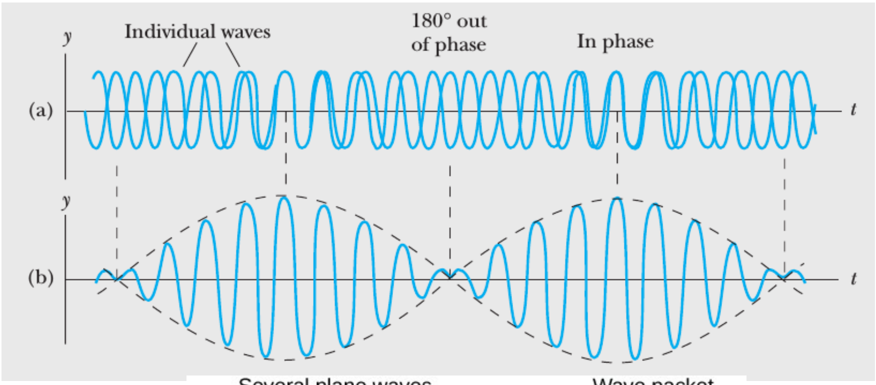
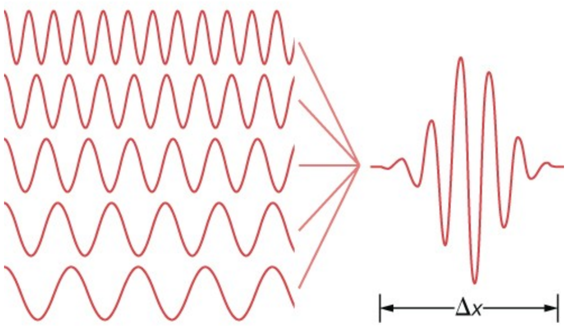

Regular Old Classical Physics
When things are fast
Newtonian Physics
Special Theory of Relativity
When things are small
When things are fast as well as small
Quantum Physics
Quantum Field Theory

Recap: Representation of Matter through waves



Several plane waves
Wave packet



$$\Psi(x, t) = 2A\cos\left(\frac{\Delta k}{2}x - \frac{\Delta\omega}{2}t\right)\cos(k_{av}x - \omega_{av}t)$$

where $\Delta k = k_1 - k_2$, $\Delta\omega = \omega_1 - \omega_2$, $k_{av} = (k_1 + k_2)/2$, and $\omega_{av} = (\omega_1 + \omega_2)/2$

$$\frac{\Delta k}{2}x_2 - \frac{\Delta k}{2}x_1 = \pi$$

$$\Delta\omega\Delta t = 2\pi$$

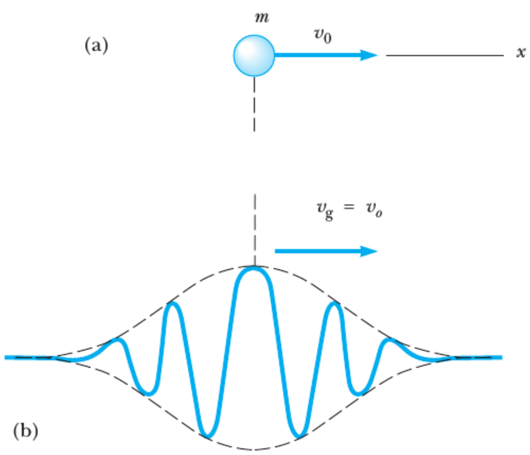
$$\Delta k\Delta x = 2\pi$$

$$\Delta E\Delta t = h$$

$$\Delta x\Delta p = h$$

In principle one can generalise the previous calculation to obtain the form of the most general wave packet.

However, we can obtain an interesting insight about the wave packet by simply considering the superposition of two waves which can also be generalised to many waves.



