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

Last time: 1. 1-D infinite box $E_n = n^2\left[\frac{h^2}{8mL^2}\right]$

continuity of $\psi(x), \frac{d\psi}{dx}, \frac{d^2\psi}{dx^2}$ $\psi_n = (2/L)^{1/2}\sin(n\pi x)$

confinement → quantization

2. δ–function well

one bound level $E = \frac{-ma^2}{2\hbar^2}$

$\psi = \pm\left(\frac{ma}{\hbar^2}\right)^{1/2} e^{-ma|x|/\hbar^2}$ (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, Δx, p_0, Δp
5. p_0, Δp from $|g(k)|$
6. x_0, Δx 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. wavepackets

$$\Psi(x,0) = \sum a_n \psi_n(x)$$ 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?

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

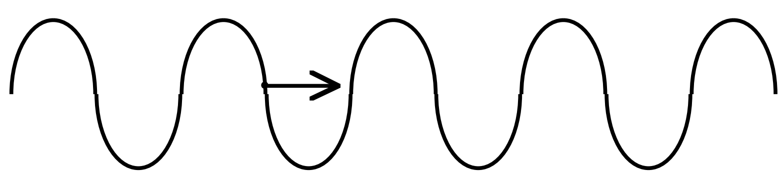
$$\Psi_{|k|}(x,t) = e^{-i\omega_k t}\left[Ae^{ikx} + Be^{-ikx}\right]e^{-iV_0 t/\hbar}$$

$$= \left[Ae^{i(kx-\omega_k t)} + Be^{-i(kx+\omega_k t)}\right]e^{-iV_0 t/\hbar}$$

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



$$v_\phi = \frac{dx_\phi}{dt} = \frac{\omega_k}{k} \leftarrow \frac{\hbar k^2}{2m} \qquad \text{phase velocity} \qquad v_\phi = \frac{\hbar k}{2m} = \frac{p}{\underset{?}{\underline{2m}}} = \frac{v}{2}$$

(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. <u>But what about the probability distribution, $\mathbf{P}(x,t)$?</u>

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

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 $\hat{p}$ $\quad < p > = \dfrac{\int \Psi^* \hat{p} \Psi dx}{\int \Psi^* \Psi dx}$?

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

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

$$\langle x \rangle = x_0$$

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

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

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

4A. <u>k_0, Δk.</u>

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

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

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

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

$$g(k) = e^{-(a^2/4)(k-k_0)^2}$$

compared to

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

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

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

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

$\Delta x\, \Delta k = 1 \quad \Delta x\, \Delta p = \hbar \quad$ 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)!

$\boxed{\text{Stationary phase argument}}$ **

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

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

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!

plot I(k) vs. k

$$I(k) = \int_{-\infty}^{k}(\text{integrand})dk$$

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.

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

stationary phase requirement

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

If we let $\left.\frac{d\alpha}{dk}\right|_{k=k_0} \equiv -x_0$, 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 $\longrightarrow$ $\delta(x, x_0)$

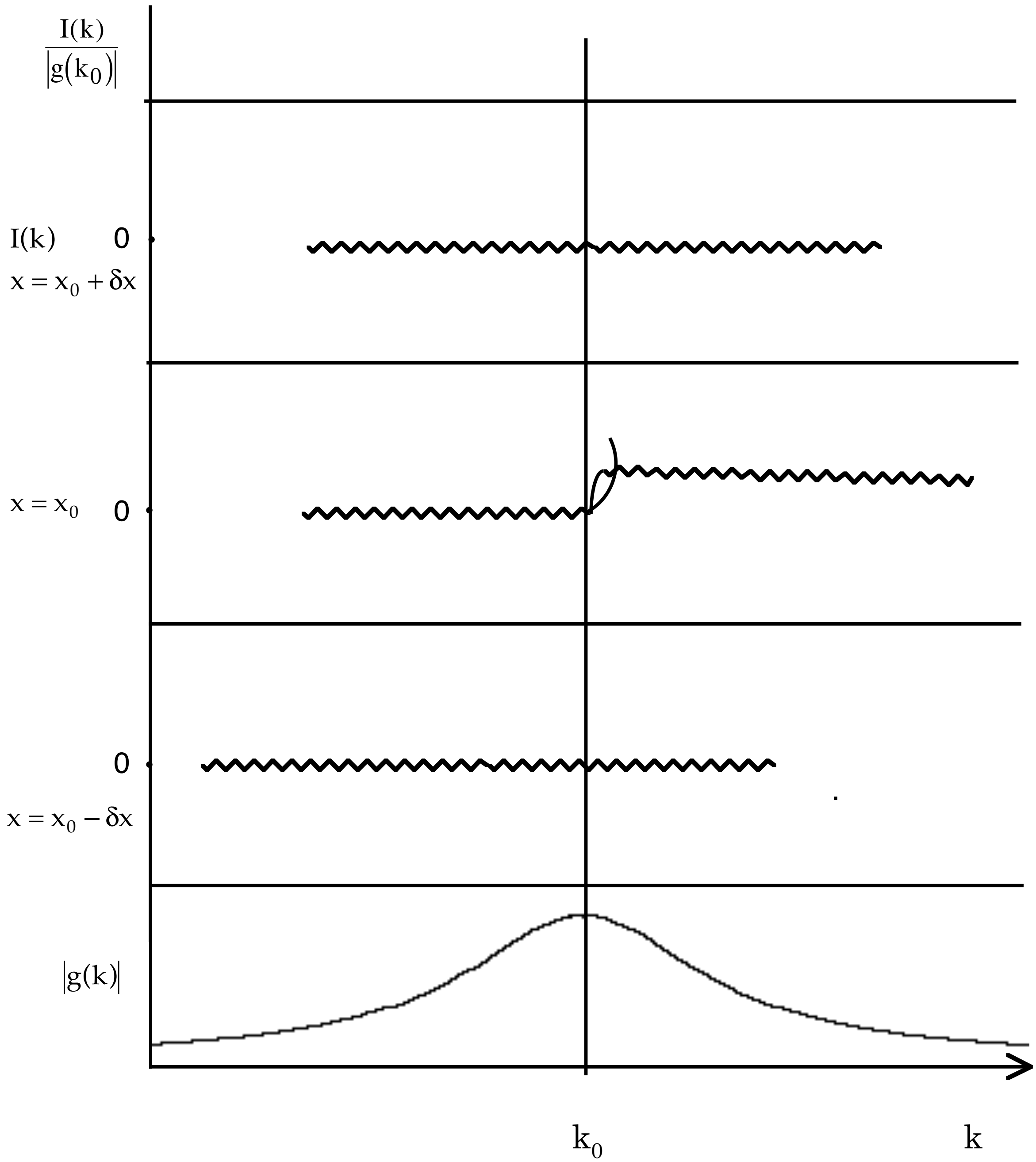
This $|\Psi|^2$ is localized at x_0, k_0, and has widths Δx, Δk,

$\Delta k = ?$ (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

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

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

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 $|\Psi(x,t)|^2$.

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

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

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

* $|g(k)|$, 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 $\langle p \rangle$ 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.