Reading Chapter 1, CTDL, pages 9-39, 50-56, 60-85

Last time:

1. 1-D infinite box $\qquad E_n = n^2\left[\frac{h^2}{8mL^2}\right]$
   continuity of $\psi(x), \frac{d\psi}{dx}, \frac{d^2\psi}{dx^2}$ $\qquad \psi_n = (2/L)^{1/2}\sin(n\pi x)$
   confinement → quantization
2. δ–function well $\qquad E = \frac{-ma^2}{2\hbar^2}$
   one bound level $\qquad \psi = \pm\left(\frac{ma}{\hbar^2}\right)^{1/2} e^{-ma|x|/\hbar^2}$ (what happens to ψ as a increases?)

Why do we know there is only one bound level?

What do we know about $\overline{\psi}(p)$? How does this depend on a ? what about <p>?

TODAY and WEDNESDAY:

1. motion → time dependent Schr. Eq.
2. motion of constant phase point on $\Psi(x,t)$ -- phase velocity
3. motion of $|\Psi(x,t)|^2$ requires non-sharp E
4. encode $\Psi(x,t)$ for $x_0, \Delta x, p_0, \Delta p$
5. $p_0, \Delta p$ from $|g(k)|$
6. $x_0, \Delta x$ from stationary phase argument
7. moving, spreading wavepacket $|\Psi(x,t)|^2$
8. group velocity ≠ phase velocity -- see CTDL, pages 28-31

1. Motion

time dependent Schr. Eq. $i\hbar\frac{\partial\Psi}{\partial t} = \mathbf{H}\Psi$ TDSE

if V(x) is time independent, then

$$\Psi_n(x,t) = \psi_n(x)e^{-iE_n t/\hbar}$$

satisifies TDSE?

can use this form of Ψ to describe time dependence of any non-eigenstate initial preparation: e.g. <u>wavepackets</u>

$$\Psi(x,0) = \sum a_n \psi_n(x)$$ superposition of **eigenstates**

$$\Psi(x,t) = \sum a_n \psi_n(x) e^{-i\omega_n t} \qquad \omega_n = E_n/\hbar$$

go back to free particle to really see motion of QM systems

$$\psi_{|k|}(x) = Ae^{ikx} + Be^{-ikx}$$

$$E_k - V_0 = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m}$$

$$\omega_k = (E_k - V_0)\Big/\hbar = \frac{\hbar k^2}{2m} \geq 0$$

WHAT ABOUT ARBITRARY ZERO OF E?

CALL IT E_0

add a phase factor which expresses the arbitrariness of the zero of energy:

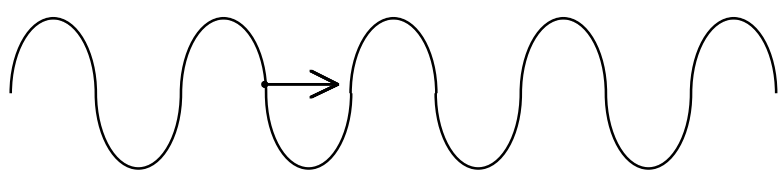
$$\Psi_{|k|}(x,t) = e^{-i\omega_k t}\left[Ae^{ikx} + Be^{-ikx}\right]e^{-iE_0 t/\eta}$$

$$= \left[Ae^{i(kx-\omega_k t)} + Be^{-i(kx+\omega_k t)}\right]e^{-iE_0 t/\hbar}$$

2. <u>How does point of constant $\begin{bmatrix}\text{argument}\\ \text{phase}\end{bmatrix}$ move?</u>

$$\text{const} = kx_\phi - \omega_k t$$

$$x_\phi(t) = +\frac{\omega_k t}{k} + x_\phi(0)$$ moves in +x direction if k > 0



$$v_\phi = \frac{dx_\phi}{dt} = \frac{\omega_k}{k} \leftarrow \frac{\hbar k^2}{2m}$$ phase velocity $$v_\phi = \frac{\hbar k}{2m} = \underset{?}{\frac{p}{\boxed{2m}}} = \frac{v}{2}$$ (half as fast as we naively expect)

first term in $\Psi(x,t)$ moves to +x (right), second to –x (left).

