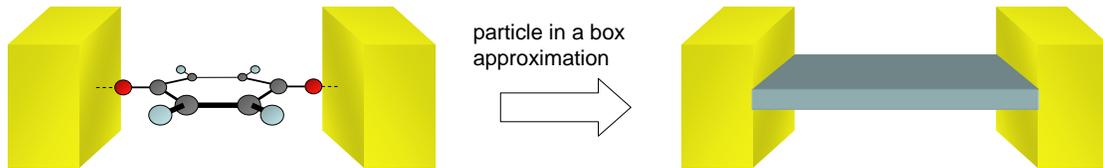


## Part 1. The Quantum Particle

This class is concerned with the propagation of electrons in conductors.

Here in Part 1, we will begin by introducing the tools from quantum mechanics that we will need to describe electrons. We will introduce probabilistic descriptions of the key physical properties: position, momentum, time and energy. In the next part we will consider electrons in the simplest possible model of a conductor – a box – *i.e.* we will ignore atoms and assume that the material is perfectly homogeneous.

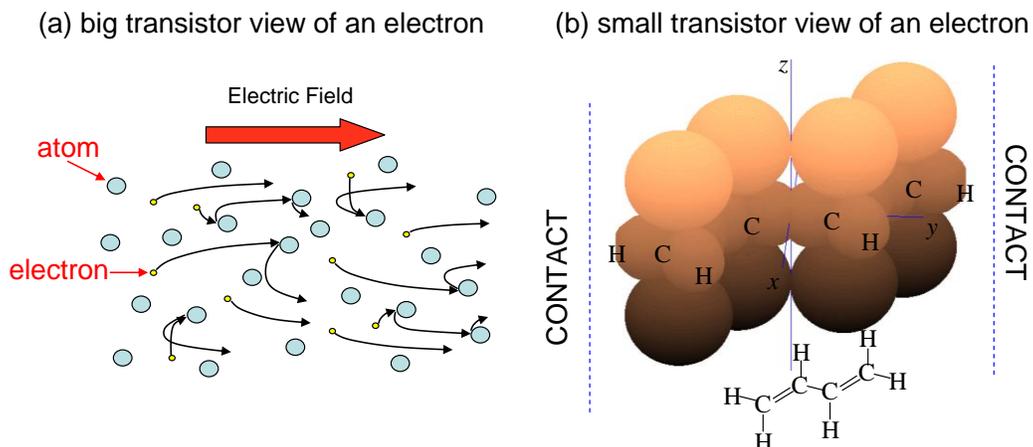


**Fig. 1.1.** The ‘particle in a box’ takes a complex structure like a molecule and approximates it by a homogeneous box. All details, such as atoms, are ignored.

This model of electrons in conductors is known as ‘the particle in a box’. It is surprisingly useful, and later in the class we will employ it to describe the behavior of modern transistors.

But first we will need a way to describe electrons. It is often convenient to imagine electrons as little projectiles pushed around by an electric field. And in many cases, this classical model yields a fairly accurate description of electronic devices.

But not always. In nanoscale devices especially, electrons are better described as waves.

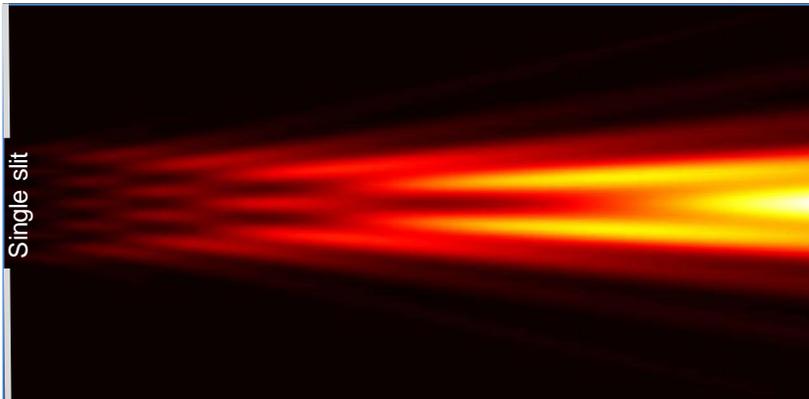


**Fig. 1.2.** Two representations of electrons in a solid. In **(a)** the electrons are represented as hard little spheres, propelled by the electric field, and bouncing off atoms. In **(b)** we draw an approximate representation of the molecule 1,3-butadiene positioned between contacts. Now the electrons are represented by probability clouds.

# Part 1. The Quantum Particle

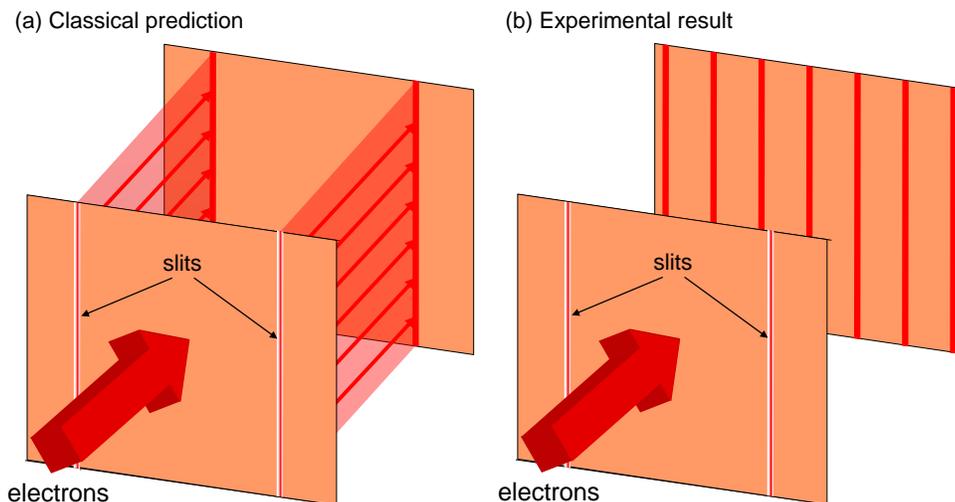
## Waves in electronics

Consider a beam of electrons propagating through a small hole - a very crude model for electrons moving from a contact into a nanoscale conductor. We might expect that the electrons would continue in straight lines after passing through the hole. But if the hole is small enough (the dimensions of a nanoscale transistor, for example), then the electrons are observed to diffract. This clearly demonstrates that we must consider the wave properties of electrons in nanoelectronic devices.



**Fig. 1.3.** A simulation of electron diffraction through a single slit. This experiment is analyzed in Problem 1.

The diffraction pattern shown above is obtained by assuming each point inside the single slit is a source of expanding waves; see Problem 1. An easier example to analyze is the double slit experiment, in which we assume there are only two sources of expanding waves. Like the single slit example, the result of a double slit experiment is consistent with electrons behaving like waves.



**Fig. 1.4.** Classically, we would predict that electrons passing through slits in a screen should continue in straight lines, forming an exact image of the slits on the rear screen. In practice, however, a series of lines is formed on the rear screen, suggesting that the electrons have been somehow deflected by the slits.

## Review of Classical Waves

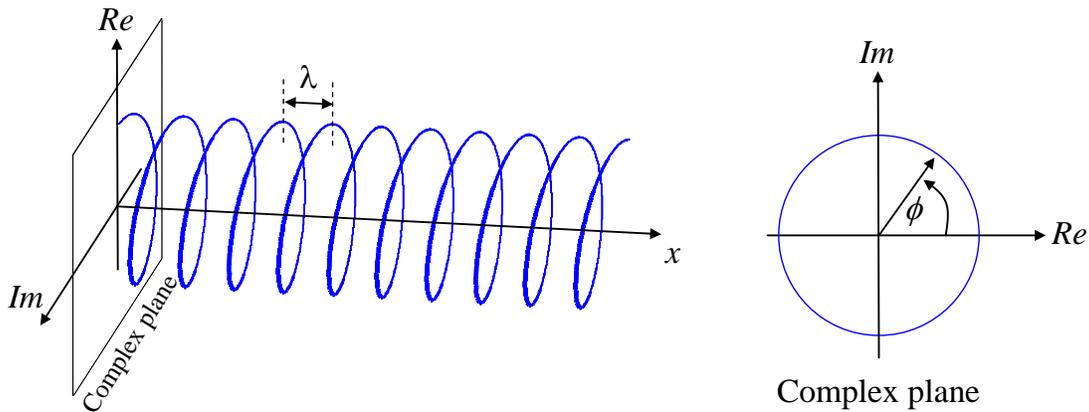
A wave is a periodic oscillation. It is convenient to describe waves using complex numbers. For example consider the function

$$\psi(x) = e^{ik_0x} \quad (1.1)$$

where  $x$  is position, and  $k_0$  is a constant known as the wavenumber. This function is plotted in Fig. 1.5 on the complex plane as a function of position,  $x$ . The phase of the function

$$\phi = k_0x \quad (1.2)$$

is the angle on the complex plane.



