Physics 371 Lecture 4

Conservation of probability

$$\rho(x,t) = \psi^*(x,t)\,\psi(x,t)$$

probability density (per unit length)

What is $\frac{\partial \rho}{\partial t}$?

$$\frac{\partial}{\partial t}\psi^*\psi = \psi^*\frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t}\psi$$

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

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

$(V^* = V)$

$$\frac{\partial \rho}{\partial t} = -\frac{\hbar}{2im}\left[\psi^*\frac{\partial^2 \psi}{\partial x^2} - \psi\frac{\partial^2 \psi^*}{\partial x^2}\right]$$

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x}\left[\frac{\hbar}{2im}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x}\right)\right] \quad 2$$

Defining the <u>probability current</u>

$$j_x(x,t) \equiv \frac{1}{2m}\left[\Psi^* \frac{\hbar}{i}\frac{\partial}{\partial x}\Psi - \Psi \frac{\hbar}{i}\frac{\partial}{\partial x}\Psi^*\right],$$

we find

$$\boxed{\frac{\partial \rho}{\partial t} + \frac{\partial j_x}{\partial x} = 0}$$

$$P(a,b) = \int_a^b dx\, |\Psi|^2$$

$$\frac{d\,P(a,b)}{dt} = \int_a^b dx\, \frac{\partial \rho}{\partial t} = -\int_a^b dx\, \frac{\partial j_x}{\partial x}$$

$$= \underbrace{j_x(a,t)}_{\text{in}} - \underbrace{j_x(b,t)}_{\text{out}}$$

In three dimensions,

$$\vec{J}(\vec{r},t) = \frac{1}{2m}\left[\psi^* \frac{\hbar}{i}\nabla\psi - \psi\frac{\hbar}{i}\nabla\psi^*\right]$$

and

$$\boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = 0 \quad \text{continuity equation}}$$

What is the meaning of $\vec{J}$?

Electric current operator

$$\vec{J}_e = -\frac{e\hbar}{2im}\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right] = -e\vec{J}$$

for electrons of charge $-e$.

The complexity of ψ

If ψ is real, then $\psi^* = \psi$.

$$\Rightarrow j_x = \frac{\hbar}{2im}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right) = 0.$$

Thus a real wavefunction cannot describe a state with a flux or flow of particles. The complexity of ψ is not a mathematical convenience, but a necessity.

Amplitude and phase

Let $\psi(x,t) = A(x,t)\, e^{i\theta(x,t)}$

A, θ = real functions

$$A(x,t) = \sqrt{\rho(x,t)}$$

$$j_x = \frac{\hbar \rho}{m} \frac{\partial \theta(x,t)}{\partial x} \qquad \text{or}$$

$$\vec{J} = \frac{\hbar \rho}{m} \nabla \theta \qquad \text{in 3D}$$

Thus the probability current (flow of particles) is determined by the gradient of the phase of the wavefunction.

Ex. Plane wave $\psi(x) = A e^{ikx}$

$$j_x = \rho \frac{\hbar k}{m} = \rho \frac{p_x}{m} = \rho v$$

Particle-like properties

So far, we have mainly talked about plane-waves, which are states of definite momentum, where the position of the particle is undefined. In order to account for the particle nature of quantum systems, we need to consider wave packets. One way to form a wave packet is simply to chop a plane

Wave

$$\psi(x) = \begin{cases} e^{ik_0 x}, & |x| < a \\ 0, & |x| > a. \end{cases}$$

This state is no longer a state of definite momentum

$$\hat{P}_x \psi(x) = i\hbar \frac{\partial}{\partial x} \psi(x) \neq \hbar k_0 \psi(x).$$

Q: What is the momentum content of $\psi(x)$?

Any function may be written as a Fourier integral

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

which is a linear <u>superposition</u> of plane waves.