But if we treat the $e^{-iV_0 t/\hbar} = e^{-i\omega_0 t}$ term explicitly,

we get $v_\phi = \frac{\omega_k + \omega_0}{k}$! Any velocity we want! IS THIS A PROBLEM? WHY NOT?

(compare v_ϕ for a +k, –k pair of free particle states)

3. But what about the probability distribution, $\mathbf{P}(x,t)$?

$$\mathbf{P}(x,t) = \Psi^*(x,t)\Psi(x,t) = |A|^2 + |B|^2 + 2\,\mathrm{Re}(A^*B)\cos 2kx + 2\,\mathrm{Im}(A^*B)\sin 2kx$$

no time dependence! lose all t-dependence because cross terms (+k, –k) still belong to same E_k! The wiggles in $\Psi^*\,\Psi$ are standing waves, not traveling waves. No ambiguity about V_0 either?

What is the expectation value of $\hat{p}$ $$<p> = \frac{\int \Psi^* \hat{p} \Psi dx}{\int \Psi^* \Psi dx}?$$

$$\langle p \rangle = \hbar k \frac{|A|^2 - |B|^2}{|A|^2 + |B|^2}$$

This is an interesting result that suggests something that is always true and a very useful inspection tool. Whenever the wavefunction is pure real or pure imaginary, $\langle p \rangle = 0$.

SO HOW DO WE ENCODE $\Psi(x,t)$ for *both* spatial localization *and* temporal motion? need several k components, not just +k, –k

**4. Recipe for encoding Gaussian Wavepacket for x_0, Δx, p_0, Δp

Start with $\Psi(x,0)$ and later build in correct $e^{-i\omega_k t}$ dependence for each k component.

THIS IS GOING TO BE SHOWN TO BE the Ψ that yields $\Psi^*\Psi$ as a Gaussian prob. distrib. in x and p

$$\Psi(x,0) = \frac{a^{1/2}}{(2\pi)^{3/4}} \int_{-\infty}^{\infty} \underbrace{e^{-\left(a^2/4\right)\left(k-k_0\right)^2}}_{g(k)} e^{ikx} dk$$

FT of a Gaussian

*form of a Gaussian in k
* superposition of many e^{ikx}

WHAT KIND OF FUNCTION IS THE SQUARE OF A GAUSSIAN? WHAT IS ITS WIDTH?

ASIDE

see Gaussian Handout

a Gaussian prob. distrib. in x

$$G\left(x;x_0,\Delta x\right) \equiv (2\pi)^{-1/2} \frac{1}{\Delta x} e^{-\left(x-x_0\right)^2 / \left[2(\Delta x)^2\right]}$$

G is normalized $\quad \int_{-\infty}^{\infty} G(x;x_0,\Delta x)dx = 1$

$$\langle x \rangle = x_0$$

$$\left\langle x^2 \right\rangle = (\Delta x)^2 + x_0^2$$

$(\Delta x)^2$ is called the variance in x

$$\left[\left\langle x^2 \right\rangle - \langle x \rangle^2\right]^{1/2} \equiv \Delta x$$

4A. $\underline{k_0, \Delta k.}$

Now what can we say about g(k) in $\Psi(x,0)$ above?

$$G(k;k_0,\Delta k) = (2\pi)^{-1/2}\left(\frac{a}{2^{1/2}}\right)g(k)$$

$$\frac{a^2}{4} \longleftrightarrow \frac{1}{2(\Delta x)^2}$$

$$\therefore \frac{a}{2^{1/2}} \longleftrightarrow \frac{1}{\Delta x}$$

$$\boxed{\begin{array}{l} g(k) = e^{-(a^2/4)(k-k_0)^2} \\ \qquad \text{compared to} \\ G(x;x_0,\Delta x) = (2\pi)^{-1/2}\dfrac{1}{\Delta x}e^{-(x-x_0)^2/\left[2(\Delta x)^2\right]} \end{array}}$$

$$\therefore \quad \langle k \rangle = k_0$$

$$\Delta k = \left(2^{1/2}/a\right)$$

you can verify by doing relevant integrals

So we already know, by inspection (rather than integration), the k_0, Δk parts for $\psi(x,0)$.

