Quantum Mechanics - Lecture 8

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The Free Particle

"V(x) = 0; No boundaries; continuous energy states"

- The time independent Schrodinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\Rightarrow \frac{d^2\psi}{dx^2} = -k^2\psi\text{ , where } k = \frac{\sqrt{2mE}}{\hbar} \qquad \text{Eq.(1)}$$

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- Let us choose the solution in a general form

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \qquad \text{Eq.(2)} \qquad \text{(A and B are the constants)}$$

"there are no boundary conditions for wave function"

$\Rightarrow$ no restrictions on the values of k

$\Rightarrow$ no restrictions on the energy particle can carry"

$\Rightarrow$ it can have any positive energy $E = \dfrac{\hbar^2 k^2}{2m}$

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- Now, the time dependent wave function (the stationary state) we can write as

$$\Psi(x,t) = \psi(x)e^{-\frac{iEt}{\hbar}} = Ae^{i\left(kx-\frac{\hbar k^2}{2m}t\right)} + Be^{-i\left(kx+\frac{\hbar k^2}{2m}t\right)}$$

$$= Ae^{i(kx-\omega t)} + Be^{-i(kx+\omega t)}$$

Where: $\frac{\hbar \quad k^2}{2m} = \frac{E}{\hbar} = \frac{2\pi E}{h} = 2\pi v = \omega$

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- We can also write in a simple form by combining the two terms as

$$\Psi_k(x,t) = Ae^{i(kx-\omega t)}, \text{ with } k = \pm\frac{\sqrt{2mE}}{\hbar}$$

→ *k>0*: wave is travelling to the right

→ *k<0*: wave is travelling to the left

Important Paradoxes

- The probability density

$$P(x,t) = |\Psi_k(x,t)|^2 = |A|^2$$

→ that is, probability is independent of position and time

→ this implies that there is a complete loss of information about position and time of the state. This is due to "definite" values of momentum ($p = \hbar k$) and energy ($E = \frac{\hbar^2 k^2}{2m}$), respectively

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2. The speed of the wave $v_{wave} = \frac{\omega}{k} = \frac{E}{\hbar} \times \frac{\hbar}{\sqrt{2mE}} = \sqrt{\frac{E}{2m}}$

The speed of the particle $v_{particle} = \sqrt{\frac{2E}{m}}$ $\Rightarrow v_{particle} = 2\, v_{wave}$ OR $v_{classical} = 2\, v_{quantum}$

→ "this means that the particle travels twice as fast as the wave that represents it"

Important Paradoxes

"V(x) = 0; No boundaries"

3. Let us normalize the wave function

$$\int_{-\infty}^{\infty} \Psi_k^*(x,t)\Psi_k(x,t)\,dx = |A|^2 \int_{-\infty}^{\infty} dx \ \rightarrow \infty$$

→ that is, wave function of free particle is not normalizable

→ this implies that $\Psi_k\ (x,t)$ is not a physical state. That is, a free particle cannot exist in a stationary state.

→ this also implies that a free particle cannot have a definite momenta and energy

Solution to Paradoxes

"wave packets NOT a plane wave

- The physical solution to free particle Schrodinger equation is represented by the "wave packets" (not the plane waves) defined as

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \phi(k)\, e^{i(kx-\omega t)}\, dk\ ,$$ (free particle's wave function)

$\phi(k)$ represents the amplitude of the wave packets, and obtained using the initial wave function $\Psi(x,0)$ using

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

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what does the above wave packet solution tell us?

→the position, momentum (or energy) of the particle are no longer known exactly

→the wave packet and the particle travels with the same speed ($v_g = \sqrt{\frac{2E}{m}}$), called the group velocity.

→the wave packet is normalizable

Phase and Group Velocities

We know that the velocity of an EM wave in a medium is

$$v = \frac{1}{\sqrt{\mu\epsilon}}$$

- If μ and ϵ of a medium does not depend on the frequency of the EM wave, the medium is called a non-dispersive medium.