How do we determine $\tilde{\Psi}(k)$?

$$\tilde{\Psi}(k) = \int_{-\infty}^{\infty} dx \; \Psi(x)\, e^{-ikx}.$$

<u>Proof</u>:

$$\int_{-\infty}^{\infty} dx \; \Psi(x)\, e^{-ikx} = \int_{-\infty}^{\infty} dx \; e^{-ikx} \int_{-\infty}^{\infty} \frac{dk'}{2\pi} \, \tilde{\Psi}(k')\, e^{ik'x}$$

$$= \int_{-\infty}^{\infty} dk' \; \tilde{\Psi}(k') \int_{-\infty}^{\infty} \frac{dx}{2\pi} \, e^{i(k'-k)x}$$

<u>Define</u> $\delta(k-k') = \int_{-\infty}^{\infty} \frac{dx}{2\pi} \, e^{+i(k-k')x}$

$\delta(k)$ is known as the <u>Dirac delta function</u>. Actually, the integral is poorly defined.

Let us write

$$\delta(k) = \lim_{\epsilon \to 0^+} \int_{-\infty}^{\infty} \frac{dx}{2\pi} e^{ikx - \epsilon x^2}$$

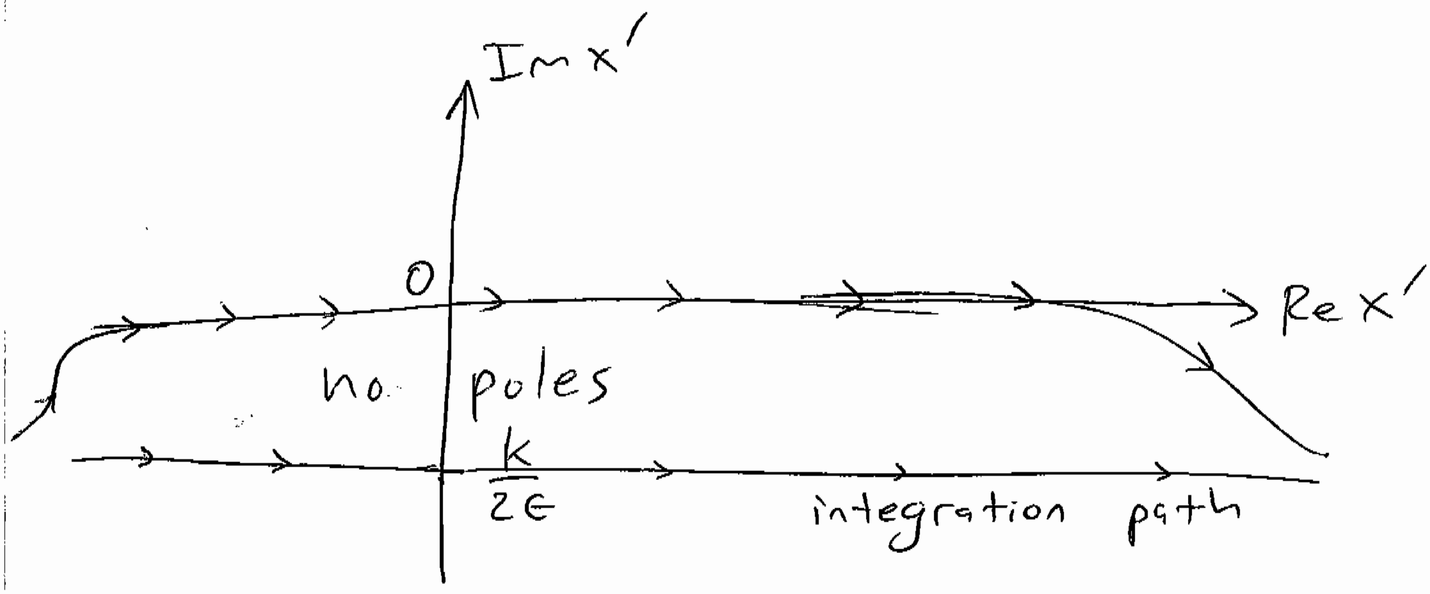
$$-\epsilon\left(x^2 - \frac{ikx}{\epsilon} - \frac{k^2}{4\epsilon^2}\right) - \frac{k^2}{4\epsilon}$$