**Fig. 1.5.** A standing wave with its phase plotted on the complex plane.

The wavelength is defined as the distance between spatial repetitions of the oscillation. This corresponds to a phase change of  $2\pi$ . From Eqns. (1.1) and (1.2) we get

$$k_0 = \frac{2\pi}{\lambda} \quad (1.3)$$

This wave is independent of time, and is known as a standing wave. But we could define a function whose phase varies with time:

$$\psi(t) = e^{-i\omega_0 t} \quad (1.4)$$

Here  $t$  is time, and  $\omega$  is the angular frequency. We define the period,  $T$ , as the time between repetitions of the oscillation

$$\omega_0 = \frac{2\pi}{T}. \quad (1.5)$$

## Plane waves

We can combine time and spatial phase oscillations to make a traveling wave. For example

$$\psi(x, t) = e^{i(k_0x - \omega_0 t)} \quad (1.6)$$

## Part 1. The Quantum Particle

We define the intensity of the wave as

$$|\psi|^2 = \psi^* \psi \quad (1.7)$$

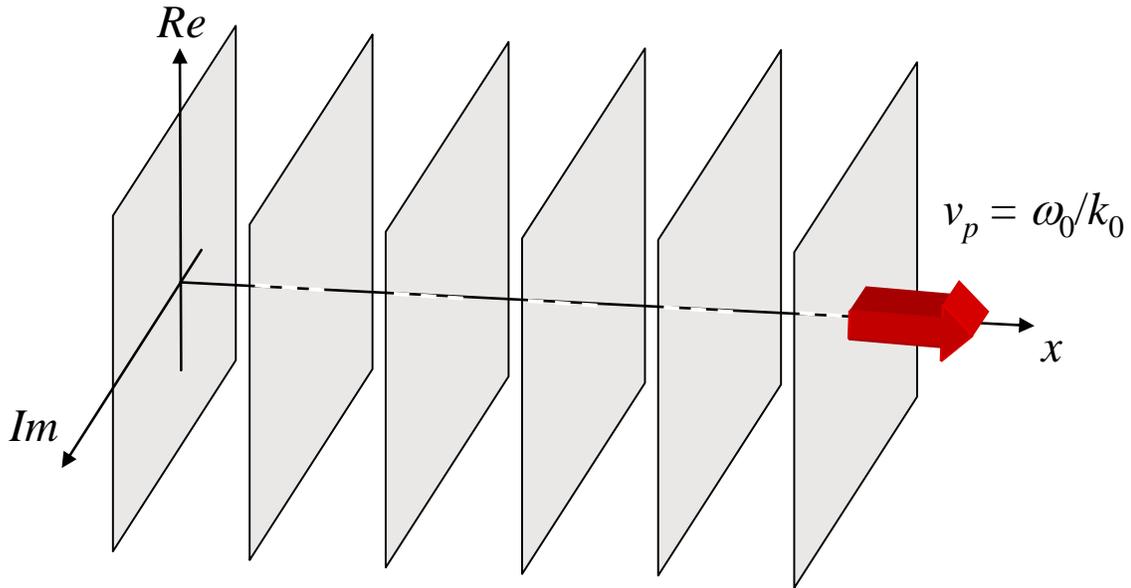
Where  $\psi^*$  is the complex conjugate of  $\psi$ . Since the intensity of this wave is uniform everywhere  $|\psi|^2 = 1$  it is known as a *plane wave*.

A plane wave has at least four dimensions (real amplitude, imaginary amplitude,  $x$ , and  $t$ ) so it is not so easy to plot. Instead, in Fig. 1.6 we plot planes of a given phase. These planes move through space at the phase velocity,  $v_p$ , of the wave. For example, consider the plane corresponding to  $\phi = 0$ .

$$k_0 x - \omega_0 t = 0 \quad (1.8)$$

Now,

$$v_p = \frac{dx}{dt} = \frac{\omega_0}{k_0} \quad (1.9)$$



**Fig. 1.6.** In a plane wave planes of constant phase move through space at the phase velocity.

### The double slit experiment

We now have the tools to model the double slit experiment described above. Far from the double slit, the electrons emanating from each slit look like plane waves; see Fig. 1.7, where  $s$  is the separation between the slits and  $L$  is the distance to the viewing screen.

At the viewing screen we have

$$\psi(x=L, t) = A \exp[i(k_0 r_1 - \omega_0 t)] + A \exp[i(k_0 r_2 - \omega_0 t)] \quad (1.10)$$

The intensity at the screen is

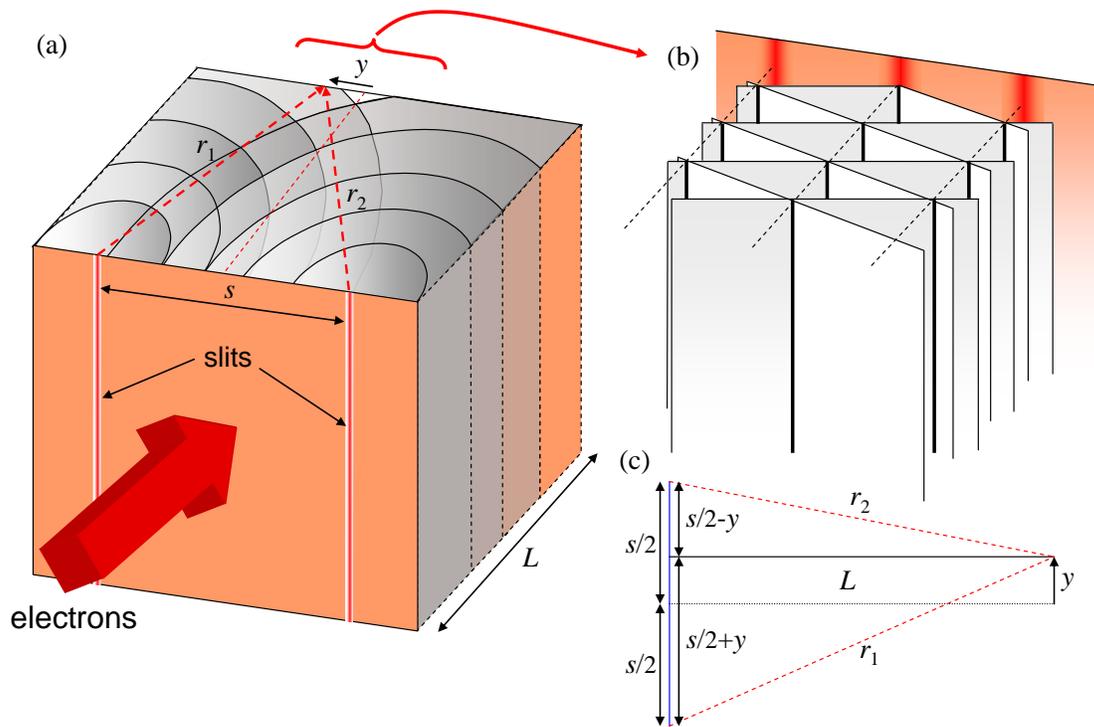
$$\begin{aligned}
 |\psi|^2 &= \left\{ A \exp[-i\omega_0 t] (\exp[ik_0 r_1] + \exp[ik_0 r_2]) \right\} \left\{ A \exp[-i\omega_0 t] (\exp[ik_0 r_1] + \exp[ik_0 r_2]) \right\}^* \\
 &= |A|^2 + |A|^2 \exp[i(k_0 r_2 - k_0 r_1)] + |A|^2 \exp[i(k_0 r_1 - k_0 r_2)] + |A|^2 \\
 &= 2|A|^2 (1 + \cos(k(r_2 - r_1)))
 \end{aligned} \tag{1.11}$$

where  $A$  is a constant determined by the intensity of the electron wave. Now from Fig. 1.7:

$$\begin{aligned}
 r_1^2 &= L^2 + (s/2 - y)^2 \\
 r_2^2 &= L^2 + (s/2 + y)^2
 \end{aligned} \tag{1.12}$$

Now, if  $y \ll s/2$  we can neglect the  $y^2$  term:

$$\begin{aligned}
 r_1^2 &\approx L^2 + (s/2)^2 - sy \\
 r_2^2 &\approx L^2 + (s/2)^2 + sy
 \end{aligned} \tag{1.13}$$



**Fig. 1.7.** Far from the double slit, the electrons from each slit can be described by plane waves. Where the planes of constant phase collide, a bright line corresponding to a high intensity of electrons is observed.

