ELEC4705 – Fall 2009

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LECTURE 4
Wave Packets

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4.1. Comparison between QM and Classical Electrons

First we shall briefly review a comparsion between Classical and QM behaviour of electrons. Table 1 briefly compares the electron behavior in QM and classical physics.

Classical physics	Quantum mechanics
electron is a point particle	electron is assumed be to be a wave
motion is described by Newton laws: • $F = ma$ • $F = -\nabla V(r)$ • $V(r)$ is the potential energy	motion is described by the Schrodinger. • $\frac{-\hbar^2}{2m}\nabla^2\Psi + V\Psi = E\Psi$ • $\Psi(r,t) = \Psi(r)e^{-jwt}$ • $E = \hbar w$ • $V(r)$ is the potential energy
• $p = mv$ • $E = \frac{1}{2}mv^2$	• $p = \hbar k$ • $E = \hbar w$
	$\Psi \cdot \Psi^*$ is the probability density of finding an electron at position r
for free electrons we have $F = 0$ which means $V(r) = cont.$	for free electrons we have $V(r) = 0$

Table 1. Comparison between electron behavior in QM and Classical Physics

4.2. Wavepackets and localized electrons

Solving the Schrodinger equation for free electrons ($V(r) = 0$) we will have the solution as:

$$\Psi(r,t) = Ce^{j(k\cdot r - wt)} \quad \textbf{traveling plane wave} \tag{4.1}$$

$$\Psi(r,t)\Psi^*(r,t) = C^2 \quad \textbf{electron is everywhere} \tag{4.2}$$

We see that this solution doesn't say anything about the position of the electrons. Classically, we know that electrons are localized, if we measure the position of an electron we will see it follows a general trajectory.

To deal with this problem we will try to represent a localized electron as a wave pulse or wavepacket which is a pulse (or packet) of probability of the electron existing at a given location.

Definition of a wave packet: A wave packet is an envelope of a wave action that travels as an unit and consists of an infinite set of waves with different wave numbers (See Figure 1).

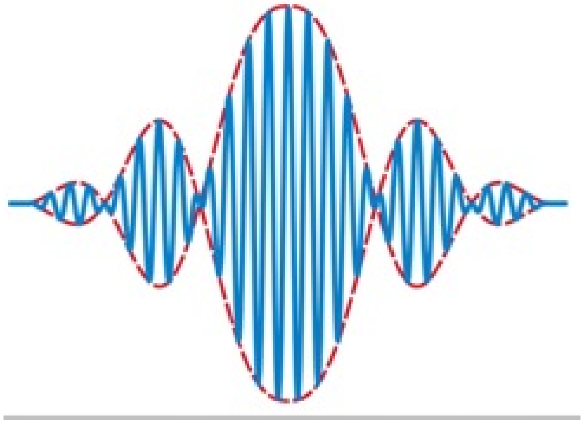

Figure 1. wavepacket, envelope

When we deal with a wave packet we need to consider two different types of phenomena:

- **Particle behavior:** The case when we study the packet as a whole.
- **Wave behavior:** The the case when we study the individual frequencies (or phases) of the wavepacket.

From Fourier transform concepts, the wavepacket can be represented as a superposition of wave with different k's (the spatial frequency). We can form wave packet just like forming a voltage pulse from temporal (time) frequency (w or f) components. A Fourier Transform can be defined in time and a localized (in time) packet would be created using a frequency spectrum given by,

$$g(w) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) e^{-jwt} dt \qquad (4.3)$$

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(w) e^{jwt} dw \qquad (4.4)$$

In the time independent QM it is useful to represent the wave function is a Fourier transform with respect to space as follows:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(k) e^{j(kx-wt)} dk \tag{4.5}$$

$$\psi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-jkx} dx \tag{4.6}$$

The spatial frequencies are referred to their wavenumber k which is given by $k = 2\pi f / v_{phase}$ where v_{phase} is the velocity of each frequency component.