4B. What about x_0, Δx for $G(k;k_0,\Delta k)$?

To do this, perform the FT implicit in defn. of $\Psi(x,0)$ [CTDL, pages 61-62]

$$\Psi(x,0) = \frac{a^{1/2}}{(2\pi)^{3/4}} \int_{-\infty}^{\infty} e^{-\left(a^2/4\right)\left(k-k_0\right)^2 + ikx} dk$$

complete the squares in the exponent (because Gaussian integrals are easy)

$$-\left(a^2/4\right)(k-k_0)^2 + ikx = -\frac{a^2}{4}\left[(k-k_0) - \frac{2ix}{a^2}\right]^2 + ik_0x - \frac{x^2}{a^2}$$

k-dependent → change variables and evaluate Gaussian integral

k-independent — take outside integral

result $\Psi(x,0) = \left(\frac{2}{\pi a^2}\right)^{1/4} e^{ik_0x} e^{-x^2/a^2}$ FT of a Gaussian is a Gaussian!

$\langle x \rangle = \langle x_0 \rangle = 0$

$\Delta x = 2^{-1/2} a$

$\left(2^{1/2}/a\right)$

(for $\Psi * \Psi$, $\Delta x = a/2$, $\Delta k = \frac{1}{a}$, and $\Delta x \Delta k = 1/2$)

ALL OF THE k_0, Δk INFORMATION IS HIDDEN

$\Delta x\ \Delta k = 1 \quad \Delta x\ \Delta p = \hbar$ minimum uncertainty!

This wavepacket: 1. minimum uncertainty
2. centered at $x_0 = 0$

5,6. <u>How to build a w.p. (not necessarily Gaussian) centered at arbitrary x_0</u>
with arbitrary Δx?

* Start again with a new g(k)

$$\Psi(x,0) = \frac{a^{1/2}}{(2\pi)^{3/4}} \int_{-\infty}^{\infty} \underbrace{|g(k)| e^{i\alpha(k)}}_{\text{complex } g(k) \text{ written in amplitude, argument form}} e^{ikx} dk$$

5. let $|g(k)|$ be sharply peaked near $k = k_0$. [It could be $e^{-(a^2/4)(k-k_0)^2}$ and then we already know k_0 and $\Delta k = 2^{1/2}/a$.]

6. Thus we really only need to look at $\alpha(k)$ near k_0 in order to find info about $\langle x \rangle$ and Δx. This is a very important simplification (or focussing of attention)!

Stationary phase argument **

Expand in $\alpha(k)$ in power series in $(k-k_0)$

$$\alpha(k) \cong \underbrace{\alpha(k_0)}_{\alpha_0} + (k - k_0) \left.\frac{d\alpha}{dk}\right|_{k=k_0}$$

Thus the exponential in integral becomes

$$e^{i\alpha_0}\underbrace{e^{i\left[\left(k-k_0\right)\frac{d\alpha}{dk}+kx\right]}}_{\text{very wiggly function of x except at a special region of x}}$$

Now <u>what we want to know is the value of x (for k near k_0) where the phase factor becomes independent of k</u>. This is because, when we integrate over k, if the wiggly factor in the integrand stops wiggling, the integral accumulates to its final value near this value of k!

$$\boxed{\begin{array}{l}\text{plot } I(k) \text{ vs. } k\\ I(k)=\int_{-\infty}^{k}(\text{integrand})dk\end{array}}$$

The value of the integral evaluated at this special value of x (that we do not yet know) $x = x_0(t)$ is $\sim g(k_0)\delta k$ where δk is the change in k required to cause the phase factor to change by π.

MOST IMPORTANT IDEA IN THE ENTIRE LECTURE!