## Part 1. The Quantum Particle

Then,

$$\begin{aligned} r_1 &\approx \sqrt{L^2 + (s/2)^2} \left( 1 - \frac{1}{2} \frac{sy}{L^2 + (s/2)^2} \right) \\ r_2 &\approx \sqrt{L^2 + (s/2)^2} \left( 1 + \frac{1}{2} \frac{sy}{L^2 + (s/2)^2} \right) \end{aligned} \quad (1.14)$$

Next, if  $L \gg s/2$

$$\begin{aligned} r_1 &\approx L - \frac{1}{2} \frac{sy}{L} \\ r_2 &\approx L + \frac{1}{2} \frac{sy}{L} \end{aligned} \quad (1.15)$$

Thus,  $r_2 - r_1 = \frac{sy}{L}$ , and

$$|\psi|^2 = 2|A|^2 \left( 1 + \cos \left( ks \frac{y}{L} \right) \right) \quad (1.16)$$

At the screen, *constructive* interference between the plane waves from each slit yields a regular array of bright lines, corresponding to a high intensity of electrons. In between each pair of bright lines, is a dark band where the plane waves interfere *destructively*, i.e. the waves are  $\pi$  radians out of phase with one another.

The spacing between the bright lines at the viewing screen is

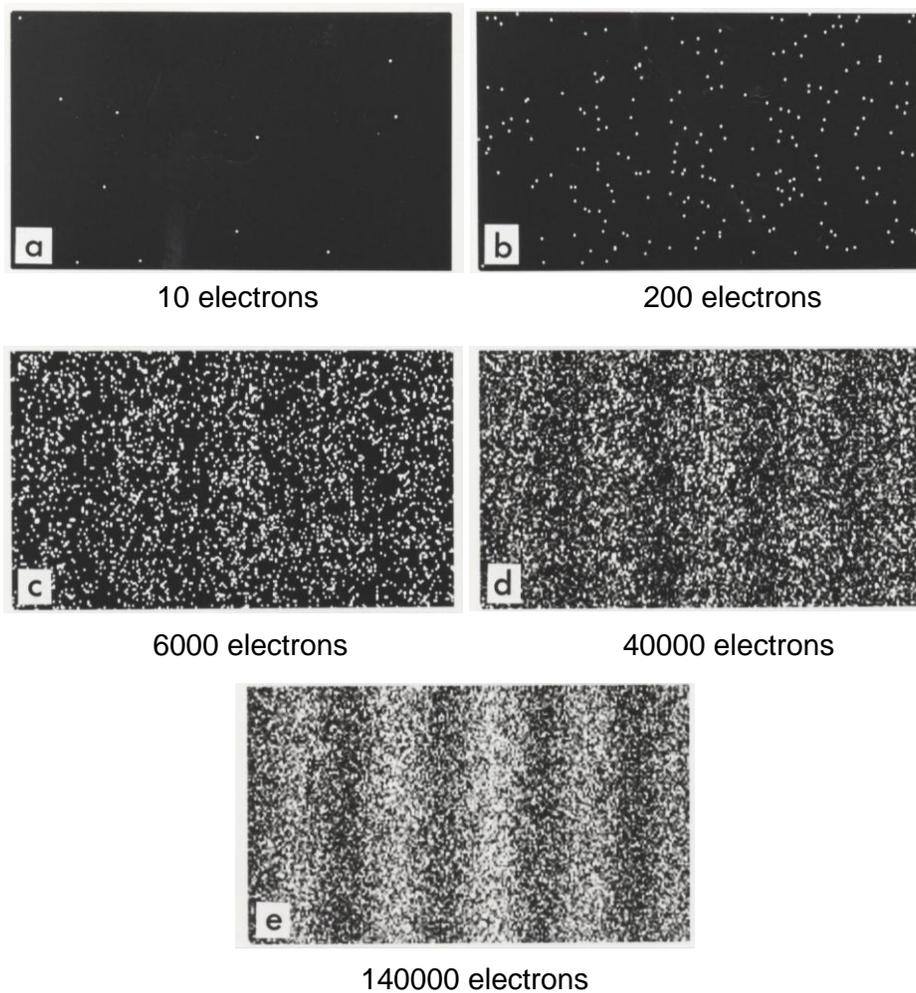
$$\frac{2\pi}{\lambda} s \frac{y}{L} = 2\pi \quad (1.17)$$

Rearranging,

$$y = \frac{L\lambda}{s} \quad (1.18)$$

## Interpretation of the double slit experiment

It is notable that the fringe pattern is independent of intensity. Thus, the interference effect should be observed even if just a single electron is fired at the slits at a time. For example, in Fig. 1.8 we show the buildup of the fringe pattern from consecutive electrons. The only conclusion is that the electron – which we are used to thinking of as a particle - also has wave properties.



**Fig. 1.8.** The cumulative electron distribution after passage through a double slit. Just a single electron is present in the apparatus at any time. From A. Tanamura, *et al.* *Am. J. Physics* **57**, 117 (1989).

# Part 1. The Quantum Particle

## The Wavefunction

The wave-like properties of electrons are an example of the ‘wave-particle duality’. Indeed, in the early 20<sup>th</sup> century, quantum mechanics revealed that a combination of wave and particle properties is a general property of everything at the size scale of an electron.

Without addressing the broader implications of this unusual observation, we will simply note that our purposes require a suitable mathematical description for the electron that can describe both its particle and wave-like properties. Following the conventions of quantum mechanics, we will define a function known as the wavefunction,  $\psi(x,t)$ , to describe the electron. It is typically a complex function and it has the important property that its magnitude squared is the probability density of the electron at a given position and time.

$$P(x,t) = |\psi(x,t)|^2 = \psi^*(x,t)\psi(x,t) \quad (1.19)$$

If the wavefunction is to describe a single electron, then the sum of its probability density over all space must be 1.

$$\int_{-\infty}^{+\infty} P(x,t) dx = 1 \quad (1.20)$$

In this case we say that the wavefunction is *normalized* such that the probability density sums to unity.

## Frequency domain and $k$ -space descriptions of waves

Consider the wavefunction

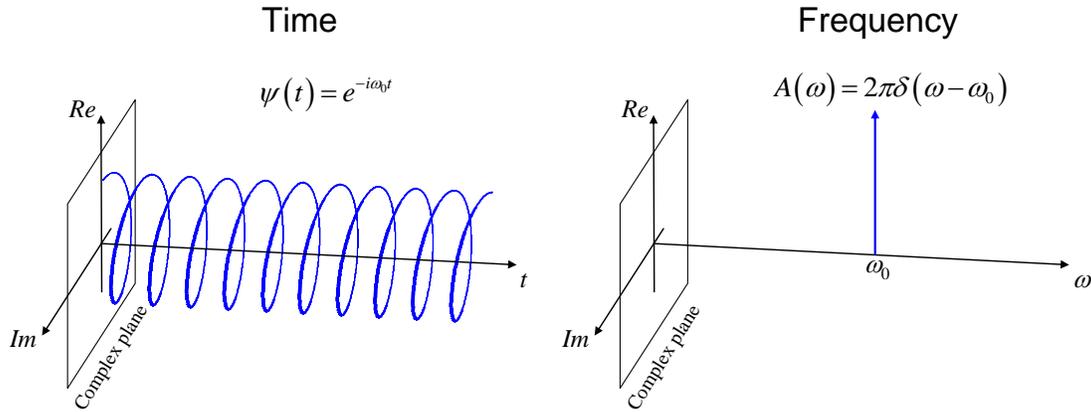
$$\psi(t) = a e^{-i\omega_0 t} \quad (1.21)$$

which describes a wave with amplitude  $a$ , intensity  $|a|^2$ , and phase oscillating in time at angular frequency  $\omega_0$ . This wave carries two pieces of information, its amplitude and angular frequency.<sup>†</sup> Describing the wave in terms of  $a$  and  $\omega_0$  is known as the frequency domain description. In Fig. 1.9, we plot the wavefunction in both the time and frequency domains.

