Wave-packets

• The De Broglie relation $\lambda = \frac{h}{p}$ is known to be valid experimentally for both photons and particles.

•This suggests that matter or quanta of radiation may perhaps be represented as localized (concentrated) wave forms $\psi(x, y, z, t)$. We will mostly be restricted within one dimension x only from now on.

• This function ψ must have the following properties:
a) It can describe a single photon or particle;
b) It is larger in magnitude where the particle or photon is 'likely' to be;
c) It can interfere with itself;

d) If a wave packet has to represent a particle of mass m, velocity v, kinetic Energy E and momentum p, then the velocity of the center of the packet must be $v = \frac{p}{m}$. For a wavepacket, this is $\frac{d\omega}{dk} = \frac{d(2\pi\nu)}{2\pi/\lambda} = \frac{dE}{dp} = \frac{d(p^2/2m)}{dp} = \frac{p}{m}$ (where we have used $E = h\nu,\ p = hk$). This is indeed the classical expression for the velocity.

Examples

- You are already familiar with Fourier series expansion:

$$f(x) = \int_{-\infty}^{\infty} dk\ g(k)\ e^{ikx}$$

- This is a linear superposition of waves of wavelength $2\pi/k$, weighted by a k-dependent factor $g(k)$.

- Choose $g(k) \sim e^{-\alpha(k-k_0)^2}$. Result:

$$
\begin{aligned}
f(x) &= \int_{-\infty}^{\infty} dk \ e^{-\alpha(k-k_0)^2} \ e^{ikx} \\
&= \int_{-\infty}^{\infty} dk \ e^{-\alpha(k-k_0)^2} \ e^{i(k-k_0)x} \ e^{ik_0x} \\
&= \sqrt{\frac{\pi}{\alpha}} e^{-\frac{1}{4\alpha}x^2+ik_0x}; \\
|f(x)|^2 &= \frac{\pi}{\alpha} e^{-\frac{1}{2\alpha}x^2}
\end{aligned}
$$

- Spreads:

$$
\Delta k \sim \frac{1}{\sqrt{2\alpha}}, \ \Delta x \sim \sqrt{2\alpha}, \ \Delta x \Delta k \sim 1!
$$

- Hence, the wave packet provides a natural realization of the Uncertainty principle!

Propagation of wave-packets

- Consider a simple plane wave: $f(x-vt) = e^{i(kx-\omega t)}$ with $v = \frac{\omega}{k}$.

- For light, $\omega = ck$. In general, for a matter particle, the propagation may be represented by a more general $\omega(k)$.

- For simplicity, we may assume that the wave is sharply peaked around some momentum $k = k_0$, allowing us to use the Taylor expansion:

$$\begin{aligned} \omega(k) &= \omega(k_0) + \frac{d\omega(k)}{dk}|_{k_0}(k-k_0) + \frac{1}{2}\frac{d^2\omega(k)}{dk^2}|_{k_0}(k-k_0)^2 + .. \\ &= \omega(k_0) + v_g(k-k_0) + \beta(k-k_0)^2 + .. \end{aligned}$$

We may assume that the variation of $\omega(k)$ is slow enough so that the terms higher the second order may be ignored.

- Then, assuming $g(k) \sim e^{-\alpha(k-k_0)^2}$ as earlier, the superposition of these waves leads to:

$$\begin{aligned}
\psi(x,t) &= \int_{-\infty}^{\infty} dk \; g(k) \; e^{i(kx-\omega(k)t} \\
&= \sqrt{\frac{\pi}{\alpha - i\beta t}} \; e^{i(k_0 x - \omega(k_0)t)} e^{-\frac{(\alpha+i\beta t)(x-v_g t)^2}{4(\alpha^2+\beta^2 t^2)}}
\end{aligned}$$

- Probability density:

$$|\psi(x,t)|^2 = \frac{\pi}{\alpha^2 + \beta^2 t^2} \; e^{-\frac{\alpha(x-v_g t)^2}{2(\alpha^2+\beta^2 t^2)}}$$

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- $|\psi(x,t)|^2$ is peaked around $x - v_g t = 0$. This implies that the center moves at a speed $v_g \sim$ group velocity, exactly what we want!

