LECTURE 4 – WAVE PACKETS

1.2 Comparison between QM and Classical Electrons

<table>
<thead>
<tr>
<th>Classical physics (particle)</th>
<th>Quantum mechanics (wave)</th>
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</thead>
<tbody>
<tr>
<td>electron is a point particle</td>
<td>electron is wavelike</td>
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<tr>
<td>motion described by $\vec{F} = m\vec{a}$</td>
<td>for energy $E$, motion described by wavefunction $\Psi(\vec{r},t) = \Psi(\vec{r})e^{-i\omega t}$ $\hbar\omega = E$</td>
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</table>

$\vec{F} = -\nabla V(\vec{r})$

where $V(\vec{r})$ – potential energy

typically $\vec{F}$ due to electric fields from other charges

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V(\vec{r})\Psi = E\Psi$$

- differential equation governing $\Psi$

$V(\vec{r})$ - (potential energy) - this is where the forces acting on the electron are taken into account

probability density of finding electron at position $\Psi(\vec{r}) \cdot \Psi^*(\vec{r})$

$p = mv, E = \frac{1}{2}mv^2$

$E = \hbar\omega, \quad p = \hbar k$

We shall now consider "free" electrons: $\vec{F} = 0 \therefore V(\vec{r}) = \text{const.} \,(\text{for simplicity, take } V(\vec{r}) = 0)$
Wavepackets and localized electrons

For free electrons we have to solve Schrodinger equation for \( V(r) = 0 \) and previously found:

\[
\Psi(r, t) = Ce^{j(k \cdot r - \omega t)} - \text{travelling plane wave}
\]

\[
\therefore \Psi \cdot \Psi^* = C^2 \quad \text{everywhere.}
\]

We can’t conclude anything about the location of the electron!

However, when dealing with real electrons, we usually have some idea where they are located! How can we reconcile this with the Schrodinger equation? Can it be correct? We will try to represent a localized electron as a wave pulse or wavepacket. A pulse (or packet) of probability of the electron existing at a given location. In other words, we need a wave function which is finite in space at a given time (i.e. \( t=0 \)).

Particle behavior is observation of the evolution of the packet as a whole.

Wave effects are an observation of the individual frequency components of the “packet”.

From Fourier transform concepts, the wavepacket can be represented as a superposition of waves with different \( k \) (the spatial frequency). Just like forming a voltage pulse from temporal (time) frequency (\( \omega \) or \( f \)) components.

A Fourier Transform can be defined in time and a localized (in time) packet created using a frequency spectrum (communications theory).

\[
g(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t)e^{j\omega t} dt
\]

\[
f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(\omega)e^{j\omega t} d\omega
\]
We can do the same for a spatial function.

i.e., \( \Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(k)e^{i(kx-\omega t)} \, dk \)  \hspace{1cm} (13)

A \( k \) “spectrum” will produce a spatially localized wave “packet”.

where \( \psi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0)e^{-jkx} \, dx \)

\( \psi(k) \) is the spatial frequency spectrum of \( \psi(x) \). A \( k \) “spectrum” will produce a spatially localized wave “packet”.

![Diagram of a wave packet](image)

where \( k_o = \frac{2\pi}{\lambda_o} \) is the average "packet wave" spatial frequency, \( x_o \) is the packet position, \( \Delta x \) is the packet size and \( \Delta k \) the packet size in \( k \) space.

It is found from Fourier math that the more tightly confined the wavepacket is in \( x \), the broader the spread in \( k \), and vice-versa, This is equivalent to needing high frequency components for a small rise time in a voltage pulse.

Fourier transform result : \( \Delta k \cdot \Delta x \geq 2\pi \) \hspace{1cm} (Formal derivation later)

\( \therefore \Delta k \cdot \frac{\Delta p}{h} \geq 2\pi \quad \Delta x \cdot \Delta p \geq h \) - called the uncertainty principle.
Formation of a wave packet by superposition of two different waves of slightly different frequencies:

As the number of waves increases, the wave packet becomes more localized in space.

Note that the wavepacket does not change its shape as time passes if all the components have the same phase velocity.

Let’s define the shift in space of the packet in time $\Delta t$ as

$$\Delta x = \frac{d\omega}{dk} \Delta t$$

Velocity of wavepacket: $\Delta x = \frac{d\omega}{dk} \Delta t$ \hspace{1cm} \therefore \hspace{1cm} V_{\text{group}} = \frac{\Delta x}{\Delta t} = \frac{d\omega}{dk}$ (16)
where $V_{\text{group}}$ is the group velocity, the velocity the packet moves at, not the velocity of the individual phases. It represents the velocity of the particle.

If the phase velocities are constant and the group velocity equals the phase velocity the packet moves with out changing shape, we call this “no dispersion”. However, if the phase velocity differs we can get packet distortion and dispersion of the packet.

Dispersion is a very important phenomenon present in several types of wave propagation. In particular, it appears in the case of EM waves propagating through matter (Optical fibers).
Compare:

For a free electron we have \( \frac{\hbar^2 k^2}{2m} = \hbar \omega = E \)

\[
\therefore \omega = \frac{\hbar k^2}{2m} \quad \text{so} \quad \frac{d\omega}{dk} = \frac{\hbar k}{m} = \sqrt{\frac{2E}{M}} \tag{17}
\]

Using Classical Physics:

\[
E = \frac{mv^2}{2} \quad \therefore v = \sqrt{\frac{2E}{M}}
\]

and we find that the energy carried at group velocity is analogous to the kinetic energy of the particle at same velocity.