In the frequency domain, the wavefunction is described by a delta function at  $\omega_0$ . Tools for the exact conversion between time and frequency domains will be presented in the next section. Note that, by convention we use a capitalized function ( $A$  instead of  $\psi$ ) to represent the wavefunction in the frequency domain. Note also that the convention in quantum mechanics is to use a negative sign in the phase when representing the angular frequency  $+\omega_0$ . This is convenient for describing plane waves of the form  $e^{i(kx - \omega t)}$ . But it is exactly opposite to the usual convention in signal analysis (i.e. 6.003). In general, when you see  $i$  instead of  $j$  for the square root of  $-1$ , use this convention in the time and frequency domains.

---

<sup>†</sup> Note the information in any constant phase offset,  $\phi$ , as in  $\psi = \exp[i\omega_0 t + i\phi]$  can be contained in the amplitude prefactor, i.e.  $\psi = a \exp[i\omega_0 t]$ , where  $a = \exp[i\phi]$ .

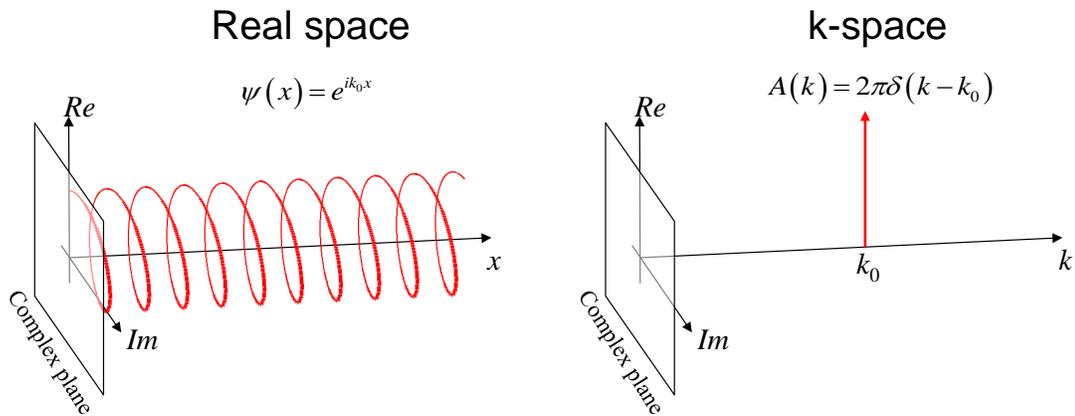


**Fig. 1.9.** Representations of the angular frequency  $\omega_0$  in time and frequency domains.

Similarly, consider the wavefunction

$$\psi(x) = a e^{ik_0 x} \quad (1.22)$$

which describes a wave with amplitude  $a$ , intensity  $|a|^2$ , and phase oscillating in *space* with spatial frequency or wavenumber,  $k_0$ . Again, this wave carries two pieces of information, its amplitude and wavenumber. We can describe this wave in terms of its spatial frequencies in *k-space*, the equivalent of the frequency domain for spatially oscillating waves. In Fig. 1.10, we plot the wavefunction in real space and k-space.



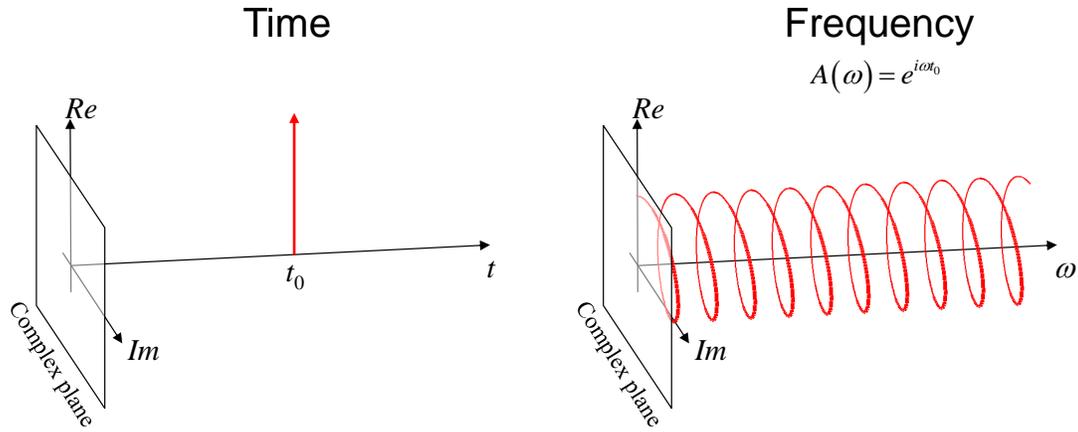
**Fig. 1.10.** Representations of wavenumber  $k_0$  in real space and k-space.

Next, let's consider the wavefunction

$$A(\omega) = a e^{i\omega t_0} \quad (1.23)$$

which describes a wave with amplitude  $a$ , intensity  $|a|^2$ , and phase oscillating in the frequency domain with period  $2\pi / t_0$ . This wave carries two pieces of information, its amplitude and the time  $t_0$ . In Fig. 1.11, we plot the wavefunction in both the time and frequency domains.

## Part 1. The Quantum Particle

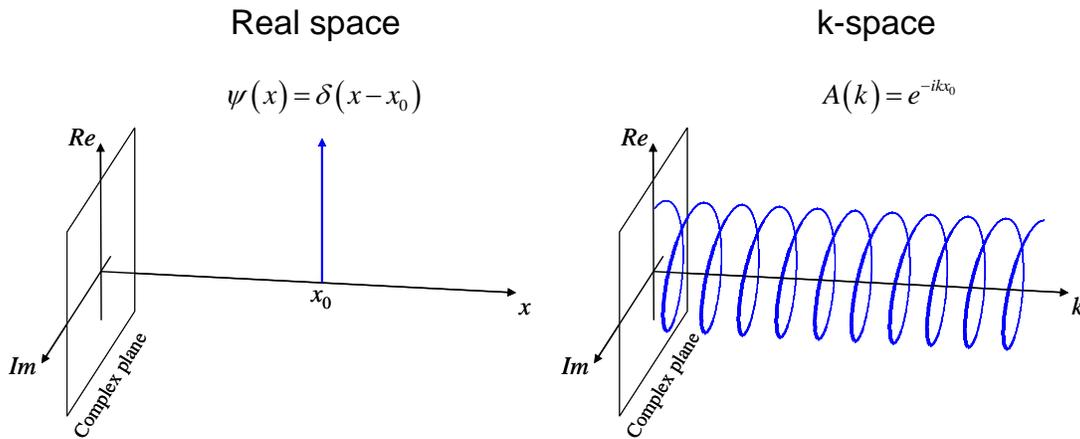


**Fig. 1.11.** Representations of time  $t_0$  in time and frequency domains.

Finally, consider the wavefunction

$$A(k) = a e^{-ikx_0} \quad (1.24)$$

which describes a wave with amplitude  $a$ , intensity  $|a|^2$ , and phase oscillating in  $k$ -space with period  $2\pi/x_0$ . This wave carries two pieces of information, its amplitude and the position  $x_0$ . In Fig. 1.12, we plot the wavefunction in both real space and  $k$ -space.



**Fig. 1.12.** Representations of position  $x_0$  in real space and  $k$ -space.

Note that, by convention we use a capitalized function ( $A$  instead of  $\psi$ ) to represent the wavefunction in the  $k$ -space domain.

Observe in Fig. 1.9-Fig. 1.12 that a precise definition of both the position in time and the angular frequency of a wave is impossible. A wavefunction with angular frequency of precisely  $\omega_0$  is uniformly distributed over all time. Similarly, a wavefunction associated with a precise time  $t_0$  contains all angular frequencies.