Matter particle moving with velocity v_0 can be represented by a wave packet with group velocity $v_g = v_0$

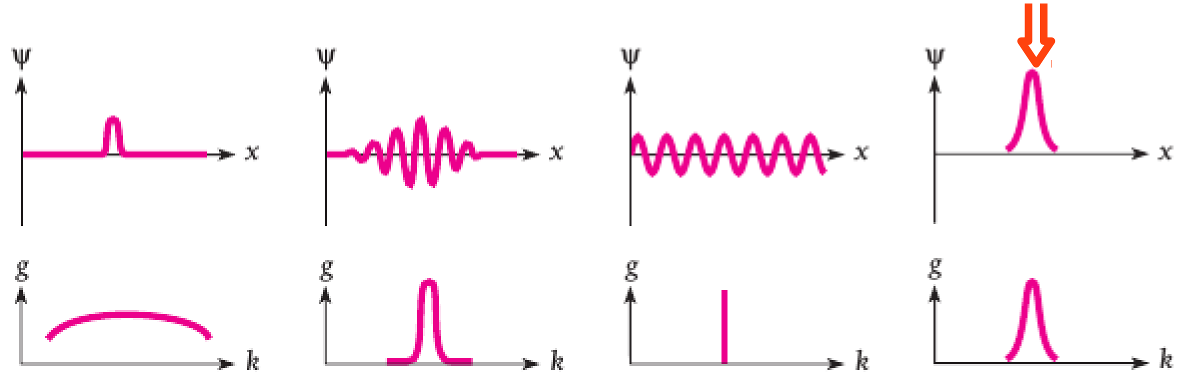
In the wave representation we can not determine the particular location of the particle exactly if momentum is given. In the similar way we can not say something definite about the momentum if we are able to make the spread of wave packet nearly zero.

Representation of Matter through waves: Uncertainty Priciple

Gaussian Wave function $\psi(x) = \dfrac{1}{\sigma\sqrt{2\pi}} e^{-(x-<x>)^2/2\sigma^2}$

Reepresentation of wave in the real space

$\sigma = \sqrt{< x^2 > - < x >^2}$ is the standard deviation in the x



Representation of wave in the wave number space

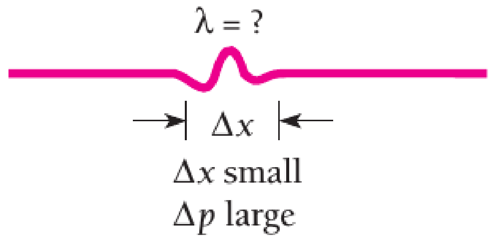
If wave is spread in the real space, it will be more localized in the wave number (or meomentum space). However, Gaussian wave packet in real space will have the form Gaussian wave-packet in the wave number space. And the relation between spread in real and moemntum space is given by

$\Delta x \Delta k = 1/2$

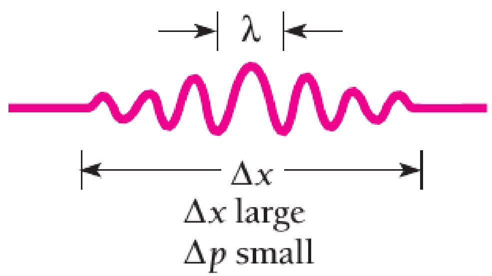
where Δx and Δk is the standard deviation in the x and k respectively and given by $\Delta x = \sqrt{< x^2 > - < x >^2}$ and $\Delta k = \sqrt{< k^2 > - < k >^2}$ where, $< . >$ represents the average (or expectation) value.

However, the wave packet is not exactly the Gaussian and the relation comes as $\Delta x \Delta k \geq 1/2$

It is impossible to know both the exact position and exact momentum of an object at the same time.



(a)



Representation of wave in position space

Representation of wave in wavenumber space

$$\Delta x \, \Delta k \geq \frac{1}{2}$$

Uncertainty Principle

$$\Delta x \Delta k \geq 1/2$$

where Δx and Δk is the standard deviation in the x and k respectively and given by $\Delta x = \sqrt{< x^2 > - < x >^2}$ and $\Delta k = \sqrt{< k^2 > - < k >^2}$ where, $< . >$ represents the average (or expectation) value.

$$k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h} \qquad p = \frac{hk}{2\pi}$$

Hence an uncertainty Δk in the wave number of the de Broglie waves associated with the particle results in an uncertainty Δp in the particle's momentum according to the formula

$$\Delta p = \frac{h\,\Delta k}{2\pi}$$

Since $\Delta x\, \Delta k \geq \frac{1}{2}$, $\Delta k \geq 1/(2\Delta x)$ and

Uncertainty principle

$$\Delta x\, \Delta p \geq \frac{h}{4\pi}$$

It states that the product of the uncertainty Δx in the position of an object at some instant and the uncertainty Δp in its momentum component in the x direction at the same instant is equal to or greater than $h/4\pi$.