- Width is $\Delta x \sim \sqrt{\alpha + \frac{\beta^2 t^2}{\alpha}}$, which grows with t

- This indicates the growing probability (with time) that the particle is far from where it was localized initially (at $t = 0$). This is also perfectly consistent.

Wave packet and Schrodinger equation

• How to obtain these packets above as solutions of an equation? The general form of any such equation should be universal for any one particle system.

• The most general possibility is: $\hat{O}\Psi = 0$ where $\hat{O}$ is some operator that may depend only on dynamical variables ($x, p_x, ..$ and t), on universal constants such as $c, \hbar$ and on invariant parameters of the system such as mass, charge etc.

• Also, the relation $E = p^2/2m$ and $p = \hbar k$ should emerge naturally.

• Further, the equation must be linear so as to allow linear superposition of solutions (construction of wave-packets).

- For instance, take a plane wave: $\psi(x,t) = e^{i(kx-\omega t)}$.

- If we define $\widehat{p} = -i\hbar\frac{\partial}{\partial x}$, then $\widehat{p}\psi(x,t) = \hbar k\psi(x,t)$.

- If we define $\widehat{E} = i\hbar\frac{\partial}{\partial t}$, then $\widehat{E}\psi(x,t) = \hbar\omega\psi(x,t)$.

- Thus, we indeed recover the correct results in the form of eigenvalues of operators.

- What should then be the equation which naturally incorporates the requirement $\widehat{E}\psi(x,t) = \frac{\widehat{p^2}}{2m}\psi(x,t)$?

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$$\begin{aligned}
\hat{E}\psi(x,t) &= i\hbar\frac{\partial}{\partial t}\psi(x,t) = \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)\left(-i\hbar\frac{\partial}{\partial x}\right) \\
&= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) \\
&= \frac{\widehat{p^2}}{2m}\psi(x,t)
\end{aligned}$$

- This must be the equation we have been searching for, which describes a single particle within this new (quantum) mechanical formulation!

- Note the following features:

a) It is linear, as it should be;
b) It is a partial DE;

c) It is not equivalent to the wave equation; If it was, the only allowed solution for a single particle wave function would have been $\psi(x,t) = \psi(vt \pm x)$. Rather, $\psi(x,t)$ is more general;
d) This equation is applicable for any $\omega = \omega(k)$ (hence includes the case of light);
e) It is first order in t-derivative; Once $\psi(x,t)$ is specified at some $t = 0$, the wave function at any subsequent time can be found out.

Separability: Time-independent Schr eqn

- This equation leads to a simplication when the wavefunction is separable into space and time part: $\psi(x,t) = \phi(x)T(t)$.

- This implies:

$$\frac{i\hbar}{T(t)}\frac{\partial T(t)}{\partial t} = -\frac{\hbar^2}{2m\phi(x)}\frac{\partial^2 \phi(x)}{\partial x^2} = E$$

where E is an arbitrary spacetime constant.

- The time-dependent part has a straightforward solution $T(t) = Ae^{-\frac{i}{\hbar}Et}$ $(A = constant)$

- The space-dependent part obeys the following equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi(x)}{\partial x^2} = E\phi(x),$$

known as the time-independent Schrodinger equation (free particle).

- Evidently, the above may also be interpreted as an eigenvalue equation in terms of the operator $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$, E being the (kinetic) energy eigenvalue.

However, there are some still some issues which need to be understood better:

a) What is the interpretation of $\psi(x,t)$, which in general may be complex (see the earlier example of the wave-packet)?

b) How to obtain discrete values for physical (observable) quantities (e.g. energy, momentum etc.) within this framework?