Solve for value of x where the phase factor stops changing, i.e. take derivative with respect to k to find extremum.

$$\frac{d}{dk}\underbrace{\left[\left(k-k_0\right)\frac{d\alpha}{dk}+kx\right]}_{\text{phase factor}}=0$$

stationary phase requirement

$$\therefore \text{ want } \frac{d\alpha}{dk}+x=0$$

$$\boxed{\text{If we let } \left.\frac{d\alpha}{dk}\right|_{k=k_0} \equiv -x_0, \text{ then the phase factor is stationary when x is near } x_0}$$

$$\Psi(x,0) = \frac{a^{1/2}}{(2\pi)^{3/4}} \int_{-\infty}^{\infty} e^{-\left(a^2/4\right)\left(k-k_0\right)^2} \underbrace{e^{-i\left(k-k_0\right)x_0} e^{ikx}}_{= \underbrace{e^{-ik\left(x-x_0\right)}}_{\delta\left(x,x_0\right)} e^{ik_0x_0}} dk$$

shifts Ψ to be sharply peaked at any x_0 $\longrightarrow$ $\delta(x, x_0)$

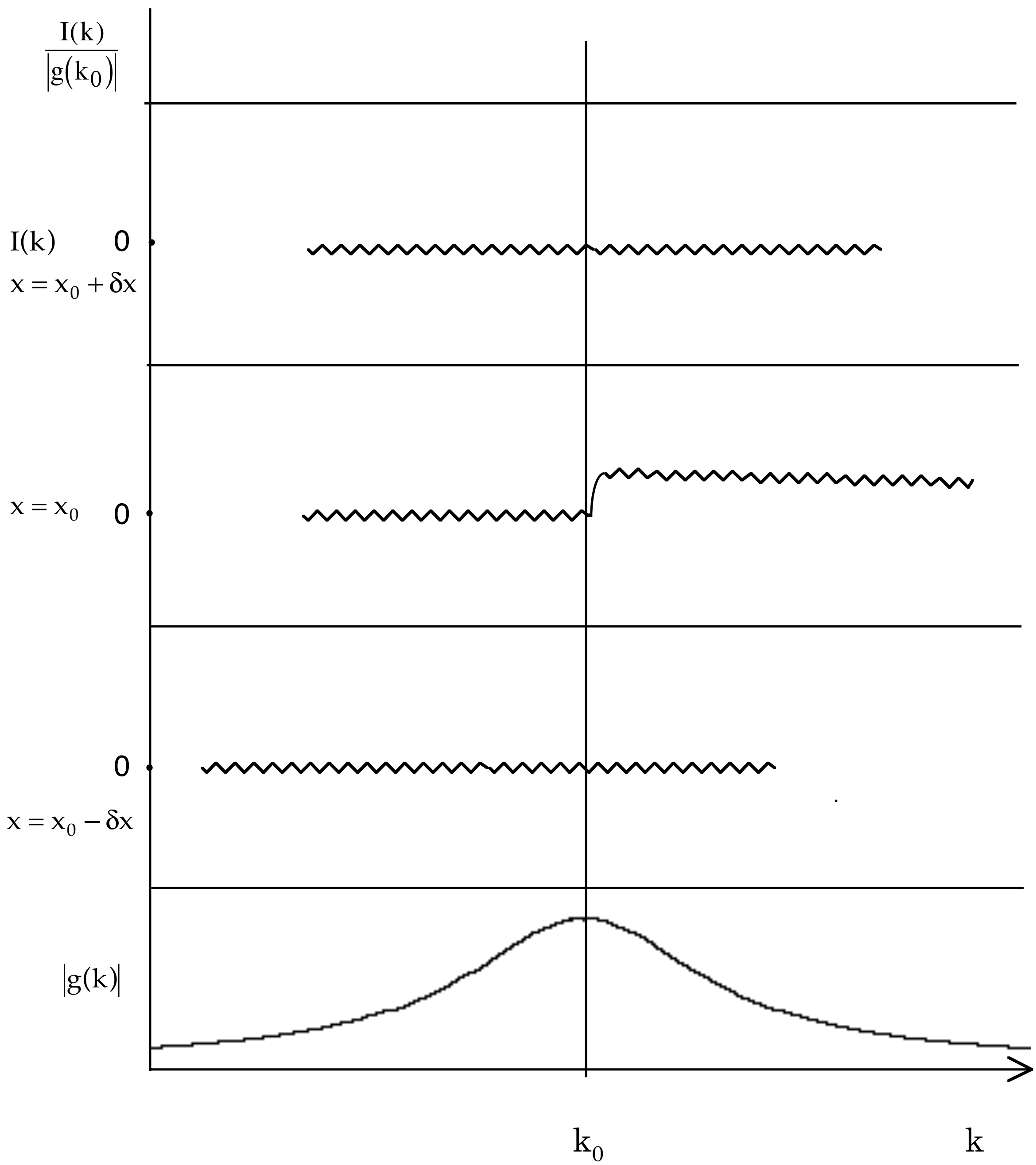
This $|\Psi|^2$ is localized at x_0, k_0, and has widths Δx, Δk,

