Lecture #4: Stationary Phase and Gaussian Wavepackets

Last time:

tdSE → motion, motion requires non-sharp E
phase velocity
began Gaussian Wavepacket

goal: $\langle x \rangle$, Δx, $\langle p \rangle = \hbar \langle k \rangle$, $\Delta p = \hbar \Delta k$ by construction or inspection

$\Psi(x,t)$ is a complex function of real variables. Difficult to visualize.

What are we trying to do here?

techniques for solving series of increasingly complex problems illustrate philosophical points along the way to solving problems.

So far: free particle, infinite well, δ - function } very artificial

* nothing particle-like
* nothing molecule-like
* no spectra

Minimum Uncertainty (Gaussian) Wavepacket -- QM version of particle. We are going to construct a $\Psi(x,t)$ for which $|\Psi(x,t)|^2$ is a Gaussian in x and the FT of $\Psi(x,t)$, gives $\Phi(k,t)$, for which $|\Phi(k,t)|^2$ is a Gaussian in k.

center of wavepacket follows Newton's Laws

extra stuff: spreading
interference
tunneling

Today: (improved repeat of material in pages 3–4 through 3–1

infer Δk by comparing g(k) to std. $G(x;\ x_0, \Delta x)$

$g(k) = |g(k)|\, e^{i\alpha(k)}$ for k near k_0

$\left.\frac{d\alpha}{dk}\right|_{k=k_0} \equiv -x_0$ STATIONARY PHASE

$|\Psi(x,t)|^2$ moving, spreading wavepacket

$v_G \neq v_\phi$ { how is it possible that the center of the wavepacket moves at a different velocity than its center k - component

Here is a normalized Gaussian (see Gaussian Handout)

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

$$\left.\begin{array}{lll} \left[\text{normalized}\right. & \left.\int_{-\infty}^{\infty} G(x;\ x_0,\Delta x)dx = 1\right] & \\ \text{center} & \langle x\rangle = x_0 & \\ \text{std. dev.} & \Delta x \equiv \left[\langle x^2\rangle - \langle x\rangle^2\right]^{1/2} & \end{array}\right\}\text{by construction}$$

Now compare this special form against

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

F.T. of a Gaussian in k

a Gaussian in k, but what width and $\langle k\rangle$?

by analogy

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

$$\boxed{\frac{a^2}{4} = \frac{1}{2(\Delta k)^2} \quad \therefore \quad \Delta k = \frac{2^{1/2}}{a}}$$

by analogy with $G(x;x_0,\Delta x)$

So casual inspection of this form of $\Psi(x,0)$ gives us $\langle k\rangle$ and Δk. Not quite so easy to get $\langle x\rangle$ and Δx.

If we actually carry out the F.T. specified in the definition of $\Psi(x,0)$ above (see bottom of page 3–4), we get

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

$$\boxed{\frac{1}{2(\Delta x)^2} = \frac{1}{a^2} \qquad \Delta x = a/2^{1/2}}$$

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

$$\Delta x = 2^{-1/2}a, \qquad \text{previously } \langle k\rangle = k_0, \Delta k = \frac{2^{1/2}}{a};$$

But the square of a Gaussian is a Gaussian and its Δx or Δk is a factor of $2^{-1/2}$ smaller than the original value.

$$\Delta x \text{ for } \Psi(x,0) \text{ is } 2^{-1/2}a, \ \Delta x \text{ for } |\Psi(x,0)|^2 \text{ is } \frac{a}{2}.$$

$$\Delta k \text{ for } \Phi(k,0) \text{ is } \frac{2^{1/2}}{a}, \ \Delta k \text{ for } |\Phi(k,0)|^2 \text{ is } \frac{1}{a}.$$

$$\Delta x \Delta k = \frac{a}{2}\frac{1}{a} = \frac{1}{2}$$

See CTDL, p. 231 [$\Delta x, \Delta k$ are defined rigorously in contrast to treatment on p. 23.]