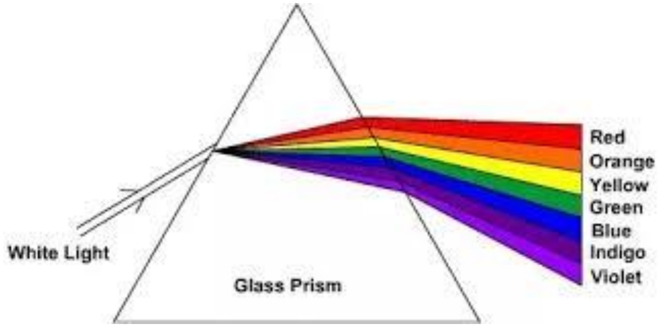
  → vacuum is an example of a non-dispersive medium"

In this case the EM wave travels at constant speed

$$v_p = \frac{\omega}{k}\,, \qquad (v_p \text{ is the phase velocity})$$

"→ all waves in a wave packet travel with the same speed leading to a **no** change in the shape of the wave packet"

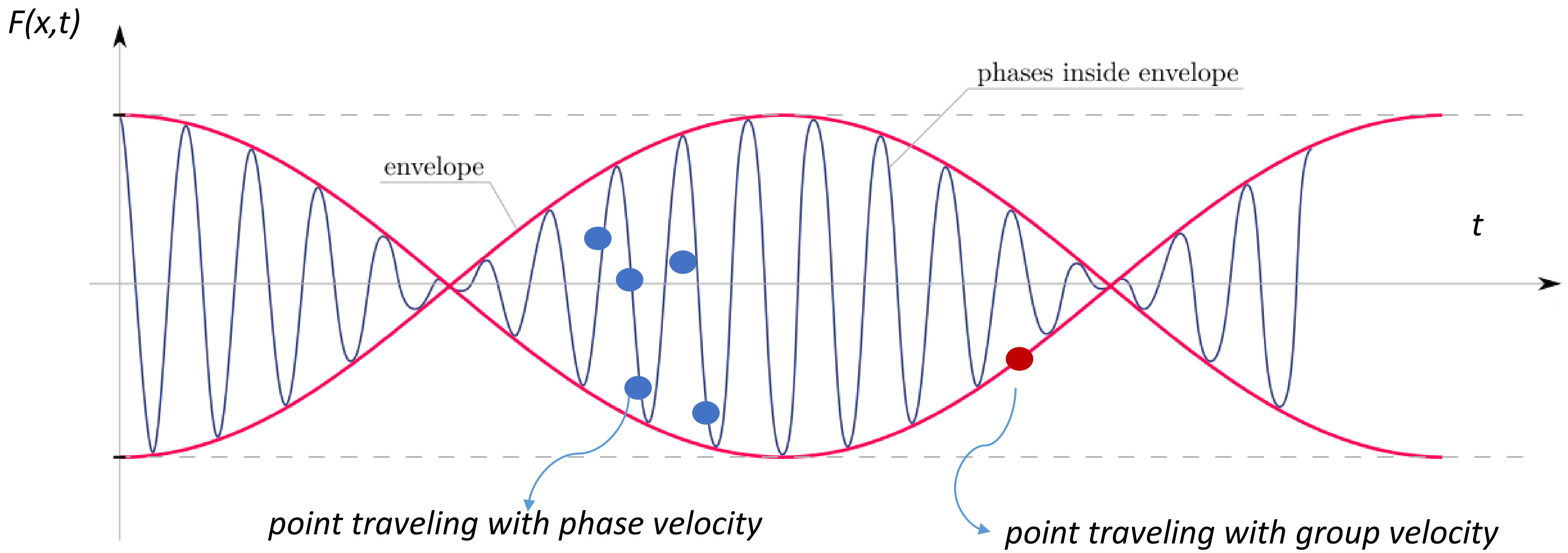
- If μ and ϵ of a medium depend on the frequency of the EM, the medium is called a dispersive medium. In this case the EM waves of different frequency travel with different speeds.
  Example: dispersion of light by a prism or a raindrop