Werner Heisenberg
German
1901-1976

It was in Copenhagen, in 1927, that Heisenberg developed his uncertainty principle, while working on the mathematical foundations of quantum mechanics.

Wave Function

Classical wave equation

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{\upsilon^2}\frac{\partial^2 y}{\partial t^2}$$

Typical solution

$$y = F\left(t \pm \frac{x}{\upsilon}\right)$$

In quantum mechanics the physical interpretation is obtained from the square of the amplitude or the probability distribution.

We can in principle assume the following form of the solution for a free particle which is moving along the X-direction .

$$\Psi = Ae^{-i\omega(t - x/\upsilon)}$$

Replacing ω in the above formula by $2\pi\nu$ and υ by $\lambda\nu$ gives

$$\Psi = Ae^{-2\pi i(\nu t - x/\lambda)}$$

$$E = h\nu = 2\pi\hbar\nu \qquad \text{and} \qquad \lambda = \frac{h}{p} = \frac{2\pi\hbar}{p}$$

$$\Psi = Ae^{-(i/\hbar)(Et - px)}$$

Schroedinger Equation

$$\Psi = Ae^{-(i/\hbar)(Et-px)}$$

$$\frac{\partial^2\Psi}{\partial x^2} = -\frac{p^2}{\hbar^2}\Psi \qquad \frac{\partial\Psi}{\partial t} = -\frac{iE}{\hbar}\Psi \qquad E = \frac{p^2}{2m} + U(x,\, t)$$

$$p^2\Psi = -\hbar^2\frac{\partial^2\Psi}{\partial x^2} \qquad E\Psi = -\frac{\hbar}{i}\frac{\partial\Psi}{\partial t} \qquad E\Psi = \frac{p^2\Psi}{2m} + U\Psi$$

$$\boxed{i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + U\Psi}$$

Schroedinger's equation in 1 dimension

$$\boxed{i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2}\right) + U\Psi}$$

Schroedinger's equation in 3 dimension

Matter-wave Mechanics

Schroedinger's equation: Non-Relativistic equation for matter wave.

$$\psi(x,t) = A\, e^{2\pi i\left(\frac{x}{\lambda} - \frac{t}{T}\right)}$$

$$\psi(x,t) = A\, \mathrm{e}^{\frac{2\pi i}{h}(p\,x - E\,t)}$$

$$\underbrace{i\hbar\frac{\partial}{\partial t}}_{\mathrm{E}}\psi(x,t) = \underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}}_{\frac{p^2}{2m}}\psi(x,t)$$

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

$$\underbrace{i\hbar\frac{\partial}{\partial t}}_{\mathrm{E}}\psi(x,t) = \underbrace{\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right)}_{\frac{p^2}{2m} + V(x,t)}\psi(x,t)$$

Relativistic equation for matter wave.

$$E^2 = p^2c^2 + m_0^2c^4$$

$$\left(i\hbar\frac{\partial}{\partial t}\right)^2\Psi(x,t) = \left(-i\hbar\frac{\partial}{\partial x}\right)^2 c^2 + m_0^2c^4\Psi(x,t)$$

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\Psi(x,t) = -\frac{\partial^2}{\partial x^2}\Psi(x,t) + \frac{m_0^2c^2}{\hbar^2}\Psi(x,t)$$

