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 <u>wave packets</u>. 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>super-position</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

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

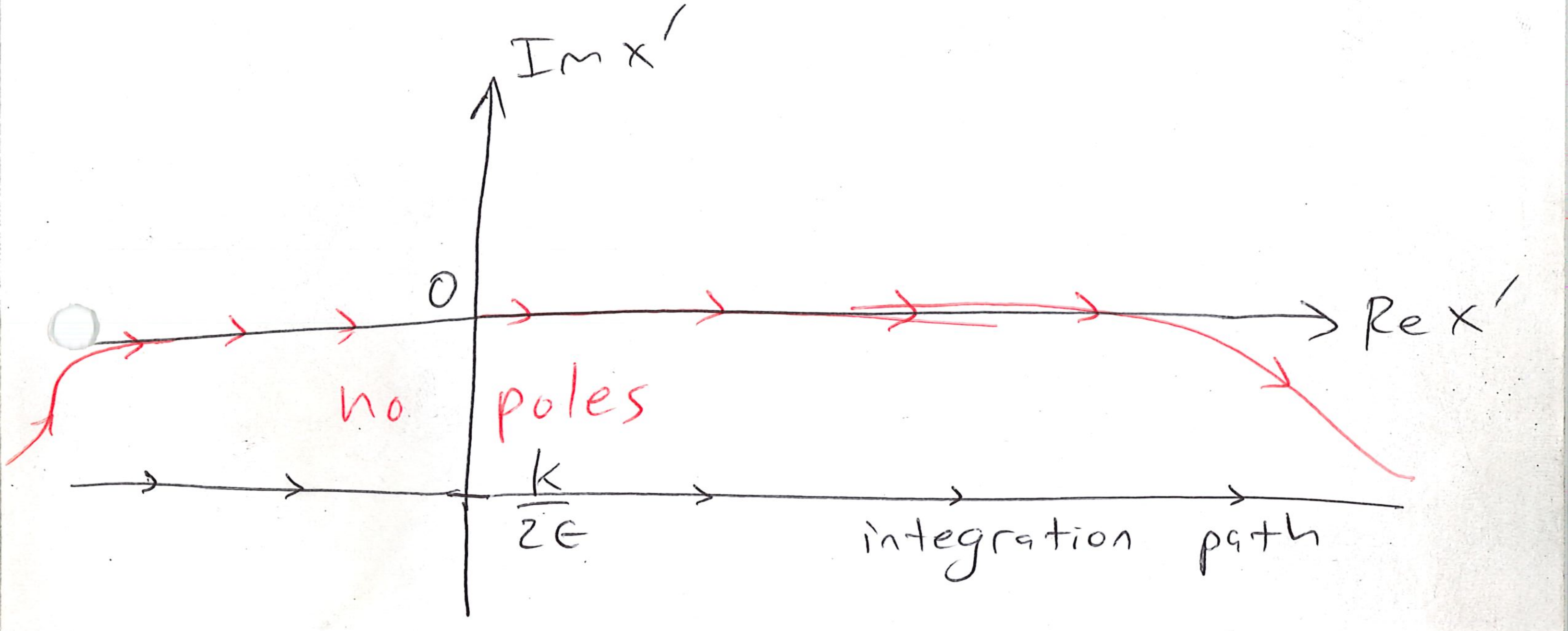
$$-\epsilon\left(x^2 - \frac{ikx}{\epsilon} - \frac{k^2}{4\epsilon^2}\right) - \frac{k^2}{4\epsilon}$$

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

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

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

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



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

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

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

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

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

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

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

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

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

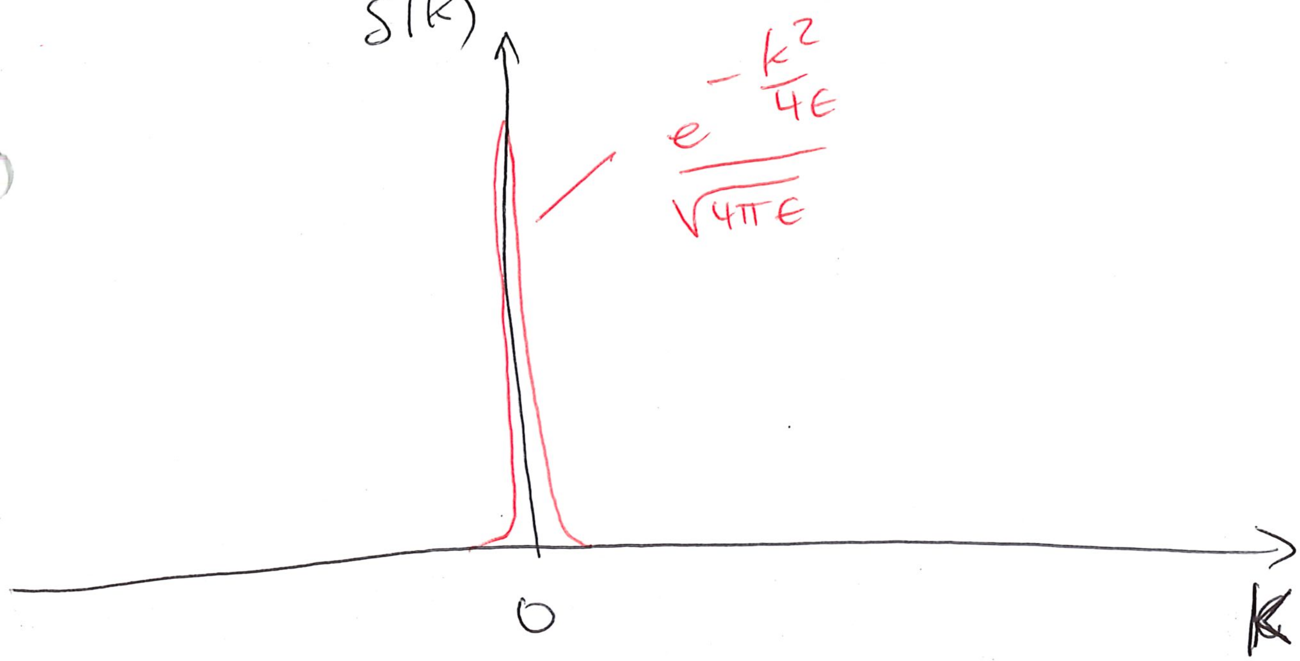
$$\delta(k) = \lim_{\epsilon \to 0^+} \frac{e^{-k^2/4\epsilon}}{\sqrt{4\pi\epsilon}}$$