This is a very special Gaussian wavepacket

* minimum uncertainty
* $x_0 = 0$

What about more general Gaussian wavepackets.?

g(k) is a <u>complex function</u> of k <u>sharply peaked</u> near $k = k_0$

$g(k) = |g(k)| e^{i\alpha(k)}$ amplitude, argument form

If $|g(k)|$ is sharply peaked near $k = k_0$, then the only relevant part of $\alpha(k)$ is the part for k near k_0

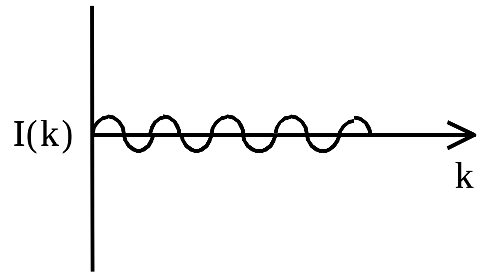
$$\text{Expand } \alpha(k) = \underbrace{\alpha(k_0)}_{\alpha_0} + (k-k_0)\left.\frac{d\alpha}{dk}\right|_{k=k_0} + \quad \text{higher terms neglected}$$

$$\Psi(x,0) = \frac{a^{1/2}}{(2\pi)^{3/4}}\int_{-\infty}^{\infty} \underbrace{|g(k)| e^{i\alpha(k)} e^{ikx}}_{|g(k)| e^{i\alpha_0} e^{i\left[(k-k_0)\left.\frac{d\alpha}{dk}\right|_{k=k_0} + kx\right]}} dk$$

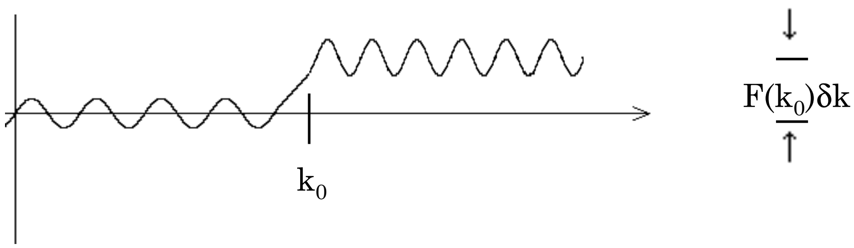
We want to "cook" $\Psi(x,0)$ so that it is localized near $x = x_0$. In order for this to happen, the factor $\left[(k-k_0)\left.\frac{d\alpha}{dk}\right|_{k=k_0} + kx\right]$, must be indpendent of k near $k = k_0$. <u>Stationary Phase</u>!

How does integral of a wiggly function accumulate?

e.g., $$I(k) = \int_{-\infty}^{k} e^{ik'x} dk'$$



but if phase factor stops wiggling near $k = k_0$



where δk is range of k over which the phase factor changes by π.

So, arrange for phase factor to become stationary near $k = k_0$

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

$$0 = \frac{d\alpha}{dk} + x$$ satisfied if $$\boxed{\left.\frac{d\alpha}{dk}\right|_{k=k_0} \equiv -x_0}\ !$$

Thus

$$\Psi(x,0)=\frac{a^{1/2}}{(2\pi)^{3/4}}e^{i\alpha_0}\int_{-\infty}^{\infty}\underbrace{e^{-\left(a^2/4\right)(k-k_0)^2}}_{|g(k)|}\underbrace{e^{-i(k-k_0)\overset{-\frac{d\alpha}{dk}\big|_{k=k_0}\downarrow}{x_0}}e^{ikx}}_{e^{ik(x-x_0)}e^{ik_0x_0}}dk$$

$\left(\text{insertion of } e^{\pm i(k-k_0)x_0} \text{ phase factor to center w.p. at } x_0.\right)$

$e^{ik(x-x_0)}e^{ik_0x_0}$ (stops wiggling only when $x \approx x_0$)