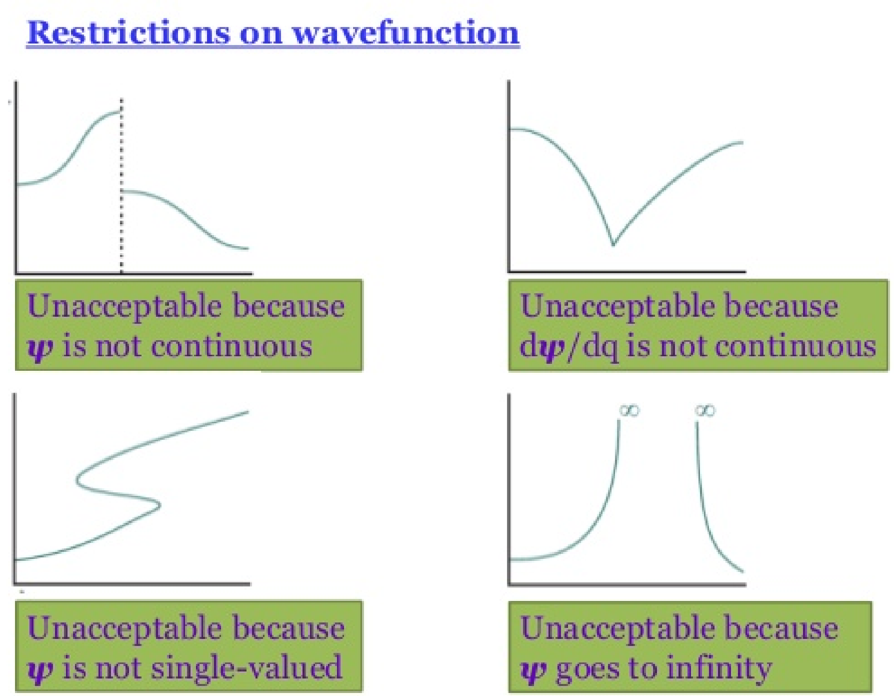
Relevant quantity is Probability density $|\psi(x,t)|^2 = |A|^2$

Wavefunction

1 Ψ must be continuous and single-valued everywhere.
2 $\partial\Psi/\partial x$, $\partial\Psi/\partial y$, $\partial\Psi/\partial z$ must be continuous and single-valued everywhere.
3 Ψ must be normalizable, which means that Ψ must go to 0 as $x \to \pm\infty$, $y \to \pm\infty$, $z \to \pm\infty$ in order that $\int |\Psi|^2 \, dV$ over all space be a finite constant.

Because there is always a finite probablity of particles existence in space, the wave function needs to be normalized.

Note that the above conditions (1, 2) may not be applicable for special cases e.g. when the potential corresponding to the force field have discontinuity.



Postulates of Quantum Mechanics

As the subject progressed, it became clear that a list of "Rules of the game" had to be urgently written down so that further progress could quickly be made. These rules go by the name of "Postulates of Quantum Mechanics" and they summarize what was known at that time (around 1927). The point of view contained in these postulates is known as the *Copenhagen Interpretation* of Quantum Mechanics since it was started by Neils Bohr and Werner Heisenberg working together in Copenhagen, Denmark between 1925-27.

1) State postulate: The state* of a quantum particle is described by a "wave function" which is denoted by $\psi(x,t)$ which is in general, a complex number and has the following meaning: $|\psi(x,t)|^2\,dx$ is the probability of finding that particle between positions x and $x+\mathrm{d}x$ at some time t. This is unlike in classical physics where the state of the particle is uniquely specified by prescribing its position x and momentum p (or velocity).

**The state of a system at a given time both in classical and quantum physics refers to that minimum amount of information needed to describe what this is at a later time assuming one knows all the forces etc that are acting in the system (i.e. the dynamics).*

Physical Interpretation of the complex matter wave

2) Observables: While position is described by just a number x other physical quantities (known as "observables") are described by operators (derivatives with respect to x,y,z if the particle moves in 3 dimensions e.g.).

Of this, the most important is the (linear) momentum $p = -i\,\hbar\,\frac{\partial}{\partial x}$ *. Since in this way of doing things, if x – the position has a well defined value, the momentum p cannot be a number with a well defined value. It has to be something that acts on the given state and leads to a number which could be the most probable value (or expectation value) for this quantity. Other observables such as angular momentum, kinetic energy etc. may be generated using the above correspondence. The average or "expected" value of an observable A is determined through the formula*

$$< A > = \int dx\, \psi^*(x,t)\, A\, \psi(x,t)$$

3) The measurement postulate: Measurement of the value of an observable in a quantum state in general yields a different result each time the measurement is performed (imagine n-copies of the same state and the same measurement being performed on all copies). All that quantum mechanics can predict are the values of these outcomes and the probabilities (or frequencies) with which they are seen. No one can know which of these outcomes will be seen in a specific attempt at measurement.