$$= -\epsilon\left(x - \frac{ik}{2\epsilon}\right)^2 - \frac{k^2}{4\epsilon}$$

$$\delta(k) = \lim_{\epsilon \to 0^+} \frac{e^{-\frac{k^2}{4\epsilon}}}{2\pi} \underbrace{\int_{-\infty}^{\infty} dx\, e^{-\epsilon\left(x - \frac{ik}{2\epsilon}\right)^2}}_{I(\epsilon)}$$

let $x' = x - \frac{ik}{2\epsilon}$, $dx = dx'$

$$I(\epsilon) = \int_{-\infty - \frac{ik}{2\epsilon}}^{\infty - \frac{ik}{2\epsilon}} dx' \, e^{-\epsilon x'^2} = \int_{-\infty}^{\infty} dx' \, e^{-\epsilon x'^2}$$



$$I(\epsilon) = \int_{-\infty}^{\infty} dx \, e^{-\epsilon x^2}$$

$$= \sqrt{\int_{-\infty}^{\infty} dx \, e^{-\epsilon x^2} \int_{-\infty}^{\infty} dy \, e^{-\epsilon y^2}}$$

$$I^2 = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \; e^{-\epsilon(x^2+y^2)}$$

let $r^2 = x^2 + y^2$, $dx\,dy \to r\,dr\,d\theta$

$$I^2 = \int_0^{\infty} r\,dr\, e^{-\epsilon r^2} \int_0^{2\pi} d\theta$$

$$= \frac{\pi}{\epsilon} \int_0^{\infty} 2\epsilon r\,dr\, e^{-\epsilon r^2}$$

$$= \frac{\pi}{\epsilon} \int_0^{\infty} e^{-u}\,du, \quad u = \epsilon r^2$$

$$= \frac{\pi}{\epsilon}$$

$$\Rightarrow \quad I(\epsilon) = \sqrt{\frac{\pi}{\epsilon}}$$

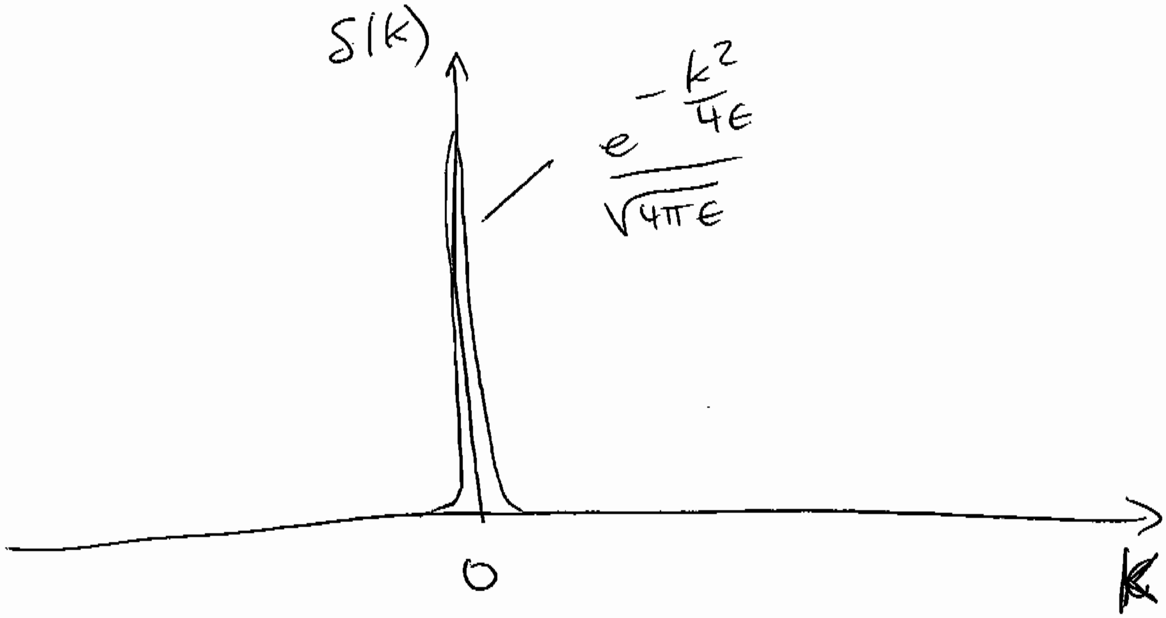
$$\delta(k) = \lim_{\epsilon \to 0^+} \frac{e^{-k^2/4\epsilon}}{\sqrt{4\pi\epsilon}}$$

