PHYS-454

The free particle

The free particle-a

- The free particle is that for which the potential V(x) is zero everywhere!
- Clasically this would just mean motion at a constant velocity. But in quantum mechanics the problem is very tricky.
- The Schroedinger equation reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \Rightarrow \frac{d^2\psi}{dx^2} = -k^2\psi, \qquad k \equiv \frac{\sqrt{2mE}}{\hbar}$$

The free particle-b

- The solutions of this equations are plane waves:

$$\psi\left(x\right) = Ae^{ikx} + Be^{-ikx}$$

- The time dependent solution is just the above solution multiplied by the standard time dependence $\exp\left(-iEt/\hbar\right)$:

$$\Psi(x,t) = Ae^{ik\left(x-\frac{\hbar k}{2m}t\right)} + Be^{-ik\left(x+\frac{\hbar k}{2m}t\right)}$$

The free particle-c

- In the above solution the first term represents a wave traveling to the *right,* and the second represents a wave (of the same energy) going to the *left.*
- Since they only differ by the *sign* in front of *k,* we might as well write:

$$\Psi_k(x,t) = Ae^{i\left(kx - \frac{\hbar k^2}{2m}t\right)}$$

$$k \equiv \pm \frac{\sqrt{2mE}}{\hbar}, \qquad \text{with} \begin{cases} k > 0 \Rightarrow & \text{traveling to the right} \\ k < 0 \Rightarrow & \text{traveling to the left} \end{cases}$$

…The free particle-d…

- The speed of these waves (the coefficient of t over the coefficient of x) is

$$v_{quantum} = \frac{\hbar |k|}{2m} = \sqrt{\frac{E}{2m}}$$

- On the other hand, the classical speed of a free particle with kinetic energy E is given by

$$v_{classical} = \sqrt{\frac{2E}{m}} = 2v_{quantum}$$

…The free particle-e…

- Apparently the quantum mechanical wave function travels at *half* the speed of the particle it is supposed to represent!
- There is also another problem: this wave function is *not normalizable.*

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

- In the case of the free particle, then, the separable solutions do not represent physically realizable states. A free particle cannot exist in a stationary state; or, to put it another way, *there is no such thing as a free particle with a definite energy.*

…The free particle-e…

- This does not mean that these solutions are of no use for us. They play a *mathematical* role that is entirely independent of their *physical* interpretation.
- The general solution to the time-dependent Schroedinger eq. is still a linear combination of separable solutions (only this time it's an integral over the continuous variable *k,* instead of a *sum* over the discrete index *n*):

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

…The free particle-f…

Where the analogy with the discrete spectrum is given by

$$c_n \to \left(1/\sqrt{2\pi}\right)\phi\left(k\right)dk$$

- Now the wavefunction *can* be normalized (for appropriate $\phi\left(k\right)$). But it has a range of k' s, and hence a range of energies and speeds. We call it a **wave packet**.

…The free particle-f…

- In the generic problem we are given $\Psi(x,0)$ and we are asked to find $\Psi(x,t)$. For a free particle the problem is how to determine $\phi(k)$ so as to match the initial wave function:

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

…The free particle-f…

- The answer is given by the **Plancherel's theorem** of Fourier analysis:

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k) e^{ikx} dk \Leftrightarrow F(k) = \frac{1}{\sqrt{2\pi}} f(x) e^{-ikx} dk$$

- $F(k)$ is called the **Fourier transform** of $f(x)$
- $f(x)$ is called the **inverse Fourier transform** of $F(k)$
- So the solution to the generic quantum problem, for the free particles is:

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

…discussion of a paradox-a…

- We return now to the paradox: the separable solution $\Psi_k(x,t)$ travels at a different speed from the particle it represents!
- We could easily avoid this problem by saying that $\Psi_k(x,t)$ is not a physically realizable state. But a further discussion reveals very interesting properties of the wave-packet and the velocity concept.

…discussion of a paradox-b…

- The essential idea is this: A wavepacket is a superposition of sinusoidal functions whose amplitude is modulated by ϕ; it consists of "ripples" contained with an "envelope". What corresponds to the particle velocity is not speed of the individuals ripples (the so called **phase velocity**), but rather the speed of the envelop (**the group velocity**) - which, depending on the nature of the waves, can be greater than, less than, or equal to, the velocity that go to make it up.

…the wave packet…