Physics 491

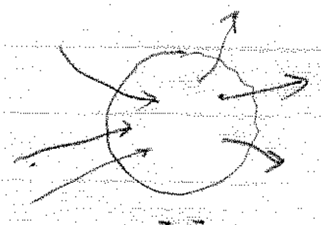
Lecture 5: Introduction to Wave Mechanics

Continuity Equation

Let us recall that, given the wave function $\psi(\vec{x},t)$, $|\psi(\vec{x},t)|^2$ is the probability density to find the particle in region near $\vec{x}$

Consider a finite volume V

flux



V

The probability to find particle in V

$$P_V(t) = \int_V d^3x \, |\psi(\vec{x},t)|^2$$

Assume the particle is neither created or destroyed (nonrelativistic) the only way the probability can change is if it move into or out of the volume. Conservation of particle

$$\Longrightarrow \quad \frac{dP_V}{dt} = -I \quad \left(\begin{matrix}\text{current out of} \\ \text{volume}\end{matrix}\right)$$

$$I = \oint_{\text{surface}} \vec{J}\cdot d\vec{a} \qquad \vec{J} = \text{probability current density}$$

$$d\vec{a} = \hat{n}\, da \quad \hat{n}\text{: normal}$$

$$= \int_V d^3x \, (\vec{\nabla}\cdot\vec{J}) \qquad \text{divergence theorem}$$

$$\therefore \int_V d^3x \, \frac{\partial}{\partial t}|\psi(\vec{x},t)|^2 = -\int_V d^3x \, (\vec{\nabla}\cdot\vec{J})$$

$$\Longrightarrow \boxed{\frac{\partial}{\partial t}|\psi(\vec{x},t)|^2 + \vec{\nabla}\cdot\vec{J} = 0} \qquad \text{Conservation of particle}$$

To ensure conservation of the particle, we thus seek a <u>first order in time</u> wave equation for $\psi(\vec{x},t)$

Recall, last time

Wave equation $\left[\frac{\partial^2}{\partial x^2} - \frac{1}{v^2}\frac{\partial^2}{\partial t^2}\right] F(x,t) = 0$

Plane wave $F(x,t) = \mathrm{Re}\left(F_0\, e^{i(kx-\omega t)}\right)$

$\Rightarrow$ Dispersion relation $\omega = v k$

Let us try to "reverse engineer" a first order in time wave equation for $\psi(\vec{x},t)$.
(Let's consider 1D for the time being)

Wave-particle duality: $E = \hbar\omega \qquad p = \hbar k$

$\omega = \frac{2\pi}{T} = 2\pi\nu \qquad k = \frac{2\pi}{\lambda}$

Free particle: $E = \text{Kinetic energy} = \frac{p^2}{2m}$

$$\Rightarrow \hbar\omega = \frac{\hbar^2 k^2}{2m} \Rightarrow \boxed{\omega = \frac{\hbar k^2}{2m}}$$ ← Dispersion relation

We seek a wave equation such that this is the dispersion relation for plane waves.

Start with $\psi(x,t) = \psi_0\, e^{i(kx-\omega t)}$

Note $\frac{\partial\psi}{\partial x} = ik\psi \Rightarrow \frac{\hbar}{i}\frac{\partial\psi}{\partial x} = \hbar k\psi = p\psi$

$\frac{\partial\psi}{\partial t} = -i\omega\psi \Rightarrow \frac{\hbar}{-i}\frac{\partial\psi}{\partial t} = \hbar\omega\psi = E\psi$

$$E = \frac{p^2}{2m} \Rightarrow \frac{\hbar}{-i}\frac{\partial}{\partial t}\psi = \frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2\psi$$

$$\Rightarrow \boxed{i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}}$$

Time dependent Schrödinger eq for free particle

If there is potential energy $V(x)$

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

Note:
- The Schrödinger equation is first order in time
- The wave function must be complex to get the dispersion relation

A good part of this class will involve solving this PDE for different potentials $V(x)$

Continuity equation:

$$\frac{\partial}{\partial t}|\psi(x,t)|^2 = \frac{\partial}{\partial t}\left(\psi^*_{(x,t)}\psi_{(x,t)}\right) = \left(\frac{\partial\psi^*}{\partial t}\right)\psi + \psi^*\left(\frac{\partial\psi}{\partial t}\right)$$

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

$$= \frac{+i\hbar}{2m}\left[\psi^*\frac{\partial^2\psi}{\partial x^2} - \left(\frac{\partial^2\psi^*}{\partial x^2}\right)\psi\right]$$

$$= -\frac{\partial}{\partial x}\left[\underbrace{\frac{\hbar}{2im}\left(\psi^*\frac{\partial}{\partial x}\psi - \left(\frac{\partial\psi^*}{\partial x}\right)\psi\right)}_{J(x,t)}\right]$$

$J(x,t)$ ← Current density

"Momentum - space wave function"

For plane waves $\frac{\hbar}{i}\frac{\partial \psi}{\partial x} = \hbar k \, \psi_{(x,t)} = p \, \psi_{(x,t)}$

The differential "operator" $\frac{\hbar}{i}\frac{\partial}{\partial x}$ thus acts like multiplication by p (the momentum) for plane waves.