$\Delta k = ?$ (easy: by inspection)

$\Delta x = ?$ (must perform Fourier transform)

This prescription does not permit free specification of Δx. Δx must still be $\Delta x = 2^{-1/2}a$ if $|g(k)|$ is a Gaussian [shortcut: $\Delta x \Delta k = 1$].

[N.B. We are talking about the shape of $\Psi(x,0)$, not the QM Δx and Δp associated with a particular Ψ.]



Integral accumulates near $k = k_0$ but only when $x \approx x_0$.

7. Now we are ready to let $\Psi(x,t)$ evolve in time

$$\Psi(x,t) = \frac{a^{1/2}}{(2\pi)^{3/4}} \int_{-\infty}^{\infty} |g(k)| e^{-i(k-k_0)x_0} e^{ikx} e^{-i\omega_k t} dk$$

$$\omega_k = \frac{E_k}{\hbar} = \boxed{\frac{\hbar^2 k^2}{2m\hbar} = \frac{\hbar k^2}{2m}}$$

SPECIAL CHOICE OF ZERO OF E, $V_0 = 0$

See CTDL, page 64 for evaluation of $\int dk$ integral and simplification of $\Psi(x,t)$ and $|\Psi(x,t)|^2$. Arbitrary choice of zero of E drops out of $|\Psi(x,t)|^2$.

$$|\Psi(x,t)|^2 = \underbrace{\left(\frac{2}{\pi a^2}\right)^{1/2} \left(1 + \frac{4\hbar^2 t^2}{m^2 a^4}\right)^{-1/2}}_{\substack{\text{t-dependent} \\ \text{normalization} \\ \text{factor}}} \exp - \underbrace{\left[\frac{2a^2 \left(x - \overbrace{\frac{\hbar k_0}{m} t}^{x_{0t}}\right)^2}{a^4 + \frac{4\hbar^2 t^2}{m^2}}\right]}_{\text{spreading}}$$

Complicated: * Δx depends on t, reaching minimum value when t = 0
* x_{0t}, the center of the wavepacket, moves as

$$x_{0t} = \underbrace{\frac{\hbar k_0}{m}}_{v_{\text{group}} \neq v_{\text{phase}} = \frac{\hbar k_0}{2m}!} t$$

* $|g(k)|$, which is independent of time, contains all info about p_0, Δp.

Therefore these quantities do not evolve in time for a free wavepacket. They do evolve if V(x) is not constant.

Think about chopping up the Fourier transform of $|\Psi(x,t)|^2$ into pieces corresponding to different values of p. If there is no force acting on the wavepacket, the <p> for each piece of the original $|\Psi(x,t)|^2$ remains constant.

Summary

We know how to encode a wavepacket for p_0, Δp, x_0 (and since Δx is an explicit function of time, we can let $\Psi(x,t)$ evolve until it has the desired Δx and then shift x_{0t} back to the desired location where Δx has the now specified value).

We also know how to inspect an arbitrary Gaussian $\Psi(x,t)$ to reveal its x_{0t}, Δx, p_{0t}, Δp without evaluating any integrals.