$\Psi(k)$ is the spatial frequency spectrum of $\psi(x)$. A *k spectrum* will produce a spatially localized wave *packet*, see figure 2

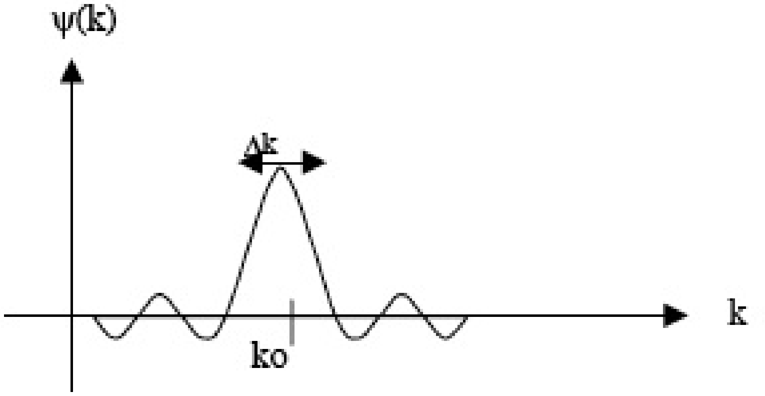

Figure 2. k spectrum

where

$k_0 = \frac{2\pi}{\lambda_0}$: average spatial frequency of the wave packet
Δk : packet size in space
x_0 : position of the packet
Δx : packet size

Note that according to equations 4.5 and 4.6 we have two distributions of Ψ – one in space and one in the frequency domain k. Often in QM each spatial frequency can be attributed with a component of the particles momentum p, where $p = \hbar k$. Under these conditions the frequency domain is often called the momentum space. The two distributions of Ψ basically reveal to us that if we measure the distribution of the electrons momentum and position in space we will only obtain the probability of the electron being at a particular place or velocity.

Notes and conclusions from Fourier Math:

- The more tightly confined the wavepacket is in x, the broader the spread in k, and vice-versa. For example to have a voltage pulse with small rise time we need to have high frequency components in voltage.
$$\Delta k \cdot \Delta x \geq 2\pi \tag{4.7}$$
- From above we have:
$$\frac{\Delta p}{\hbar} \cdot \Delta x \geq 2\pi \Longrightarrow \Delta x \cdot \Delta p \geq h \tag{4.8}$$
which is the uncertainty principle.
- Figure 3 shows the formation of a sequence wave packets by superposition of two different waves with slightly different frequencies.