This defines the "momentum operator" $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$

Notation: Hats = Operators

To solidify this interpretation consider the equation of motion for $\langle x \rangle$ for a free particle.

Classically $\frac{dx}{dt} = \frac{p}{m}$ (velocity)

Quantum $\langle x \rangle_t = \int_{-\infty}^{\infty} dx \; x \, |\psi_{(x,t)}|^2 = \int_{-\infty}^{\infty} dx \; \psi^*_{(x,t)} \, x \, \psi_{(x,t)}$

$$\frac{d}{dt}\langle x \rangle_t = \int_{-\infty}^{\infty} dx \; x \, \underbrace{\frac{\partial}{\partial t}\left(|\psi(x,t)|^2\right) = -\int_{-\infty}^{\infty} dx \; x \left(\frac{\partial}{\partial x} J(x,t)\right)}_{\text{Continuity Eq}}$$

$$\underset{\substack{\uparrow \\ \text{integration} \\ \text{by parts}}}{=} \int_{-\infty}^{\infty} dx \left(\frac{\partial}{\partial x} x\right) J(x,t) + \underbrace{\cancel{\left[x \, J(x,t)\right]_{-\infty}^{\infty}}}_{\substack{\text{current vanishes} \\ \text{at } \infty}} \rightarrow 0$$

$$= \int_{-\infty}^{\infty} dx \; J(x,t)$$

$$\Rightarrow \frac{d}{dt}\langle x\rangle_t = \int_{-\infty}^{\infty} dx\, J(x,t) = \frac{1}{2m}\Big[\int_{-\infty}^{\infty} \psi^* \frac{\hbar}{i}\frac{\partial}{\partial x}\psi\, dx + \underbrace{\int_{-\infty}^{\infty}\left(\frac{\hbar}{i}\frac{\partial \psi}{\partial x}\right)^* \psi\, dx}_{\text{Integrate by parts}}\Big]$$

$$\Rightarrow \frac{d}{dt}\langle x\rangle_t = \frac{1}{m}\int_{-\infty}^{\infty} dx\, \psi^*_{(x,t)}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\psi_{(x,t)} = \frac{\langle p\rangle_t}{m}$$

$$\therefore \boxed{\begin{aligned}\langle p\rangle_t &= \int_{-\infty}^{\infty} dx\, \psi^*_{(x,t)}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\psi_{(x,t)} \\ &= \int_{-\infty}^{\infty} dx\, \psi^*_{(x,t)}\, \hat{p}\, \psi_{(x,t)}\end{aligned}}$$

Let us plug in for $\psi_{(x,t)}$ in terms of it's Fourier transform (Free particle $E = \frac{p^2}{2m}$, $\omega = \hbar\frac{k^2}{2m}$)

$$\psi(x,t) = \int_{-\infty}^{\infty}\frac{dk}{\sqrt{2\pi}}\,\tilde{\psi}(k)\, e^{i(kx-\omega(k)t)}$$

$$\Rightarrow \langle p\rangle_t = \int_{-\infty}^{\infty}\frac{dx\,dk\,dk'}{2\pi}\left(\tilde{\psi}^*_{(k)}\, e^{-ikx}\right)\frac{\hbar}{i}\frac{\partial}{\partial x}\left(\psi(k')\, e^{ik'x}\right) e^{i(\omega_k-\omega_{k'})t}$$

$$= \int dk\,dk'\,\hbar k'\,\tilde{\psi}^*(k)\,\tilde{\psi}(k')\, e^{i(\omega_k-\omega_{k'})t}\int\frac{dx}{2\pi}\, e^{i(k'-k)x}$$

Aside: $\int_{-\infty}^{\infty} \frac{dx}{2\pi} e^{i(k'-k)x} = \delta(k-k')$

$$\Rightarrow \langle p \rangle_t = \int_{-\infty}^{\infty} dk \, (\hbar k) \, |\tilde{\Psi}(k)|^2$$

Let $p = \hbar k$ $\quad \tilde{\phi}(p) \equiv \frac{1}{\sqrt{\hbar}} \tilde{\Psi}(k = p/\hbar)$

$$\Rightarrow \boxed{\langle p \rangle_t = \int_{-\infty}^{\infty} dp \; p \; |\tilde{\phi}(p)|^2}$$