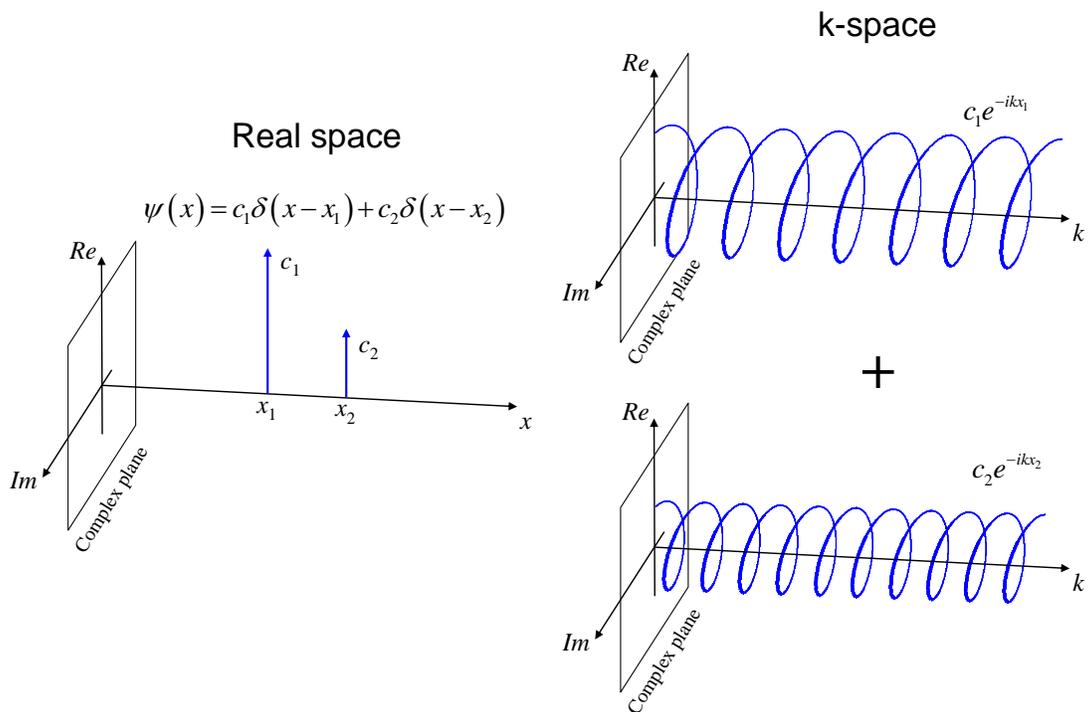
In real and  $k$ -space we also cannot precisely define both the wavenumber and the position. A wavefunction with a wavenumber of precisely  $k_0$  is uniformly distributed over

all space. Similarly, a wavefunction localized at a precise position  $x_0$  contains all wavenumbers.

## Linear combinations of waves

Next, we consider the combinations of different complex exponential functions. For example, in Fig. 1.13 we plot a wavefunction that could describe an electron that equiprobable at position  $x_1$  and position  $x_2$ . The  $k$ -space representation is simply the *superposition* of two complex exponential functions corresponding to  $x_1$  and  $x_2$ .<sup>†</sup>

$$\psi(x) = c_1\delta(x-x_1) + c_2\delta(x-x_2) \Leftrightarrow A(k) = c_1e^{-ikx_1} + c_2e^{-ikx_2} \quad (1.25)$$



**Fig. 1.13.** The  $k$ -space wavefunction corresponding to two positions  $x_1$  and  $x_2$  is simply the superposition of the  $k$ -space representations of  $\delta(x-x_1)$  and  $\delta(x-x_2)$ .

We can also generalize to an arbitrary distribution of positions,  $\psi(x)$ . If  $\psi(x)$  describes an electron, for example, the probability that the electron is located at position  $x$  is  $|\psi(x)|^2$ . Thus, in  $k$ -space the electron is described by the sum of complex exponentials  $e^{-ikx}$  each oscillating in  $k$ -space and weighted by amplitude  $\psi(x)$ .

$$A(k) = \int_{-\infty}^{+\infty} \psi(x) e^{-ikx} dx \quad (1.26)$$

You may recognize this from 6.003 as a Fourier transform. Similarly, the inverse transform is

<sup>†</sup> Note that this wave function is not actually normalizable.

## Part 1. The Quantum Particle

$$\psi(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} A(k) e^{ikx} dk. \quad (1.27)$$

To convert between time and angular frequency, use

$$A(\omega) = \int_{-\infty}^{+\infty} \psi(t) e^{i\omega t} dt \quad (1.28)$$

and

$$\psi(t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} A(\omega) e^{-i\omega t} d\omega. \quad (1.29)$$

Note that the factors of  $1/2\pi$  are present each time you integrate with respect to  $k$  or  $\omega$ . Note also that when converting between complex exponentials and delta functions, the following identity is useful:

$$2\pi\delta(u) = \int_{-\infty}^{+\infty} \exp[iux] dx. \quad (1.30)$$

### Wave packets and uncertainty

We now have two ways to describe an electron. We could describe it as a plane wave, with precisely defined wavenumber and angular frequency:

$$\psi(x, t) = e^{i(k_0x - \omega_0t)}. \quad (1.31)$$

But as we have seen, the intensity/probability density of the plane wave is uniform over all space (and all time). Thus, the position of the electron is perfectly uncertain – its probability distribution is uniform everywhere in the entire universe. Consequently, a plane wave is not usually a good description for an electron.

On the other hand, we could describe the electron as an idealized point particle

$$\psi(x, t) = \delta(x - x_0, t - t_0) \quad (1.32)$$

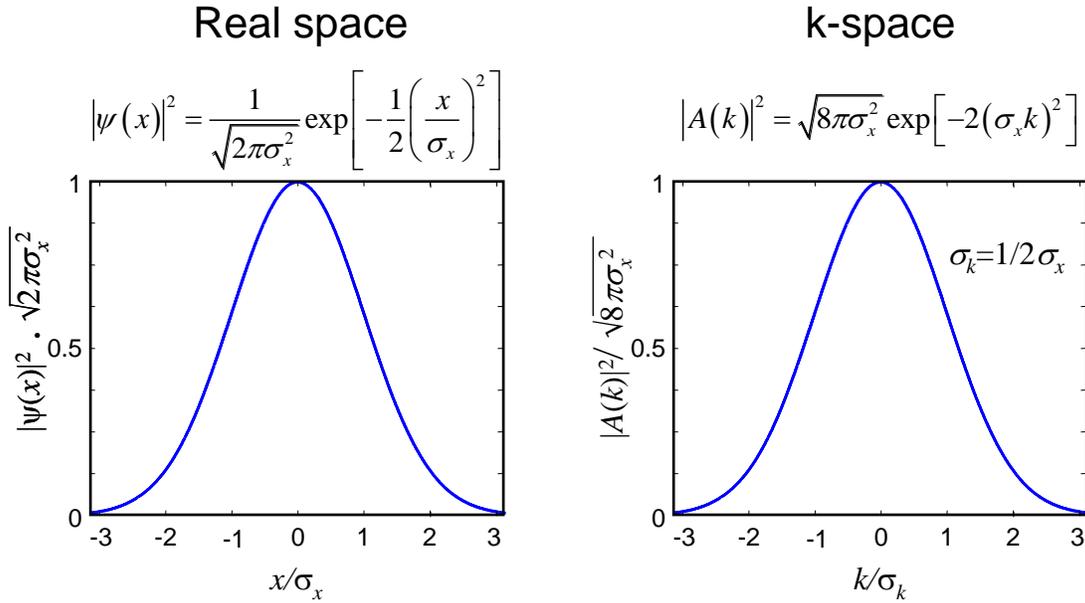
existing at a precisely defined position and time. But the probability density of the point particle is uniform over all of  $k$ -space and the frequency domain. We will see in the next section that this means the energy and momentum of the electron is perfectly uncertain, i.e. arbitrarily large electron energies and momenta are possible.

The only alternative is to accept an imprecise description of the electron in both real space and  $k$ -space, time and the frequency domain. A localized oscillation in both representations is called a *wave packet*. A common wavepacket shape is the Gaussian.

