Lecture - 8 PHY114 Jan 19, 2024

Agenda

- Remaining discussion on Propagation of wavepackets (Focus on time to spread significantly.)

- Ex. 8.1. Gaussian Wavepacket
- Problems of Normalizing Plane Waves: Two strategies to deal with.

- Why look for another wave equation?
- QM is a Probabilistic Theory.

- Motivating differential operators.

How does the wavepacket evolve with time?

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} e^{i k_0 (x - v_{ph} t)} \int_{-\infty}^{\infty} g(k-k_0)\, e^{i(k-k_0)(x - v_g t)}\, e^{-i(k-k_0)^2 \alpha t + \cdots}\, dk$$

Linear approx. : neglect k^2 term i.e. $\boxed{(k-k_0)^2 \alpha \ll 1}$

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \underbrace{e^{i k_0 (x - v_{ph} t)}} \int_{-\infty}^{\infty} g(k-k_0)\, e^{i(k-k_0)(x - v_g t)}\, dk$$

$$\psi_0(x - v_g t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k')\, e^{i(x - v_g t)\Delta k + i k_0 (x - v_g t)}\, dk'$$

modulated amplitude

where $k' = k - k_0$

$$\Rightarrow \quad |\psi(x,t)|^2 = |\psi_0(x - v_g t)|^2$$

→ wavepacket v_g is particle v

→ Size of the wavepacket?

Travelling to right without distortion in the linear approximation.

→ No distortion as long as $\alpha(k-k_0)^2$ is negligible.

Question: In case quadratic term is there, what is the time required for 'significant' distortion?

Let us think of significant distortion as spreading the width becomes equal to the width originally say $t=0$.

When does significant distortion set in?

Retain $(k-k_0)^2 \alpha t$ term.

$$\psi(x,t) = e^{i k_0 (x - v_{ph} t)} f(x,t)$$

$$f(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k')\, e^{i k'(x - v_g t)}\, e^{-i(k')^2 \alpha t}\, dk'$$

$$\boxed{k' = k - k_0}$$

The wavepacket will remain undistorted for $t \ll t_0$

$$t_0 = \left| \frac{1}{\alpha (\Delta k)^2} \right| = \left| \frac{2}{(\Delta p)^2 \frac{d^2\omega}{dp^2}} \right|$$

For a non-relativistic particle

$$\hbar\omega = \frac{p^2}{2m} = E \quad \Rightarrow \quad \frac{d^2\omega}{dp^2} = \frac{1}{m\hbar}$$

or, $$t_0 = \frac{2m\hbar}{(\Delta p)^2} \approx \frac{2m(\Delta x)^2}{\hbar}$$ $\Delta x \Delta p \sim \hbar$

Qualitative Argument: Two parts differing by $\frac{\Delta p}{2}$

$$\Delta x \sim \left(\frac{\Delta p}{2m}\right) t \longleftarrow$$ significant spreading if $\Delta x \sim \Delta x_0$

$$\boxed{t_0 \approx \frac{2m\Delta x}{\Delta p} \approx \frac{2m(\Delta x)^2}{\hbar}}$$

show it for a Gaussian wavepacket.

- Notice initially tighter spreads faster!

Example: Gaussian Wavepacket

$$\psi(x,0) = A \exp\left(-\frac{x^2}{2a^2} + ik_0 x\right)$$

a) Express as superposition of planewaves

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x,0)\, e^{-ikx}\, dx$$

$$= \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left(\frac{x^2}{2a^2} + ik_0 x - ikx\right) dx$$

$$\int_{-\infty}^{\infty} e^{-\xi^2} d\xi = \sqrt{\pi}$$

Completing the square

$$\phi(k) = \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left[-\left(\frac{x}{\sqrt{2}a} + \frac{ia(k-k_0)}{\sqrt{2}}\right)^2\right] \exp\left(-\frac{a^2(k-k_0)^2}{2}\right) dx$$