Physical Interpretation of the complex matter wave

4) Collapse postulate: In general, it is not possible in quantum mechanics to perform measurements on a physical system without altering the state of the system. When a measurement of a certain physical quantity is performed, the state of the system changes abruptly to a new state where the quantity just measured has a well defined value equal to the outcome of the measurement.

e.g. You make a measurement of the position of the electron in a hydrogen atom. The state of the electron now abruptly changes to a new state such that subsequent measurements of the position made immediately afterwards yield the same result for the position. In classical physics this is not surprising. In quantum physics the position of the electron in general has a range of values with the corresponding probabilities - but having measured the position once, any measurements of position made immediately after this will not lead to new values for the position.

5) Non-commutativity: In general any two measurements are not commutative i.e. the answers depend on the order in which they are made.

e.g. Imagine I measure the momentum of an electron in the hydrogen atom and then measure its position and note down the readings. I choose another hydrogen atom and reverse the order in which I make the measurements i.e. I first measure the position. But now I may or may not get the same value for the position I got when I did it with the earlier specimen. I keep choosing new specimens (all in the same state as the first specimen) and keep making position measurements until I get the outcome of the first specimen. Then I immediately measure the momentum. In classical physics the value of the momentum that I measured in the new specimen will be the same as in the first specimen but not so in the quantum world. This is called non-commutativity.

6) Evolution postulate: The state of a system in quantum mechanics evolves (changes in time) consistent with **Schrodinger's equation** *until interrupted by a measurement.*

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

Operators

Quantity	Operator
Position, x	x
Linear momentum, p	$\frac{\hbar}{i}\frac{\partial}{\partial x}$
Potential energy, $U(x)$	$U(x)$
Kinetic energy, $\mathrm{KE} = \frac{p^2}{2m}$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
Total energy, E	$i\hbar\frac{\partial}{\partial t}$
Total energy (Hamiltonian form), H	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)$

Expectation Value

the average position $\bar{x}$ of a number of identical particles distributed along the x axis in such a way that there are N_1 particles at x_1, N_2 particles at x_2, and so on? The average position in this case is the same as the center of mass of the distribution, and so

$$\bar{x} = \frac{N_1x_1 + N_2x_2 + N_3x_3 + \cdots}{N_1 + N_2 + N_3 + \cdots} = \frac{\sum N_i x_i}{\sum N_i}$$

When we are dealing with a single particle, we must replace the number N_i of particles at x_i by the probability P_i that the particle be found in an interval dx at x_i. This probability is

$$P_i = |\Psi_i|^2\, dx$$

where Ψ_i is the particle wave function evaluated at $x = x_i$. Making this substitution and changing the summations to integrals, we see that the expectation value of the position of the single particle is

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x|\Psi|^2\, dx}{\int_{-\infty}^{\infty} |\Psi|^2\, dx}$$

Expectation value for position

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

Expectation value

$$\langle G(x) \rangle = \int_{-\infty}^{\infty} G(x)|\Psi|^2\, dx$$

Expectation value of an operator

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

Expectation Value

$$\langle p \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{p} \Psi \, dx = \int_{-\infty}^{\infty} \Psi^* \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi \, dx = \frac{\hbar}{i} \int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x} \, dx$$

$$\langle E \rangle = \int^{\infty} \Psi^* \hat{E} \Psi \, dx = \int^{\infty} \Psi^* \left(i\hbar \frac{\partial}{\partial t} \right) \Psi \, dx = i\hbar \int^{\infty} \Psi^* \frac{\partial \Psi}{\partial t} \, dx$$

The other alternatives are

$$\int_{-\infty}^{\infty} \hat{p} \Psi^* \Psi \, dx = \frac{\hbar}{i} \int_{-\infty}^{\infty} \frac{\partial}{\partial x} (\Psi^* \Psi) \, dx = \frac{\hbar}{i} \Big[\Psi^* \Psi \Big]_{-\infty}^{\infty} = 0$$

since Ψ^* and Ψ must be 0 at $x = \pm\infty$, and

$$\int_{-\infty}^{\infty} \Psi^* \Psi \hat{p} \, dx = \frac{\hbar}{i} \int_{-\infty}^{\infty} \Psi^* \Psi \frac{\partial}{\partial x} \, dx$$

Expectation value of an operator

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

Expectation Value : Example

A particle limited to the x axis has the wave function $\Psi = ax$ between $x = 0$ and $x = 1$; $\Psi = 0$ elsewhere. (*a*) Find the probability that the particle can be found between $x = 0.45$ and $x = 0.55$. (*b*) Find the expectation value $\langle x \rangle$ of the particle's position.