For example, instead of the delta function, we could describe the electron's position as

$$\psi(x) = a \exp\left[-\frac{1}{4}\left(\frac{x}{\sigma_x}\right)^2\right]. \quad (1.33)$$

This function was chosen such that the probability distribution of the electron is



**Fig. 1.14.** A normalized Gaussian. The Gaussian has the same shape in real space and  $k$ -space. Note that a Gaussian approximates a delta function in the limit  $\sigma_x \rightarrow 0$ .

$$|\psi(x)|^2 = |a|^2 \exp\left[-\frac{1}{2}\left(\frac{x}{\sigma_x}\right)^2\right] \quad (1.34)$$

where  $\sigma_x$  is the standard deviation.  $\sigma_x$  measures the width of the Gaussian and is often thought of as the *uncertainty* in the position of the electron. The constant,  $a$ , is determined by normalizing the probability density over all space, i.e., integrating Eq. (1.34) over  $x$ , we get

$$a = (2\pi\sigma_x^2)^{-1/4} \quad (1.35)$$

Strictly, the uncertainty of a given quantity is defined by

$$\begin{aligned} \sigma^2 &= \langle (x - \langle x \rangle)^2 \rangle \\ &= \langle x^2 - 2x\langle x \rangle + \langle x \rangle^2 \rangle \end{aligned} \quad (1.36)$$

where  $\langle x \rangle$  signifies the average or expectation value of  $x$ . Because  $\langle x \rangle$  is a constant Eq. (1.36) may be simplified:

$$\begin{aligned} \sigma^2 &= \langle x^2 \rangle - 2\langle x \rangle \langle x \rangle + \langle x \rangle^2 \\ &= \langle x^2 \rangle - \langle x \rangle^2 \end{aligned} \quad (1.37)$$

We will leave it as an exercise to show that for the Gaussian probability density:

$$\sigma^2 = \int x^2 |\psi(x)|^2 dx = \sigma_x^2 \quad (1.38)$$

## Part 1. The Quantum Particle

Thus, the Gaussian is a convenient choice to describe a wavepacket because it has a readily defined uncertainty.

In  $k$ -space, the electron is also described by a Gaussian (this is another of the convenient properties of this function). Application of the Fourier transform in Eq. (1.26) and some algebra gives

$$A(k) = (8\pi\sigma_x^2)^{1/4} \exp[-\sigma_x^2 k^2] \quad (1.39)$$

The probability distribution in  $k$ -space is

$$|A(k)|^2 = (8\pi\sigma_x^2)^{1/2} \exp[-2\sigma_x^2 k^2] \quad (1.40)$$

Thus, the uncertainty in  $k$ -space is

$$\frac{1}{2\sigma_k^2} \equiv 2\sigma_x^2 \quad (1.41)$$

The product of the uncertainties in real and  $k$ -space is

$$|\sigma_x \sigma_k| = \frac{1}{2}. \quad (1.42)$$

The product  $|\sigma_x| |\sigma_k| \geq |\sigma_x \sigma_k|$ . Thus,

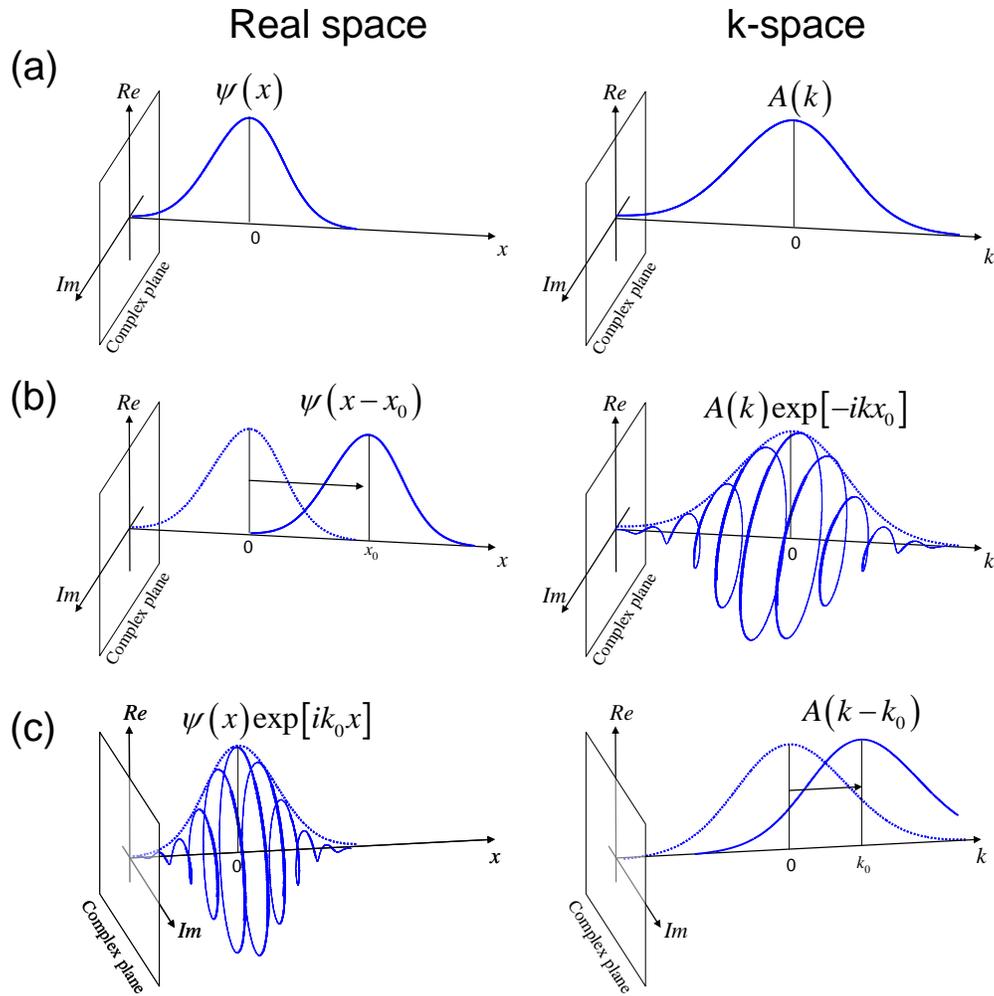
$$|\sigma_x| |\sigma_k| \geq \frac{1}{2}. \quad (1.43)$$

### Examples of wavepackets

A typical Gaussian wavepacket is shown in Fig. 1.15 in both its real space and  $k$ -space representations. Initially the probability distribution is centered at  $x = 0$  and  $k = 0$ . If we shift the wavepacket in  $k$ -space to an average value  $\langle k \rangle = k_0$ , this is equivalent to multiplying by a phase factor  $\exp[ik_0 x]$  in real space. Similarly, shifting the center of the wavepacket in real space to  $\langle x \rangle = x_0$  is equivalent to multiplying the  $k$ -space representation by a phase factor  $\exp[-ikx_0]$ .

Real coordinates ( $x, t$ )	$\iff$	Inverse coordinates ( $k, \omega$ )
shift by $x_0$	$\iff$	$\times \exp[-ikx_0]$
$\times \exp[ik_0 x]$	$\iff$	shift by $k_0$
shift by $t_0$	$\iff$	$\times \exp[i\omega t_0]$
$\times \exp[-i\omega_0 t]$	$\iff$	shift by $\omega_0$

**Table 1.1.** A summary of shift transformations in real and inverse coordinates.



**Fig. 1.15.** Three Gaussian wavepackets. In **(a)** the average position and wavenumber of the packet is  $x=0$  and  $k=0$ , respectively. In **(b)** the average position has been shifted to  $\langle x \rangle = x_0$ . In **(c)** the average wavenumber has been shifted to  $\langle k \rangle = k_0$ .

**Expectation values of position**

Given that  $P(x)$  is the probability density of the electron at position  $x$ , we can determine the average, or *expectation value* of  $x$  from

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} xP(x)dx}{\int_{-\infty}^{+\infty} P(x)dx} \tag{1.44}$$

Of course if the wavefunction is normalized then the denominator is 1.

We could also write this in terms of the wavefunction

## Part 1. The Quantum Particle

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} x |\psi(x)|^2 dx}{\int_{-\infty}^{+\infty} |\psi(x)|^2 dx} \quad (1.45)$$

Where once again if the wavefunction is normalized then the denominator is 1.

Since  $|\psi(x)|^2 = \psi(x)^* \psi(x)$ ,

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} \psi(x)^* x \psi(x) dx}{\int_{-\infty}^{+\infty} \psi(x)^* \psi(x) dx} \quad (1.46)$$

### Bra and Ket Notation

Also known as Dirac notation, Bra and Ket notation is a convenient shorthand for the integrals above.