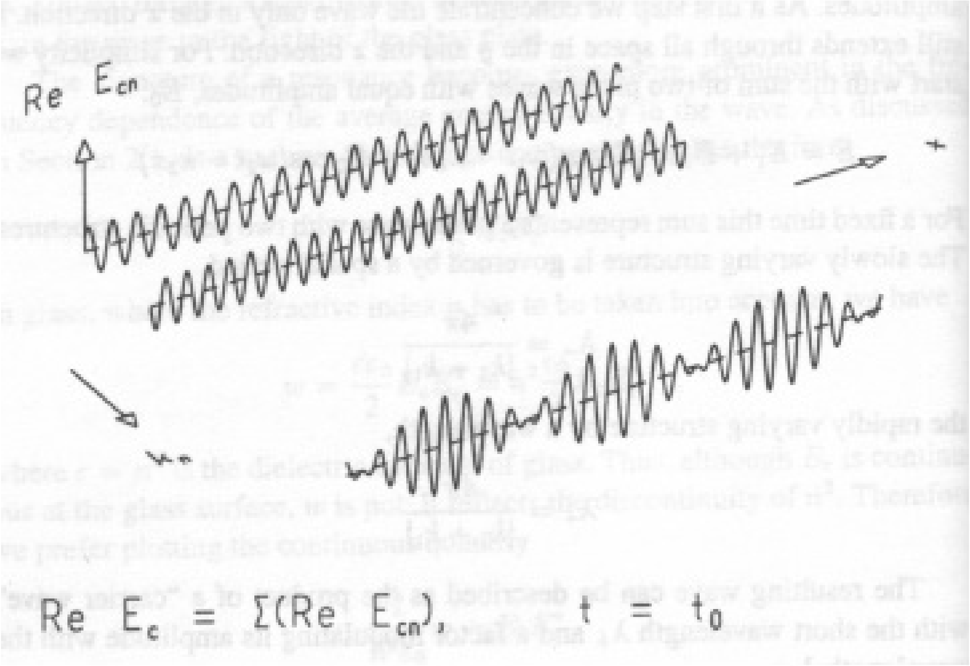

Figure 3. Superposition of the waves to build a sequence of wave packets

- As the number of waves increases, the wave packet becomes more localized in space, see figure 4.

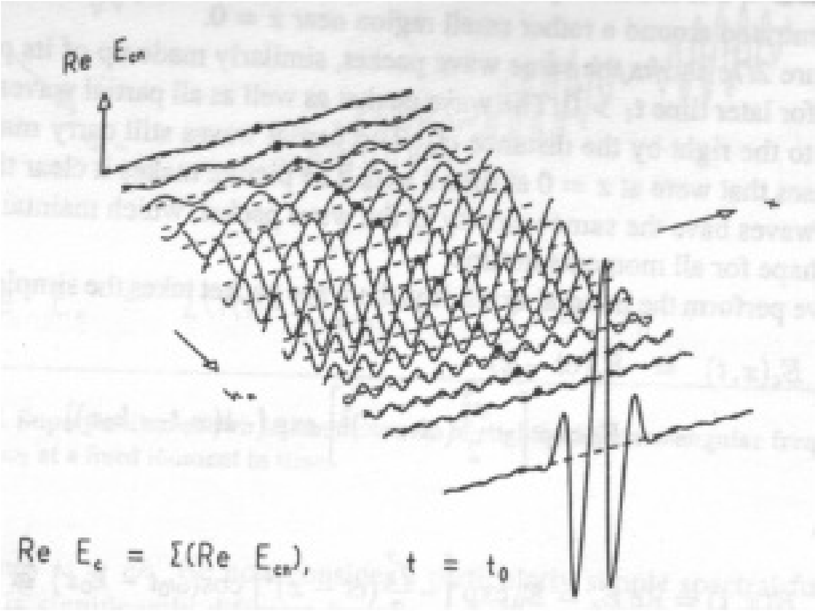

Figure 4. relation between the number of waves and the localization of the constructed wave packet

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- If all the components have the same phase velocity the shape of the wave packet will not change it as time passes.

4.3. Group velocity and the wave packet shift in space

We define the shift in space of the packet in time Δt as:

$$\Delta x = \frac{\partial w}{\partial k}\Delta t \tag{4.9}$$

So for the group velocity we will have:

$$\Delta x = \frac{dw}{dk}\Delta t \quad \Longrightarrow \quad v_{group} = \frac{\Delta x}{\Delta k} = \frac{dw}{dk} \tag{4.10}$$

Note that v_{group} is the velocity of the wave packet not the velocity of individual phases (the phase velocity). If the phase velocities are constant and equal to the group velocity, then the wave packet will move without changing shape, we call refer to this as being *no dispersion*, otherwise we will have wave packet distortion, see figure 6