Solution

(*a*) The probability is

$$\int_{x_1}^{x_2} |\Psi|^2 \, dx = a^2 \int_{0.45}^{0.55} x^2 dx = a^2 \left[\frac{x^3}{3} \right]_{0.45}^{0.55} = 0.0251a^2$$

(*b*) The expectation value is

$$\langle x \rangle = \int_0^1 x|\Psi|^2 \, dx = a^2 \int_0^1 x^3 dx = a^2 \left[\frac{x^4}{4} \right]_0^1 = \frac{a^2}{4}$$

Time independent Schroedinger's equation

$$\Psi = Ae^{-(i/\hbar)(Et-px)} = Ae^{-(iE/\hbar)t}e^{+(ip/\hbar)x} = \psi e^{-(iE/\hbar)t}$$

$$\mathrm{H}\psi e^{-(iE/\hbar)t} = E\psi e^{-(iE/\hbar)t} = -\frac{\hbar^2}{2m}e^{-(iE/\hbar)t}\frac{\partial^2\psi}{\partial x^2} + U\psi e^{-(iE/\hbar)t}$$

Dividing through by the common exponential factor gives

Steady-state Schrödinger equation in one dimension

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(E-U)\psi = 0$$

Physical Interpretation of the complex matter wave

Basis states of the Hamiltonian: In the Schrodinger equation we encountered an expression $\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x,t)\right)$. This is called the Hamiltonian operator or Hamiltonian for short. It acts on functions of x (and possibly t) and gives other functions as the end result. We denote the Hamiltonian by the symbol H.

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

Consider the case when the potential energy is independent of time i.e. we write V(x) instead of V(x,t). Just as in rigid bodies, the moment of inertia matrix $\mathbf{I}$ had specific directions $e_1, e_2\ and\ e_3$ so that $\mathbf{I}\ e_j = I_j\ e_j$ called eigenvectors, we could also ask if there are special functions $\varphi_j(x)$ that have the eigenvector property.

$$H\varphi_j(x)=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)\varphi_j(x)=E_j\ \varphi_j(x)$$

Physical Interpretation of the complex matter wave

Then the functions $\varphi_j(x)$ would be analogous to finding the "principal directions" of the Hamiltonian. Just as in rigid bodies the three directions $e_1, e_2\ and\ e_3$ were linearly independent and any other vector may be expressed as a linear combination of these directions viz. $\mathrm{v} = \sum_j c_j\, e_j$ here too we may write for any function $\psi(x,t)$,

$$\psi(x,t) = \sum_j c_j(t)\, \varphi_j(x)$$

Physical Interpretation of the complex matter wave

Specifically we want $\psi(x,t)$ to obey Schrodinger's equation. This means,

$$i\,\hbar\frac{\partial}{\partial t}\psi(x,t) = \sum_j i\,\hbar\,\frac{d}{dt}c_j(t)\varphi_j(x)\;\; and \;\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right)\psi(x,t) = \sum_j E_j c_j(t)\,\varphi_j(x)$$

or,

$$i\,\hbar\,\frac{d}{dt}c_j(t) = E_j c_j(t)\;\; which\, means\;\; c_j(t) = e^{-\frac{i}{\hbar}E_j\,t}\; c_j(0)$$

If we assume that $c_j(0) = 0$ for all j except one special j = n where $c_n(0) = 1$ then we obtain a stationary state.

$$\psi(x,t) = e^{-\frac{i}{\hbar}E_n\,t}\;\varphi_n(x)$$

This has the property that the probability density $|\psi(x,t)|^2$ is independent of time. It also means all expectation values are independent of time.

$$< A > = \int dx\;\psi^*(x,t)\;A\;\psi(x,t) \;= \int dx\;\varphi_n^*(x)\;A\;\varphi_n(x)$$