Replacing the exponent by $-\xi^2$

$$\phi(k) = \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\xi^2} \sqrt{2}\, a \exp\left(-\frac{a^2(k-k_0)^2}{2}\right) d\xi$$

$$= \frac{A}{\sqrt{2\pi}} \sqrt{2}\, a \exp\left(-\frac{a^2(k-k_0)^2}{2}\right) \sqrt{\pi}$$

$$= A a \exp\left(-\frac{a^2(k-k_0)^2}{2}\right)$$

Again a Gaussian

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$$\psi(x) = A \exp\left(-\frac{x^2}{2a^2} + ik_0x\right) \quad \Big| \begin{array}{l}\text{width}\\ \Delta x \approx a\end{array}$$

$$\phi(k) = A a \exp\left(-\frac{a^2(k-k_0)^2}{2}\right) \quad \Big| \begin{array}{l}\text{width}\\ \Delta k \approx \frac{1}{a}.\end{array}$$

$$\boxed{\Delta x \cdot \Delta k \sim 1}$$

b) Use dispersion relation to find $\psi(x,t)$ for any t.

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{i(kx-\omega t)}\, dx$$

$$\omega(k) = \frac{\hbar k^2}{2m}$$

$$\psi(x,t) = \frac{Aa}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\frac{a^2(k-k_0)^2}{2} + ikx - i\frac{\hbar k^2}{2m}t\right) dk$$

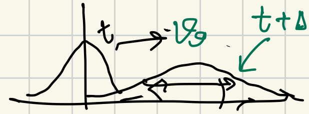
Again completing the square, and using the error integral

$$\psi(x,t) = \frac{A}{\sqrt{1+i\frac{\hbar t}{ma^2}}} \exp\left(\frac{x^2 - 2i\,a^2k_0x + i\,(a^2\hbar k_0^2/m)t}{2a^2\left[1+i\left(\frac{\hbar t}{ma}\right)^2\right]}\right)$$

$$|\psi(x,t)|^2 = \frac{|A|^2}{1+\left(\frac{\hbar t}{ma^2}\right)^2} \exp\left(-\frac{\left[x-\left(\frac{\hbar k_0}{m}\right)t\right]^2}{a^2\left[1+\left(\frac{\hbar t}{ma^2}\right)^2\right]}\right)$$

The max is at $x = \frac{\hbar k_0}{m} \cdot t$

It moves with $v_g = \frac{\hbar k_0}{m}$



But, the wavepacket flattens:

At $t=0$, the width of $|\psi^2|$ is just a.

At t, its width is $\boxed{a' = a\sqrt{1+\left(\frac{\hbar t}{ma^2}\right)^2}}$

$$|\psi(x,t)|^2 = \frac{|A|^2}{1+\left(\frac{\hbar t}{ma^2}\right)^2} \exp\left(-\frac{\left[x-\left(\frac{\hbar k_0}{m}\right)t\right]^2}{a^2\left[1+\left(\frac{\hbar t}{ma^2}\right)^2\right]}\right)$$

c) Independent of time, normalization is

$$1 = \int_{-\infty}^{\infty} |\psi(x,t)|^2\, dx = |A|^2 a \int_{-\infty}^{\infty} e^{-\xi^2}\, d\xi$$

$$= |A|^2 a\sqrt{\pi}$$

$$\therefore \boxed{A = \frac{1}{(a\sqrt{\pi})^{1/2}}}$$

absolute value only.
the phase remains underdetermined.

Normalization of Plane Waves: Problematic

Consider plane wave with a definite momentum $p = \hbar k$.

$$\psi_k(x) = A \, e^{i(kx - \omega t)}$$

- Is this a physically possible wavefunction?

  * Try normalizing it. Objection No. 1

$$\int_{-\infty}^{\infty} \psi^* \psi \, dx = 1$$

$$\Rightarrow \quad A^2 \int_{-\infty}^{\infty} dx = \infty \quad \| \text{ Not acceptable}$$

All functions must be square integrable.

  * Unacceptable from HUP: $[\Delta x \, \Delta p]$ product not defined.

- But, since we build wavepackets by superposition of such pure states, they are very useful.

* Strategy I to normalize: Particle in a large box.

  Put it in a 'large' three dimensional box.

$$\psi_{\vec{k}} = A \, e^{i(\vec{k}\cdot\vec{r} - \omega t)}$$

Then $A = \dfrac{1}{\sqrt{L^3}} = \dfrac{1}{\sqrt{V}}$, V the volume

But note that the very fact that it is inside a box, $\vec{k}$ becomes discrete.