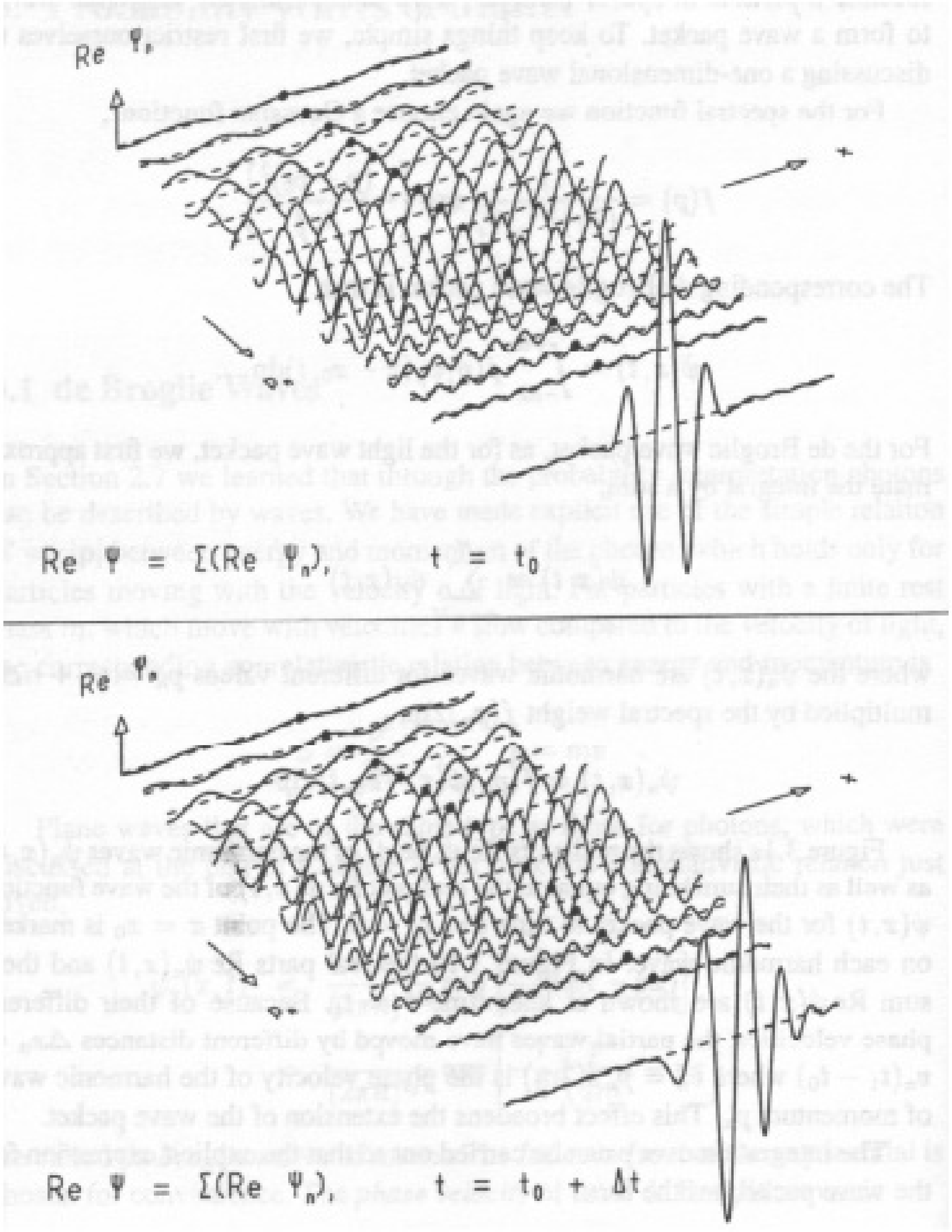

Figure 5. Top figure initial packet at t_0. Bottom figure packet after propagation for time of Δt. Second figure shows distortion of the wave packet

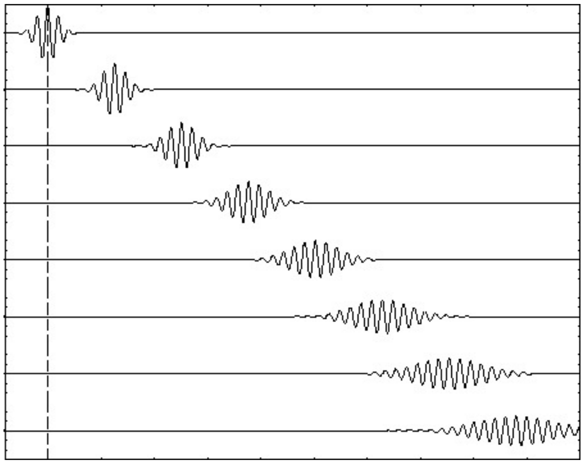

Figure 6. Wave packet during propagation showing dispersion.

