Lecture #4: Stationary Phase and Gaussian Wavepackets

Last time:

\[ \text{tdSE} \rightarrow \text{motion, motion requires non-sharp E} \]
phase velocity
began Gaussian Wavepacket

goal: \( \langle x \rangle, \Delta x, \langle p \rangle = \hbar \langle k \rangle, \Delta p = \hbar \Delta k \) by construction or inspection
\[ \Psi(x,t) \text{ is a complex function of real variables. Difficult to visualize.} \]

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
\-
\( \delta \)-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 \( \Delta k \) by comparing \( g(k) \) to std. \( G(x; x_0, \Delta x) \)

\[ g(k) = |g(k)| e^{ikx_0} \text{ for } k \text{ near } k_0 \]

\[ \frac{d\alpha}{dk} \bigg|_{k=k_0} = -x_0 \] \text{ STATIONARY PHASE}

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

\[ v_G \neq v_0 \] how is it possible that the center of the wavepacket

\[ \text{moves at a different velocity than its center k - component} \]
Here is a normalized Gaussian (see Gaussian Handout)

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

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

center \( \langle x \rangle = x_0 \) by construction

std. dev. \( \Delta x \equiv \left[ \langle x^2 \rangle - \langle x \rangle^2 \right]^{1/2} \)

Now compare this special form against

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

F.T. of a Gaussian in \( k \)

by analogy

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

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

\[
\frac{a^2}{4} = \frac{1}{2(\Delta k)^2}
\]

\[
\therefore \Delta k = \frac{a}{2^{1/2}}
\]

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

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

\[
\Psi(x,0) = \left( \frac{2}{\pi a^2} \right)^{1/4} e^{ik_0 x} e^{-x^2/a^2}
\]

\[
\langle x \rangle = x_0 = 0
\]

\[
\Delta x = 2^{-1/2} a, \quad \text{previously} \quad \langle k \rangle = k_0, \Delta k = \frac{2^{1/2}}{a}
\]
But the square of a Gaussian is a Gaussian and its $\Delta x$ or $\Delta k$ is a factor of $2^{-1/2}$ smaller than the original value.

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

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

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

This is a very special Gaussian wavepacket

* minimum uncertainty

* $x_0 = 0$

What about more general Gaussian wavepackets?

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<tr>
<th>$g(k)$ is a complex function of $k$ sharply peaked near $k = k_0$</th>
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$g(k) = |g(k)| e^{i\alpha(k)}$ 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 $k_0$

Expand $\alpha(k) = \alpha(k_0) + (k - k_0) \frac{d\alpha}{dk} \bigg|_{k=k_0}$

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

We want to “cook” $\Psi(x,0)$ so that it is localized near $x = x_0$. In order for this to happen, the factor $\left[ (k-k_0) \frac{d\alpha}{dk} \bigg|_{k=k_0} + kx \right]$, must be independent of $k$ near $k = k_0$. Stationary Phase!
How does integral of a wiggly function accumulate?

\[ I(k) = \int_{-\infty}^{k} e^{ik'x} \, dk' \]

but if phase factor stops wiggling near \( k = k_0 \)

where \( \delta k \) is range of \( k \) over which the phase factor changes by \( \pi \).

So, arrange for phase factor to become stationary near \( k = k_0 \)

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

\[
0 = \frac{d\alpha}{dk} + x \quad \text{satisfied if} \quad \left. \frac{d\alpha}{dk} \right|_{k=k_0} \equiv -x_0
\]

\[ F(k_0) \delta k \]
Thus

\[ \Psi(x, 0) = \frac{a^{1/2}}{(2\pi)^{3/4}} e^{i\alpha_0} \int_{-\infty}^{\infty} e^{-\frac{(a^2/4)(k-k_0)^2}{2g(k)}} e^{-i(k-k_0)x_0} e^{ikx} dk \]

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

\[ \frac{-d\alpha}{dk} \bigg|_{k=k_0} \]

\[ \delta(x-x_0) \text{ shifts } \Psi \text{ to any desired } x_0 \]

Now put in time-dependence by adding

\[ e^{-i\omega_k t} \text{ factor} \]

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

\[ \omega_k = \frac{\hbar k^2}{2m} \]

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

(eigenstate of \( H \))
This FT is evaluated and simplified in CTDL, page 64

\[
i\Psi(x,t)^2 = \left(\frac{2}{\pi a^2}\right)^{1/2} \left(1 + \frac{4\hbar^2 t^2}{m^2 a^4}\right) \exp\left[-\frac{2a^2(x - \frac{\hbar k_0}{m} t)^2}{a^4 + \frac{4\hbar^2 t^2}{m^2}}\right]
\]

Maximum of Gaussian occurs when numerator of \(\exp[-\cdot]\) is 0.

**MOTION:** \[0 = x - \frac{\hbar k_0}{m} t\]
\[x_0(t) = \frac{\hbar k_0}{m} t\]
\[v_G = \frac{d}{dt} x_0(t) = \frac{\hbar k_0}{m} = \frac{p_0}{m} = v_{\text{classical}}\]

This is 2\(\times\) larger than \(v_\phi\).

Classically expect free particle to move at constant \(v = \frac{p}{m}\)

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

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

\(\langle x \rangle\) and \(\Delta x\) are time dependent, but what about \(\langle k \rangle\) and \(\Delta k\)?

recall original definition of \(\Psi(x,0)\) (page 4-2), where \(\Psi(x,0)\)

is written as the FT of a Gaussian in \(k\)

\[g(k, t) = e^{-i\omega_k t} g(k, 0)\]
We know free particle must have time independent $k_0$ and $\Delta k$
(no forces — divide w.p. into $\Delta k$ 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 $x_0$, $k_0$, $\Delta k$ 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

$$\frac{d\alpha}{dk} \bigg|_{k=k_0}$$

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

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

if we want a value of $\Delta x$ 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 $\overline{\Psi}(k, 0) = \int_{-\infty}^{\infty} \overline{g}(x) e^{-ikx} dx$

and then encoded $k_0$ in $\overline{g}(x)$ thru

$$\frac{d\alpha}{dx} \bigg|_{x=x_0} = +k_0$$

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.