In fact this strategy has worked wonders in understanding properties of solids wherein you can describe electrons as free particles as in a good metal such as sodium.

Strategy II : Allow it to be described by a Dirac delta fn. i.e. we demand that prob. density when integrated over all space, such that $\int_{-\infty}^{\infty} \psi^* \psi \, dx = \delta(p-p')$

In 1-D,

$$\psi_p(x) = N e^{i\left(\frac{p}{\hbar}x - \omega t\right)}$$

$$N^2 \int_{-\infty}^{\infty} \psi_{p'}^* \psi_p \, dx = \delta(p-p')$$

Whenever it is found, it is at p!

$$\Rightarrow N^2 \int_{-\infty}^{\infty} e^{-i\left(\frac{p'}{\hbar}x - \omega t\right)} e^{i\left(\frac{p}{\hbar}x - \omega t\right)} dx$$

$$= N^2 \int_{-\infty}^{\infty} e^{i\left(\frac{p-p'}{\hbar}\right)x} dx$$

$$= N^2 \lim_{g\to\infty} \int_{-g}^{g} e^{i\frac{(p-p')}{\hbar}} dx$$

$$= 2N^2\pi \lim_{g\to\infty} \frac{1}{\pi} \frac{\sin\left(g\frac{p-p'}{\hbar}\right)}{\left(\frac{p-p'}{\hbar}\right)}$$

$$= 2N^2\pi\, \delta\left(\frac{p-p'}{\hbar}\right) = 2N^2\pi\hbar\, \delta(p-p')$$

$$\therefore \boxed{N = \frac{1}{\sqrt{2\pi\hbar}}}$$

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$$\frac{1}{\sqrt{2\pi\hbar}}\, e^{i\left(\frac{p}{\hbar}x - \omega t\right)} \quad \text{—— (1D)}$$

$$\psi_{\vec{p}}(\vec{r}) = \frac{1}{(2\pi\hbar)^{3/2}}\, e^{i\left(\frac{\vec{p}\cdot\vec{r}}{\hbar} - \omega t\right)} \quad \text{—— (3D)}$$

Q. 1. particle-wave or wavy particle Ψ

Physical Observables $E, \vec{r}, \vec{L}, \vec{p}$

How are they related?

Q.2. How does it interact with environment?

Reflected, Refracted as in EM waves?

Coulomb Interaction, Current, Voltage?

Q.3. Corpuscular & Wave character of EM waves – can they be reconciled?

i.e. Is it possible to put Maxwell's Equations into QM formalism?

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So far, I have discussed

- TWO BIG Physics ideas: HUP, Complementarity, $\hbar$
- TWO Convenient Math Tools: Dirac δ fn. & Fourier Transform

We now go on to the central QM: Schrödinger Wave Equation.

Q: Why do we need another wave eqn.?

$$\frac{\partial^2 f}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 f}{\partial t^2}$$

f: - $\vec{E}$ or $\vec{B}$ in EMT
- Waves on String: transverse displacement
- Sound Waves: Longitudinal local pressure differences.

$$f = A e^{i(kx - \omega t)}$$ | A familiar soln.

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But, $E = \hbar\omega$ & $\vec{p} = \hbar\vec{k}$

& $E = \dfrac{p^2}{2m} + V(x,t)$

$$\Psi(x,t) = A\, e^{i(kx-\omega t)}$$

$$\boxed{i\hbar \frac{\partial}{\partial t}}\Psi = E\,\boxed{\Psi}$$

$$\boxed{-i\hbar \frac{\partial}{\partial x}}\Psi = \hbar k\, \Psi$$

Differential Operators

$i\hbar \dfrac{\partial}{\partial t} \rightarrow \hat{E}$

$-i\hbar \dfrac{\partial}{\partial x} \longrightarrow \hat{p}_x$

Operator Ψ = constant Ψ || Eigenfunctions

Define differential operators $i\hbar \dfrac{\partial}{\partial t}$ for Energy

and $-i\hbar \dfrac{\partial}{\partial x}$ for P_x

Observables:

QM constructs Operators (Linear) for each physically observable quantity such that the measured quantity is a real eigenvalue of the operator in the space of its eigenfunctions.

To discuss more later.

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