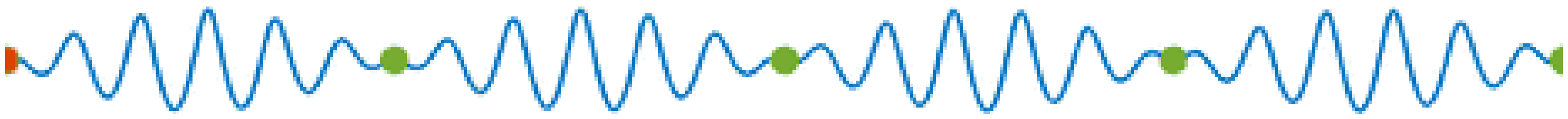


- The wave packet as a whole, however, travels with the same velocity called the group velocity.

$$v_g = \frac{d\omega}{dk} \,, \qquad (v_g \text{ is the group velocity})$$

Phase and group velocities





Example Problem 6: The initial wave function of a free particle is given as

$$\Psi(x,0) = A\, e^{-a|x|}$$, A and a are positive real constants. Then

(a) Find the value of A

(b) Find the amplitude of wave packets, $\phi(k)$

(c) Find $\Psi(x,t)$

(d) Discuss the limiting cases: i) a is very large ii) a is very small

Example Problem 6: The initial wave function of a free particle is given as

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(a) Find the value of *A*

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(c) Find $\Psi(x,t)$

(d) Discuss the limiting cases: i) *a* is very large ii) *a* is very small

Solution: (a) Since $\Psi(x,0)$ is a quantum mechanical system wavefunction, it must be normalizable.

$$1 = \int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx = 2|A|^2 \int_0^{\infty} e^{-2ax} dx = 2|A|^2 \frac{e^{-2ax}}{-2a}\Big|_0^{\infty} = \frac{|A|^2}{a} \Rightarrow A = \boxed{\sqrt{a}.}$$

$\Rightarrow$ The normalize wave function is $\Psi(x,0) = \sqrt{a}\, e^{-a|x|}$

(b) The amplitude of the wave packet is given by

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$$\phi(k) = \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-a|x|} e^{-ikx}\, dx = \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-a|x|} (\cos kx - i \sin kx) dx.$$

The cosine integrand is even, and the sine is odd, so the latter vanishes and

$$\begin{aligned}
\phi(k) &= 2\frac{A}{\sqrt{2\pi}} \int_{0}^{\infty} e^{-ax} \cos kx\, dx = \frac{A}{\sqrt{2\pi}} \int_{0}^{\infty} e^{-ax} \left(e^{ikx} + e^{-ikx}\right) dx \\
&= \frac{A}{\sqrt{2\pi}} \int_{0}^{\infty} \left(e^{(ik-a)x} + e^{-(ik+a)x}\right) dx = \frac{A}{\sqrt{2\pi}} \left[\frac{e^{(ik-a)x}}{ik-a} + \frac{e^{-(ik+a)x}}{-(ik+a)} \right]\Bigg|_{0}^{\infty} \\
&= \frac{A}{\sqrt{2\pi}} \left(\frac{-1}{ik-a} + \frac{1}{ik+a} \right) = \frac{A}{\sqrt{2\pi}} \frac{-ik-a+ik-a}{-k^2-a^2} = \boxed{\sqrt{\frac{a}{2\pi}} \frac{2a}{k^2+a^2}}.
\end{aligned}$$

(c) The dependent wave function is

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

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} 2\sqrt{\frac{a^3}{2\pi}} \int_{-\infty}^{\infty} \frac{1}{k^2+a^2} e^{i(kx-\frac{\hbar k^2}{2m}t)} dk = \boxed{\frac{a^{3/2}}{\pi} \int_{-\infty}^{\infty} \frac{1}{k^2+a^2} e^{i(kx-\frac{\hbar k^2}{2m}t)} dk.}$$

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d) **Case I:** If *a* is very large: $\Psi(x,0)$ will be sharp narrow spike wave function, AND

$$\phi(k) \cong \sqrt{\frac{2}{\pi a}}, \text{ a broad and flat wave function}$$

→ position of the particle is well defined but momentum is ill-defined

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Case II: If *a* is very small: $\Psi(x,0)$ will be broad and flat wave function, AND

$$\phi(k) \cong \sqrt{\frac{2a^3}{\pi}} \times \frac{1}{k^2}, \text{ will be sharp narrow spike wave function}$$

→ position of the particle is ill-defined but momentum is well defined