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).

Example 1. Find the group velocity for free electrons.

For free electrons we have

$$\begin{aligned} E &= \hbar w = \frac{\hbar^2 k^2}{2m} \\ w &= \frac{\hbar k^2}{2m} \\ v_{group} &= \frac{dw}{dk} = \frac{\hbar k}{m} \end{aligned} \tag{4.11}$$

Using Classical Physics we have:

$$E = \frac{1}{2} m v_{group}^2 \Longrightarrow v_{group} = \sqrt{\frac{2E}{M}} \tag{4.12}$$

It is concluded that the energy carried at group velocity is analogous to the kinetic energy of the particle at same velocity.

4.4. Gaussian Wave Packet

Back to equations 4.5 and 4.6, we can use a Guassian electron probability distribution for Ψ, see figure 7. The Gaussian wave packet produces a well-localized particle and mathematically is easy to deal with. It is a good idealized model of a QM electron.

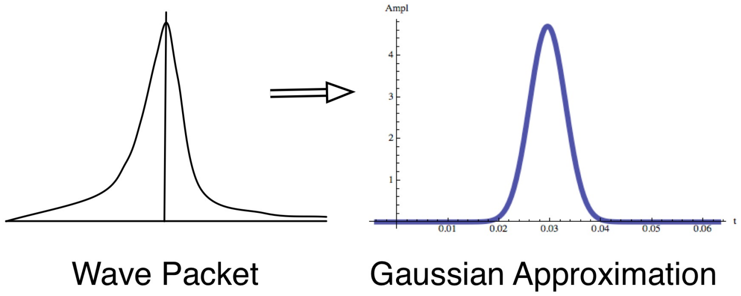

Figure 7. Guassian approximation of a wave packet.

For a Gaussian wave packet we assume ψ to be defined in space domain as

$$\psi(x) = e^{-x^2/2(\Delta x)^2} \tag{4.13}$$

which is a Gaussian distribution centered at $x = 0$ with a width Δx. Then for k domain we will have

$$\psi(k) = \int_{-\infty}^{\infty} \psi(x) e^{-jkx} dx = \int_{-\infty}^{\infty} e^{-x^2/2(\Delta x)^2} e^{-jkx} dx \tag{4.14}$$

from there we have

$$\psi(k) \propto e^{\frac{k^2}{2(\Delta x)^2}} \tag{4.15}$$

where

$$\hbar k = p \qquad \Delta k = 1/\Delta x \qquad \Delta p = \hbar/\Delta x \tag{4.16}$$

It is illustrated in figure 8. According to equations in 4.16 for smaller Δx we will get larger Δk in special case for $\psi(x) = \Delta(x)$, $\psi(p)$ will be flat (constant) as shown in figure 9.

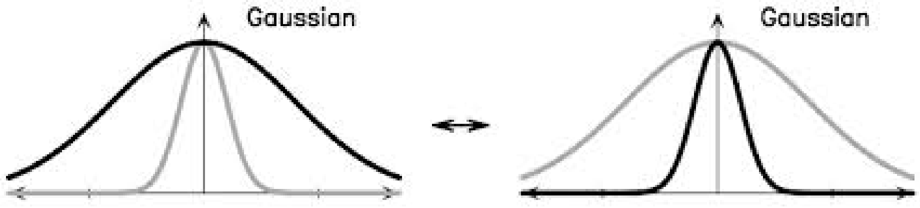

Figure 8. Gaussian distributions in x and p domain using the transform to go between the two “spaces”.