Note $\langle p \rangle_t$ is independent of t for free particle

$\Rightarrow$ $\tilde{\phi}(p)$ is the "momentum space wavefunction"

$|\tilde{\phi}(p)|^2$ is the probability density to find the particle with momentum p in the interval $p \to p + dp$

Units $[\tilde{\phi}] = \frac{1}{\sqrt{\text{momentum}}}$

Thus, with the correct units, the Fourier transform of $\Psi(x)$ is the momentum space wave function.

$$\boxed{\Psi(x) = \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi\hbar}} \tilde{\phi}(p) \, e^{ipx/\hbar}}$$

$$\boxed{\tilde{\phi}(p) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\hbar}} \Psi(x) \, e^{-ipx/\hbar}}$$

Wave packets and the uncertainty principle

Recall, the standard deviation associated with a probability distribution $P(x)$ is

$$\Delta x = \sqrt{\underset{\text{variance}}{\Delta x^2}} = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$$

$$\Rightarrow \quad \Delta x^2 = \int_{-\infty}^{\infty} dx \; x^2 \, |\Psi(x)|^2 - \left[\int_{-\infty}^{\infty} dx \; x \, |\Psi(x)|^2\right]^2$$

The variance in momentum is most easily calculated in "momentum space"

$$\Delta p = \hbar \Delta k$$

$$\Delta k^2 = \underbrace{\int_{-\infty}^{\infty} dk \; k^2 \, |\tilde{\Psi}(k)|^2}_{\langle k^2\rangle} - \underbrace{\left[\int_{-\infty}^{\infty} dk \; k \, |\tilde{\Psi}(k)|^2\right]^2}_{\langle k\rangle^2}$$

Using Fourier transform $\tilde{\Psi}(k) = \int_{-\infty}^{\infty} dx \, \Psi(x) \dfrac{e^{-ikx}}{\sqrt{2\pi}}$

can prove

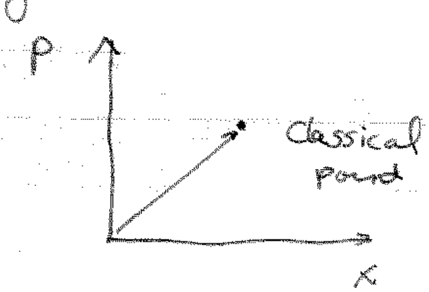
$$\boxed{\Delta x \, \Delta k \geq \frac{1}{2}}$$ Fourier "uncertainty principle"

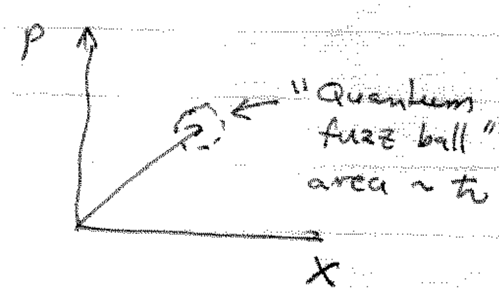
> If we want to localize the wave packet (decrease Δx) we must increase the distribution of wave lengths Δk

Implications of Fourier uncertainty in Quantum theory : $\Delta p = \hbar \Delta k$

$$\Rightarrow \boxed{\Delta x \, \Delta p \geq \frac{\hbar}{2}}$$ Heisenberg's uncertainty principle

This shakes the foundation of classical physics. There, we have trajectories in phase space specified by points (x, p). The uncertainty principle says it is <u>impossible</u> to assign perfect knowledge of both x and p simultaneously to a particle. The best we can possibly do is "fuzz out" of assignment to cells in phase space of order $\hbar$





It is sometimes stated that it is impossible to simultaneously measure x and p. This is incorrect. We can always do it, but the answer we get <u>cannot be predicted with certainty</u>. After the measurement we must make a new probability assignment (think Bayes rule) and the uncertainty principle says if you obtain more information about x you ~~lose~~ lose information about p.