Q. A stationary state of a quantum particle has an eigen function described by,

$$\varphi_0(x) \begin{cases} \sqrt{\frac{2}{L}}\,\sin\left(\frac{\pi\, x}{L}\right) \;;\; 0 < x < L \\ 0\;; \quad \text{otherwise} \end{cases}$$

a) Find the expectation value of the position.

$$< x > = \int_0^L \varphi_0(x)\, x\, \varphi_0(x)\;dx = \frac{L}{2}$$

b) Find the expectation value of the momentum.

$$< p > = \int_0^L \varphi_0(x)(-i\,\hbar\frac{\partial}{\partial x})\,\varphi_0(x)\;dx = 0$$

This is because the waves are moving in both directions.

c) Find the expectation value of the kinetic energy.

$$< KE > = \frac{1}{2m}\int_0^L \varphi_0(x)\left(-i\,\hbar\frac{\partial}{\partial x}\right)^2 \varphi_0(x)\ dx = \frac{\hbar^2\,\pi^2}{2m\,L^2}$$

d) Find the probability that the particle is between 0 and L/4

probability = $\int_0^{L/4} \varphi_0(x)\ \varphi_0(x)\ dx\ = \frac{\pi-2}{(4\,\pi)} = 0.09$

e) Estimate the size of the deviation of the position of the particle from its expected value.

Deviation from expected value = $x - \frac{L}{2}$

But is as likely for the particle to be to the left of $x = \frac{L}{2}$ as it is to the right of this value.

We want to know how far in absolute terms it can be found far away from $x = \frac{L}{2}$. For this we can do one of two things. We could calculate the average of $|x - \frac{L}{2}|$. This means we could say,

$$\Delta x = \int_0^L \varphi_0(x)\, |x - \frac{L}{2}|\, \varphi_0(x)\ dx$$

which is possible but the absolute value is a mathematically clumsy operation since we have to take into account the cases $x > \frac{L}{2}$ and $x < \frac{L}{2}$ separately while performing the above integral [do it as a homework]. What is usually done is to find the average of the square of $x - \frac{L}{2}$ and then we get a quantity whose units is [length]^2 but represents the deviation from the average value. To get a quantity with units of length we simply take the square root at the end. This is called RMS value.

$$(\Delta x)^2 = \int_0^L \varphi_0(x) \left(x - \frac{L}{2}\right)^2 \varphi_0(x)\ dx$$

In the present example we may evaluate this to get, **Δx = 0.18 L**. Hence the quantum particle is most likely to be found between 0.5 L - 0.18 L and 0.5 L + 0.18 L.

Next natural question is how likely is most likely? The probability that the particle is found between 0.5 L - 0.18 L and 0.5 L + 0.18 L is,

$$\text{probability} = \int_{0.5\,L - 0.18\,L}^{0.5\,L + 0.18\,L} \varphi_0(x)\ \varphi_0(x)\ dx = 0.65$$

or 65% probability. If you want a higher probability choose, the interval to be $\frac{L}{2} - 2\,\Delta x\ \ and\ \ \frac{L}{2} + 2\,\Delta x$. The probability that the particle is in this interval now is much higher.

$$\text{probability} = \int_{0.5\,L - 0.36\,L}^{0.5\,L + 0.36\,L} \varphi_0(x)\ \varphi_0(x)\ dx = 0.97$$

or 97% probability.

e) Estimate the size of the deviation of the momentum of the particle from its expected value.

This is easier to do since the expected value of momentum is zero.

$$(\Delta p)^2 \;=\; \int_0^L \varphi_0(x)\left(-i\,\hbar\frac{\partial}{\partial x}-0\right)^2 \varphi_0(x)\;dx = < p^2 > = 2m < KE > = \frac{\hbar^2\,\pi^2}{L^2}$$

or $\boldsymbol{\Delta p}$ **=** $\frac{\hbar\,\boldsymbol{\pi}}{\boldsymbol{L}}$ Combining with the earlier result namely, $\boldsymbol{\Delta x}$ **= 0.18 L** we conclude that

$$\Delta \boldsymbol{x}\,\Delta \boldsymbol{p} = \mathbf{0.565}\,\hbar > \hbar/\mathbf{2}$$

which is consistent with **Heisenberg's uncertainty principle.**