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

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

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

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



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

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

Q.E.D.

Back to the wave packet:

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

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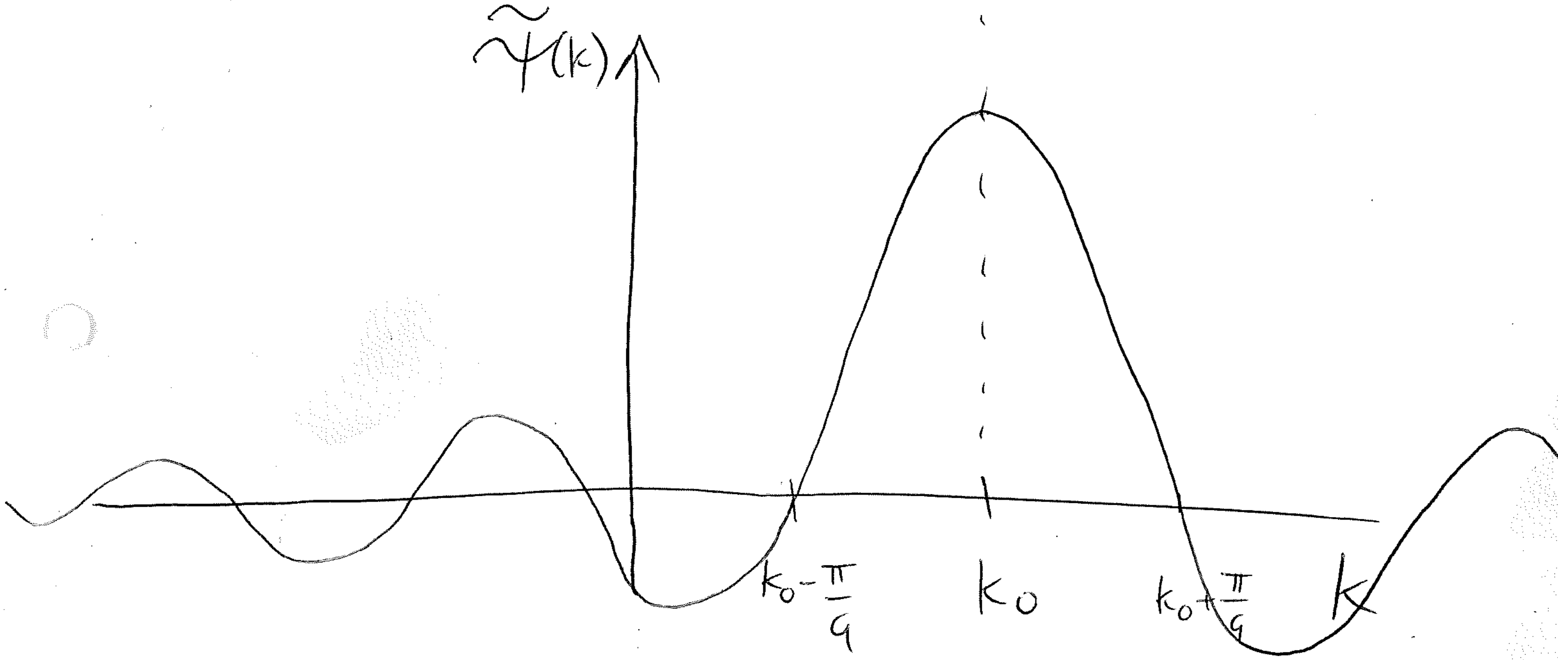
$$\tilde{\psi}(k) = \frac{e^{i(k_0-k)a} - e^{-i(k_0-k)a}}{i(k_0-k)}$$

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



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. <u>This is the essence of the uncertainty principle.</u>

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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