The wavefunction is represented by a Ket:

$$\psi(x) \rightarrow |\psi\rangle \quad (1.47)$$

The complex conjugate is represented by a Bra:

$$\psi^*(x) \rightarrow \langle \psi | \quad (1.48)$$

Together, the bracket  $\langle \psi | \psi \rangle$  (hence Bra and Ket) symbolizes an integration over all space:

$$\int_{-\infty}^{+\infty} \psi^*(x) \psi(x) dx \rightarrow \langle \psi | \psi \rangle \quad (1.49)$$

Thus, in short form the expectation value of  $x$  is

$$\langle x \rangle = \frac{\langle \psi | x | \psi \rangle}{\langle \psi | \psi \rangle} \quad (1.50)$$

### Parseval's Theorem

It is often convenient to normalize a wavepacket in  $k$  space. To do so, we can apply Parseval's theorem.

Let's consider the bracket of two functions,  $f(x)$  and  $g(x)$  with Fourier transform pairs  $F(k)$  and  $G(k)$ , respectively..

$$\langle f | g \rangle = \int_{-\infty}^{\infty} f(x)^* g(x) dx \quad (1.51)$$

Now, replacing the functions by their Fourier transforms yields

$$\int_{-\infty}^{\infty} f(x)^* g(x) dx = \int_{-\infty}^{\infty} \left[ \frac{1}{2\pi} \int_{-\infty}^{\infty} F(k') e^{-ik'x} dk' \right]^* \left[ \frac{1}{2\pi} \int_{-\infty}^{\infty} G(k) e^{-ikx} dk \right] dx \quad (1.52)$$

Rearranging the order of integration gives

$$\begin{aligned} \int_{-\infty}^{\infty} \left[ \frac{1}{2\pi} \int_{-\infty}^{\infty} F(k') e^{-ik'x} dk' \right]^* \left[ \frac{1}{2\pi} \int_{-\infty}^{\infty} G(k) e^{-ikx} dk \right] dx \\ = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(k')^* G(k) \frac{1}{2\pi} e^{-i(k-k')x} dx dk' dk \end{aligned} \quad (1.53)$$

From Eq. (1.30) the integration over the complex exponential yields a delta function

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(k')^* G(k) \frac{1}{2\pi} e^{-i(k-k')x} dx dk' dk = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(k')^* G(k) \delta(k-k') dk' dk \quad (1.54)$$

Thus,

$$\int_{-\infty}^{\infty} f(x)^* g(x) dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(k)^* G(k) dk \quad (1.55)$$

It follows that if a wavefunction is normalized in real space, it is also normalized in  $k$ -space, i.e.,

$$\langle \psi | \psi \rangle = \langle A | A \rangle \quad (1.56)$$

where

$$\langle A | A \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} A(k)^* A(k) dk \quad (1.57)$$

### Expectation values of $k$ and $\omega$

The expectation value of  $k$  is obtained by integrating the wavefunction over all  $k$ . This must be performed in  $k$ -space.

$$\langle k \rangle = \frac{\frac{1}{2\pi} \int_{-\infty}^{+\infty} A(k)^* k A(k) dk}{\frac{1}{2\pi} \int_{-\infty}^{+\infty} A(k)^* A(k) dk} = \frac{\langle A | k | A \rangle}{\langle A | A \rangle} \quad (1.58)$$

From the Inverse Fourier transform in  $k$ -space

$$\psi(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} A(k) e^{ikx} dk \quad (1.59)$$

note that

$$-i \frac{d}{dx} \psi(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} k A(k) e^{ikx} dk \quad (1.60)$$

Thus, we have the following Fourier transform pair:

$$-i \frac{d}{dx} \psi(x) \Leftrightarrow k A(k) \quad (1.61)$$

## Part 1. The Quantum Particle

It follows that<sup>†</sup>

$$\langle k \rangle = \frac{\langle A|k|A \rangle}{\langle A|A \rangle} = \frac{\langle \psi | -i \frac{d}{dx} | \psi \rangle}{\langle \psi | \psi \rangle} \quad (1.62)$$

Similarly, from the Inverse Fourier transform in the frequency domain

$$\psi(t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} A(\omega) e^{-i\omega t} d\omega \quad (1.63)$$

We can derive the Fourier transform pair:

$$i \frac{d}{dt} \psi(t) \Leftrightarrow \omega A(\omega) \quad (1.64)$$

It follows that

$$\langle \omega \rangle = \frac{\langle A|\omega|A \rangle}{\langle A|A \rangle} = \frac{\langle \psi | i \frac{d}{dt} | \psi \rangle}{\langle \psi | \psi \rangle}. \quad (1.65)$$

We define two *operators*

$$\hat{k} = -i \frac{d}{dx} \quad (1.66)$$

and

$$\hat{\omega} = i \frac{d}{dt}. \quad (1.67)$$

Operators only act on functions to the right. To signify this difference we mark them with a caret.

We could also define the (somewhat trivial) position operator

$$\hat{x} = x. \quad (1.68)$$

### The Commutator

One must be careful to observe the correct order of operators. For example,

$$\hat{x} \hat{k} \neq \hat{k} \hat{x} \quad (1.69)$$

but

$$\hat{x} \hat{\omega} = \hat{\omega} \hat{x}. \quad (1.70)$$

In quantum mechanics we define the commutator:

$$[\hat{q}, \hat{r}] = \hat{q} \hat{r} - \hat{r} \hat{q} \quad (1.71)$$

We find that the operators  $\hat{x}$  and  $\hat{\omega}$  commute because  $[\hat{x}, \hat{\omega}] = 0$ .

Considering the operators  $\hat{x}$  and  $\hat{k}$ :

$$[\hat{x}, \hat{k}] = -ix \frac{d}{dx} + i \frac{d}{dx} x \quad (1.72)$$

---

<sup>†</sup> We have applied Parseval's theorem; see the Problem Sets.

## Introduction to Nanoelectronics

To simplify this further we need to operate on some function,  $f(x)$ :

$$\begin{aligned} [\hat{x}, \hat{k}] f(x) &= -ix \frac{df}{dx} + i \frac{d}{dx}(xf) \\ &= -ix \frac{df}{dx} + if \frac{dx}{dx} + ix \frac{df}{dx} \\ &= if \end{aligned} \tag{1.73}$$

Thus, the operators  $\hat{x}$  and  $\hat{k}$  do not commute, i.e.

$$[\hat{x}, \hat{k}] = i \tag{1.74}$$

Although we used Fourier transforms, Eq. (1.43) can also be derived from the relation (1.74) for the non-commuting operators  $\hat{x}$  and  $\hat{k}$ . It follows that all operators that do not commute are subject to a similar limit on the product of their uncertainties. We shall see in the next section that this limit is known as ‘the uncertainty principle’.

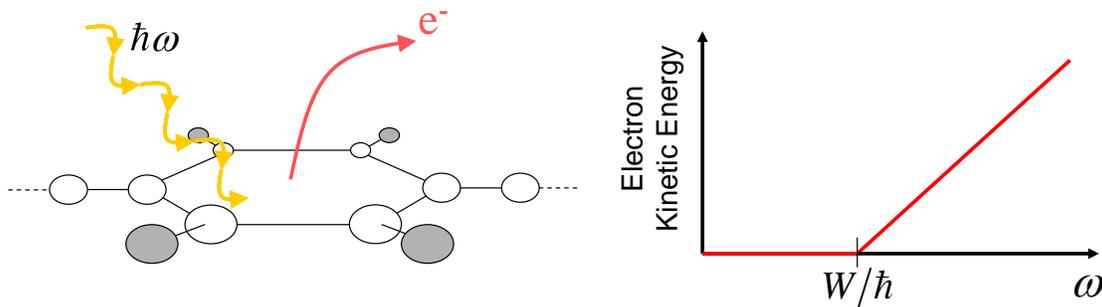
# Part 1. The Quantum Particle

## Momentum and Energy

Two key experiments revolutionized science at the turn of the 20<sup>th</sup> century. Both experiments involve the interaction of light and electrons. We have already seen that electrons are best described by wavepackets. Similarly, light is carried by a wavepacket called a photon. The first phenomenon, the photoelectric effect, was explained by assuming that a photon's energy is proportional to its frequency. The second phenomenon, the Compton effect, was explained by proposing that photons carry momentum. That light should possess particle properties such as momentum was completely unexpected prior to the advent of quantum mechanics.

### (i) The Photoelectric Effect

It is not easy to pull electrons out of a solid. They are bound by their attraction to positive nuclei. But if we give an electron in a solid enough energy, we can overcome the binding energy and liberate an electron. The minimum energy required is known as the work function,  $W$ .