What does this mean? Well if we know the position of the electron very well then we do not know the momentum of the electron very precisely. On the other hand if we know the momentum (velocity $p =$

Figure 9. Gaussian distributions for delta function

mv) of the electron well then the position of the electron is not very well defined. This relationship is known as the uncertainty law and using the assumption of a Gaussian we find that we can define a product.

$$\Delta k = 1/\Delta x \tag{4.17}$$

$$\Delta p = \hbar/\Delta x \tag{4.18}$$

$$\Delta x \cdot \Delta p \approx h \tag{4.19}$$

Which indicates the magnitude of this uncertainty.

This is the uncertainty principle it predicts a limit on the knowability of position and velocity of QM objects.

As we said before the electron can be defined to have two velocities a group and phase velocity (just like an electromagnetic pulse in a wire). The phase velocity is associated with a particular frequency component of the electron and is the velocity of a monochromatic wave, and in free space is

$$V_{phase} = f\lambda = \omega/k \tag{4.20}$$

The group velocity is the velocity of the electron i.e. the center of the distribution function or packet. Just as in an electromagnetic pulse along a wire or down a fiber the group velocity is different from the phase velocity. If there is not a linear relationship between ω and k it can be found that the group velocity of a wave is (as we defined it before),

$$V_{group} = \frac{\partial \omega}{\partial k} \tag{4.21}$$

For a single matter wave component we have (See solution of SE for a free electron):

$$\begin{aligned} E &= p^2 = mv^2 && (4.22) \\ E &= \hbar^2 k^2/2m && (4.23) \\ E &= \hbar\omega = k^2/2m && (4.24) \end{aligned}$$

$$\omega = \frac{\hbar k^2}{2m} \Rightarrow \omega \propto k^2 \textbf{(nonlinear, dispersion)} \qquad (4.25)$$

$$\begin{aligned} V_{phase} &= \omega k = \hbar k/2m && (4.26) \\ V_{group} &= \hbar k/m && (4.27) \end{aligned}$$

The phase velocity of the matter wave is one half the group velocity!

The group velocity ($V_{group)}$) does not equal phase velocity (V_{phase}) and the wave packet exhibits dispersion.

Remember however that the group velocity equals the electrons velocity.

$$V_{group} = \frac{\partial\omega}{\partial k} = \frac{\hbar}{\hbar}\frac{\partial E}{\partial p} = \frac{p}{m} \qquad (4.28)$$

Ah! the group velocity is equal to the classical velocity $v = p/m$. That makes sense.

As a comparison, consider an equivalent EM wave in vacuum (this is the wave equation introduced in lecture 2).

$$\frac{1}{\mu_0\epsilon_0}\nabla^2\vec{E} = \frac{\partial^2\vec{E}}{\partial^2 t} \textbf{ where } \vec{E}\textbf{- electric field variable} \qquad (4.29)$$

Consider 1-D only $E = (Ex, 0, 0)$, and $E_x = E_x e^{j(kx-\omega t)}$ (EM wave moving in x direction). The terms in the wave equation reduce to,

$$\begin{aligned} \frac{\partial^2\vec{E}}{\partial x^2} &= -k^2 E_x && (4.30) \\ \frac{\partial^2\vec{E}}{\partial t^2} &= -\omega^2 E_x && (4.31) \\ & && (4.32) \end{aligned}$$

so substituting in the above equation we have

$$\frac{k^2}{\mu_0\epsilon_0}E_x = \omega^2 E_x \qquad (4.33)$$

or

$$\begin{aligned}
\omega &= \frac{k}{\sqrt{\mu_0 \epsilon_0}} \qquad (4.34) \\
&\Rightarrow \omega \propto k \textbf{(linear relationship − no dispersion)} \\
V_{group} &= \frac{\partial \omega}{\partial k} = \frac{1}{\mu_0 \epsilon_0} = C \textbf{ speed of light} \qquad (4.35) \\
V_{phase} &= \frac{\omega}{k} = \frac{1}{\mu_0 \epsilon_0} = C \textbf{ - speed of light} \qquad (4.36)
\end{aligned}$$

for an EM wave in vacuum, $V_{phase} = V_{group}$ no dispersion and we can say that a light wave packet (photon) in free space will not exhibit dispersion.