$\downarrow$

$\delta(x-x_0)$ shifts Ψ to any desired x_0

Now put in time-dependence by adding

$e^{-i\omega_k t}$ factor

$$\omega_k=\frac{E_k}{\hbar}=\left(\frac{\hbar^2k^2}{2m}\right)\frac{1}{\hbar}$$

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

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

This FT is evaluated and simplified in CTDL, page 64

$$|\Psi(x,t)|^2 = \left(\frac{2}{\pi a^2}\right)^{1/2} \underbrace{\left(1+\frac{4\hbar^2 t^2}{m^2 a^4}\right)}_{\text{time dependent normalization}} \exp - \underbrace{\left[\frac{2a^2\left(x-\frac{\hbar k_0}{m}t\right)^2}{a^4+\frac{4\hbar^2 t^2}{m^2}}\right]}_{\text{Gaussian with time dependent width and center position}}$$

Maximum of Gaussian occurs when numerator of exp –[ ] is 0.

MOTION: $0 = x - \frac{\hbar k_0}{m}t \qquad x_0(t) = \frac{\hbar k_0}{m}t$

$$v_G = \frac{d}{dt}x_0(t) = \frac{\hbar k_0}{m} = \frac{p_0}{m} = v_{\text{classical}}$$

This is 2× larger than v_ϕ.
Classically expect free particle to move at constant $v = \frac{p}{m}$

WIDTH: compare coefficient of $(x - x_0(t))^2$ in exp – [ ] to standard $G(x;x_0,\Delta x)$ in handout

$$\frac{1}{2(\Delta x)^2} = \frac{2a^2}{a^4 + \frac{4\hbar^2 t^2}{m^2}}$$

$$\Delta x = \left[\frac{a^4 + 4\hbar^2 t^2/m^2}{4a^2}\right]^{1/2} \approx \underbrace{\frac{a}{2}}_{\text{minimum width at } t=0} + \underbrace{\left|\frac{\hbar t}{ma}\right|}_{\text{width increases linearly in t at long time (quadratically at early time).}}$$

$\langle x\rangle$ and Δx are time dependent, but what about $\langle k\rangle$ and Δk?

recall original definition of $\Psi(x,0)$ (page 4-2), where $\Psi(x,0)$ is written as the FT of a Gaussian in k

$$g(k,t) = e^{-i\omega_k t} g(k,0)$$

$$\therefore |\Phi(k,t)|^2 \text{ has } \left.\begin{matrix} \langle k \rangle = k_0 \\ \Delta k = \frac{1}{a} \end{matrix}\right\} \text{time independent}$$

We know free particle must have time independent k_0 and Δk
(no forces — divide w.p. into Δk slices)

$$\Delta x \Delta k = \frac{1}{2}\left[1 + \frac{4\hbar^2 t^2}{m^2 a^4}\right]^{1/2}$$ minimum uncertainty at $t = 0$ (and linearly increasing at long t).

For free particle, build w.p. with any desired x_0, k_0, Δk starting from

$$\Psi(x,t) = \int_{-\infty}^{\infty} g(k) e^{ikx} e^{-i\omega_k t} dk \quad \omega_k = \frac{\hbar k^2}{2m}$$

find x_0 from $-\left.\frac{d\alpha}{dk}\right|_{k=k_0}$

$$x_0(t) = x_0 + v_G t \qquad v_G = \frac{\hbar k_0}{m}$$

$$\Delta x = \frac{a}{2}\left[1 + \frac{4\hbar^2 t^2}{m^2 a^4}\right]^{1/2}$$

if we want a value of Δx other than a/2 at t = 0, replace x by $x' = x + \delta$ such that when the w.p. reaches x_0 at t = 0 it has the desired width.

Could have started with $\overline{\Psi}(k,0) = \int_{-\infty}^{\infty} \underbrace{\overline{g}(x)}_{\text{Gaussian in x}} \underbrace{e^{-ikx}}_{\text{inverse F.T.}} dx$

and then encoded k_0 in $\overline{g}(x)$ thru $\left.\frac{d\alpha}{dx}\right|_{x=x_0} = +k_0$

where $\alpha(x)$ is the argument of $\overline{g}(x) = |\overline{g}(x)| e^{i\alpha(x)}$

For next class read C-TDL pages 103-107, 1468-1476.