$$\delta(k) = \begin{cases} 0, & k \neq 0 \\ \infty, & k = 0 \end{cases}$$

$$\int_{-\infty}^{\infty} dk\, \delta(k) = \lim_{\epsilon \to 0^+} \int_{-\infty}^{\infty} \frac{e^{-\frac{k^2}{4\epsilon}}\, dk}{\sqrt{4\pi\epsilon}}$$

$$\lim_{\epsilon \to 0^+} \frac{1}{\sqrt{4\pi\epsilon}}\, I\left(\frac{1}{4\epsilon}\right) = 1$$

Thus $\delta(k)$ is zero everywhere except at $k=0$, and the area under the peak at $k=0$ is 1.



Consequently, $\int_{-\infty}^{\infty} dk \; \delta(k) \, f(k) = f(0).$

Back to page 8:

$$\int_{-\infty}^{\infty} dk' \, \tilde{\psi}(k') \; \delta(k-k') = \tilde{\psi}(k)$$

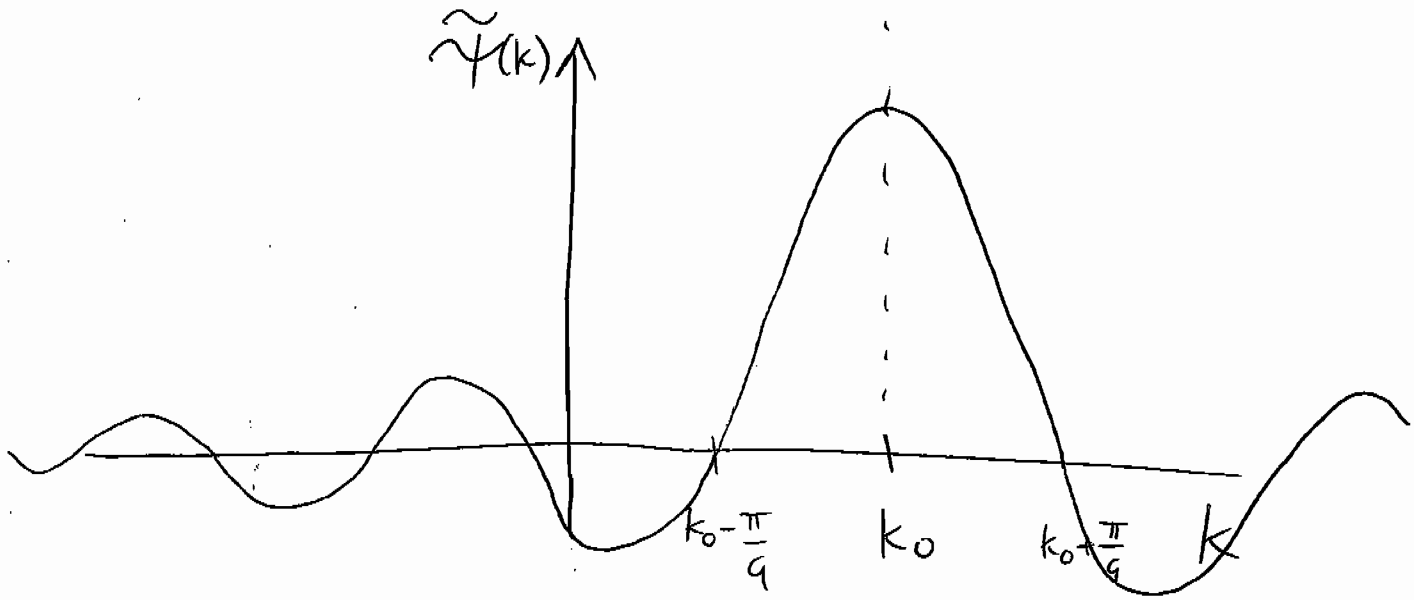
Q.E.D.