Examples:

(1) Plane wave: $\psi(x) = \psi_0 \, e^{ik_0 x} = \psi_0 \, e^{ip_0/\hbar\, x}$

- Momentum space wave function

$$\tilde{\phi}(p) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\hbar}} \, \psi(x) \, e^{-ip/\hbar\, x}$$

$$= \frac{\psi_0}{\sqrt{2\pi\hbar}} \underbrace{\int_{-\infty}^{\infty} dx \, e^{i\left(\frac{p_0}{\hbar} - \frac{p}{\hbar}\right)x}}_{=2\pi\delta\left(\frac{p_0 - p}{\hbar}\right) = 2\pi\hbar\,\delta(p_0 - p)}$$

$$\Rightarrow \boxed{\tilde{\phi}(p) = \sqrt{2\pi\hbar}\, \psi_0 \, \delta(p_0 - p)}$$ Delta function localized in p

- $\hat{p}\,\psi(x) = \frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x) = \hbar k_0 \, \psi(x) = p_0 \, \psi(x)$

$$\Rightarrow \langle \hat{p} \rangle = \int dx \, \psi^* \hat{p}\, \psi = p_0 \int dx \, |\psi(x)|^2 = p_0$$

$$\langle \hat{p}^2 \rangle = \int dx \, \psi^* \hat{p}^2 \psi = p_0^2 \int dx \, |\psi(x)|^2 = p_0$$

$$\Rightarrow \boxed{\Delta p = 0}$$ Perfectly well defined momentum

$$\langle \hat{x} \rangle = \int_{-\infty}^{\infty} dx \, \psi^* x \, \psi = \int_{-\infty}^{\infty} dx \, x = 0$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} dx \, \psi^* x^2 \psi = \int_{-\infty}^{\infty} dx \, x^2 \quad \infty!$$

$$\Rightarrow \boxed{\Delta x = \infty}$$ Completely indeterminate position

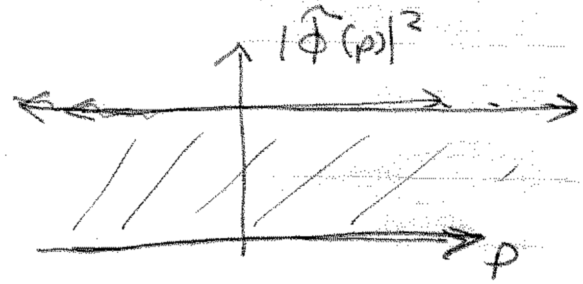
(ii) <u>Delta function</u> $\quad \psi(x) = \psi_0 \, \delta(x - x_0)$

Momentum space wave function

$$\tilde{\Phi}(p) = \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi\hbar}} \, \psi(x) \, e^{-i\frac{px}{\hbar}}$$

$$\tilde{\Phi}(p) = \frac{\psi_0}{\sqrt{2\pi\hbar}} \; e^{-i\frac{x_0}{\hbar}p}$$

$$|\tilde{\Phi}(p)|^2 = \text{Constant}$$



$$\Rightarrow \quad \boxed{\begin{aligned} \Delta p &= \infty \\ \Delta x &= 0 \end{aligned}}$$

Perfectly well defined position, indeterminant momentum

<u>Note</u>: The plane and delta function are "duals" of each other:
- plane wave in position $\Rightarrow$ delta function in momentum
- delta function position $\Rightarrow$ plane wave in momentum

Neither of these states are <u>physical</u>.

A particle cannot be complete delocalized over all space. The probability distributions are not <u>normalizable</u>. Nonetheless they are useful idealizations ~~to~~ think about, and mathematically useful, for example, in Fourier integrals.

(iii) Gaussian wave packet

Let $\psi(x) = \frac{1}{(2\pi\sigma_x^2)^{1/4}} e^{-\frac{(x-x_0)^2}{4\sigma_x^2}} e^{ip_0 x/\hbar}$

This is a <u>normalized</u> wave packet

$$\int_{-\infty}^{\infty} dx\, |\psi(x)|^2 = \int_{-\infty}^{\infty} dx \underbrace{\frac{e^{-\frac{(x-x_0)^2}{2\sigma_0^2}}}{\sqrt{2\pi\sigma^2}}}_{P(x)} = \underline{1}$$

Since $P(x)$ is a Gaussian, we know

$$\langle x \rangle = x_0 \qquad \Delta x = \sigma_x$$

Momentum space wave function (try this yourselves!)

$$\tilde{\phi}(p) = \frac{1}{(2\pi\sigma_p^2)^{1/4}} e^{-\frac{(p-p_0)^2}{4\sigma_p^2}} e^{-ix_0 p/\hbar}$$

where $\sigma_p = \frac{\hbar}{2\sigma_x}$

$|\tilde{\phi}(p)|^2$ is also a Gaussian $= \frac{e^{-\frac{(p-p_0)^2}{2\sigma_p^2}}}{\sqrt{(2\pi\sigma_p^2)}}$

$$\langle p \rangle = p_0 \qquad \Delta p = \sigma_p = \frac{\hbar}{2\sigma_x}$$

$\Rightarrow$ $\boxed{\Delta x \, \Delta p = \frac{\hbar}{2}}$ Minimum uncertainty wave packet