Back to the wave packet:

$$\tilde{\psi}(k) = \int_{-\infty}^{\infty} dx \; \psi(x) e^{-ikx} = \int_{-\infty}^{\infty} dx \; e^{i(k_0 - k)x}$$

$$\tilde{\psi}(k) = \frac{e^{i(k_0-k)a} - e^{-i(k_0-k)a}}{i(k_0-k)}$$

$$= 2\frac{\sin(k-k_0)a}{(k-k_0)}$$



The width of the main peak is $\Delta k = \frac{2\pi}{a}$. The width of the wave packet in real space was $\Delta x = 2a$.

$\Delta x \, \Delta k = 4\pi$

$\Delta p_x = \hbar \Delta k$

$\Delta x \, \Delta p_x = 4\pi \hbar = 2h.$

The narrower we make the wave packet in x, the broader it becomes in momentum.

This is the essence of the uncertainty principle.

The best we can do in terms of minimizing the product $\Delta x \, \Delta p_x$

is with a <u>Gaussian wavepacket</u>:

$$\tilde{\psi}(k) = A\, e^{-\frac{(k-k_0)^2}{4\sigma_k^2}} \Rightarrow 16'$$

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

$$= A \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, e^{ikx - \frac{(k-k_0)^2}{4\sigma_k^2}}$$

$$-\frac{1}{4\sigma_k^2}\Big[(k-k_0)^2 - i4\sigma_k^2 x(k-k_0) + (i2\sigma_k^2 x)^2\Big] - \sigma_k^2 x^2$$

$$\psi(x) = \frac{A}{2\pi}\, e^{ik_0 x - \sigma_k^2 x^2} \underbrace{\int_{-\infty}^{\infty} d\tilde{k}\, e^{-\frac{\tilde{k}^2}{4\sigma_k^2}}}_{\sqrt{\pi 4\sigma_k^2}}$$

Q: What is the normalization of $\tilde{\psi}(k)$?

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} \left|\tilde{\psi}(k)\right|^2$$

$$= \int_{-\infty}^{\infty} \frac{dk}{2\pi} \int_{-\infty}^{\infty} dx\, \psi(x)\, e^{-ikx} \int_{-\infty}^{\infty} dx'\, \psi^*(x')\, e^{ikx'}$$

$$= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx'\, \psi(x)\, \psi^*(x') \underbrace{\int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(x'-x)}}_{\delta(x-x')}$$

$$= \int_{-\infty}^{\infty} dx\, |\psi(x)|^2 = 1$$

Thus $|\tilde{\psi}(k)|^2 = \rho(k)$ gives the probability density in k-space. [measure $= \frac{dk}{2\pi}$]

$$\psi(x) = B\, e^{i k_0 x - \sigma_k^2 x^2}$$

$$\rho(x) = |\psi(x)|^2 = B^2 e^{-2\sigma_k^2 x^2}$$

$$1 = \int_{-\infty}^{\infty} \rho(x)\, dx = B^2 \sqrt{\frac{\pi}{2\sigma_k^2}}$$

$$B^2 = \sqrt{\frac{2\sigma_k^2}{\pi}}$$

$$\rho(x) = C\, e^{-\frac{x^2}{2\sigma_x^2}}$$

$$\frac{1}{2\sigma_x^2} = 2\sigma_k^2$$

$$2\sigma_x \sigma_k = \underline{1}$$

$$\Delta x = \sigma_x \qquad \Delta k = \sigma_k$$

$$\Delta x\, \Delta k = \frac{1}{2} \quad \text{c.f. } \Delta\omega\Delta t \geq \frac{1}{2}$$

$$\boxed{\Delta x\, \Delta p_x = \frac{\hbar}{2}}$$

This is the absolute minimum. We will prove this later, using matrix mechanics. The uncertainty principle states

$$\boxed{\Delta x\, \Delta p_x \geq \frac{\hbar}{2}}.$$