**Fig. 1.16.** The photoelectric effect: above a critical frequency, light can liberate electrons from a solid.

By bombarding metal surfaces with light, it was observed that electrons could be liberated only if the frequency of the light exceeded a critical value. Above the minimum frequency, electrons were liberated with greater kinetic energy.

Einstein explained the photoelectric effect by postulating that, in a photon, the energy was proportional to the frequency:

$$E = \hbar\omega \tag{1.75}$$

Where  $h = 6.62 \times 10^{-34}$  Js is Planck's constant, and  $\hbar$  is shorthand for  $\hbar = h/2\pi$ . Note the units for Planck's constant – energy  $\times$  time. This is useful to remember when checking that your quantum calculations make sense.

Thus, the kinetic energy of the emitted electrons is given by

$$\text{electron kinetic energy} = \hbar\omega - W. \tag{1.76}$$

This technique is still used to probe the energy structure of materials

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Note that we will typically express the energy of electrons in ‘electron Volts (eV)’. The SI unit for energy, the Joule, is typically much too large for convenient discussion of electron energies. A more convenient unit is the energy required to move a single electron through a potential difference of 1V. Thus,  $1 \text{ eV} = q \text{ J}$ , where  $q$  is the charge on an electron ( $q \sim 1.602 \times 10^{-19} \text{ C}$ ).

### (ii) The Compton Effect

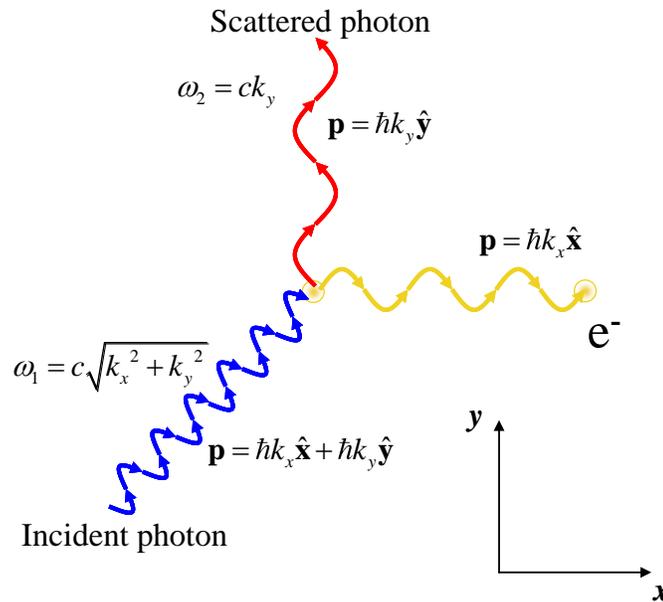
If a photon collides with an electron, the wavelength and trajectory of the photon is observed to change. After the collision the scattered photon is red shifted, i.e. its frequency is reduced and its wavelength extended. The trajectory and wavelength of the photon can be calculated by assuming that the photon carries momentum:

$$p = \hbar k, \tag{1.77}$$

where the wavenumber  $k$  is related to frequency by

$$k = \frac{2\pi}{\lambda} = \frac{\omega}{c}, \tag{1.78}$$

where  $c$  is the speed of light.



**Fig. 1.17.** The wavelength shift of light after collision with an electron is consistent with a transfer of momentum from a photon to the electron. The loss of photon energy is reflected in a red shift of its frequency.

These two relations:  $E = \hbar\omega$  and  $p = \hbar k$  are strictly true only for plane waves with precisely defined values of  $\omega$  and  $k$ . Otherwise we must employ operators for momentum and energy. Based on the operators we defined earlier for  $k$  and  $\omega$ , we define operators for momentum

$$\hat{p} = -i\hbar \frac{d}{dx} \tag{1.79}$$

## Part 1. The Quantum Particle

and energy

$$\hat{E} = i\hbar \frac{d}{dt} \quad (1.80)$$

Recall that each operator acts on the function to its right; and that  $\hat{p}\psi$  is not necessarily equal to  $\psi\hat{p}$ .

### The Uncertainty Principle

Now that we see that  $k$  is simply related to momentum, and  $\omega$  is simply related to energy, we can revisit the uncertainty relation of Eq. (1.43)

$$|\sigma_x| |\sigma_k| \geq \frac{1}{2}, \quad (1.81)$$

which after multiplication by  $\hbar$  becomes

$$\Delta p \cdot \Delta x \geq \frac{\hbar}{2}. \quad (1.82)$$

This is the celebrated Heisenberg uncertainty relation. It states that we can never know both position and momentum exactly.

For example, we have seen from our Fourier transform pairs that to know position exactly means that in  $k$ -space the wavefunction is  $\Psi(k) = \exp[-ikx_0]$ . Since  $|\Psi(k)|^2 = 1$  all values of  $k$ , and hence all values of momentum are equiprobable. Thus, momentum is perfectly undefined if position is perfectly defined.

### Uncertainty in Energy and Time

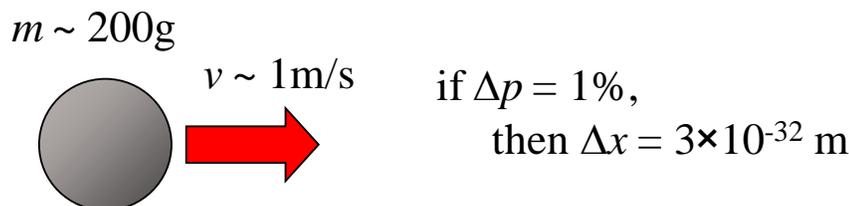
For the time/frequency domain, we take Fourier transforms and write

$$\Delta E \cdot \Delta t \geq \frac{\hbar}{2}. \quad (1.83)$$

However, time is treated differently to position, momentum and energy. There is no operator for time. Rather it is best thought of as a parameter. But the expression of Eq. (1.83) still holds when  $\Delta t$  is interpreted as a lifetime.

### Application of the Uncertainty Principle

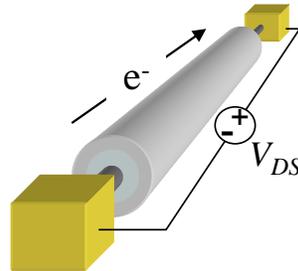
The uncertainty principle is not usually significant in every day life. For example, if the uncertainty in momentum of a 200g billiard ball traveling at a velocity of 1m/s is 1%, we can in principle know its position to  $\Delta x = (\hbar/2)/(0.2/100) = 3 \times 10^{-32}$  m.



**Fig. 1.18.** The uncertainty principle is not very relevant to everyday objects.

In nanoelectronics, however, the uncertainty principle can play a role.

For example, consider a very thin wire through which electrons pass one at a time. The current in the wire is related to the transit time of each electron by



**Fig. 1.19.** A nanowire that passes one electron at a time.

$$I = \frac{q}{\tau}, \quad (1.84)$$

where  $q$  is the charge of a single electron.

To obtain a current of  $I = 0.1$  mA in the wire the transit time of each electron must be

$$\tau = \frac{q}{I} \approx 1.6 \text{ fs}, \quad (1.85)$$

The transit time is the time that electron exists within the wire. Some electrons may travel through the wire faster, and some slower, but we can approximate the uncertainty in the electron's lifetime,  $\Delta t = \tau = 1.6$  fs.<sup>†</sup>

From Eq. (1.83) we find that  $\Delta E = 0.2$  eV. Thus, the uncertainty in the energy of the electron is equivalent to a random potential of approximately 0.2 V.<sup>§</sup> As we shall see, such effects fundamentally limit the switching characteristics of nano transistors.

## Schrödinger's Wave Equation

The energy of our electron can be broken into two parts, kinetic and potential. We could write this as

$$\text{total energy} = \text{kinetic energy} + \text{potential energy} \quad (1.86)$$

Now kinetic energy is related to momentum by

$$\text{kinetic energy} = \frac{1}{2} mv^2 = \frac{p^2}{2m} \quad (1.87)$$

Thus, using our operators, we could write

$$\hat{E}\psi(x,t) = \frac{\hat{p}^2}{2m}\psi(x,t) + \hat{V}\psi(x,t) \quad (1.88)$$

<sup>†</sup> Another way to think about this is to consider the addition of an electron to the nanowire. If current is to flow, that electron must be able to move from the wire to the contact. The rate at which it can do this (i.e. its lifetime on the wire) limits the transit time of an electron and hence the current that can flow in the wire.

<sup>§</sup> Recall that modern transistors operate at voltages  $\sim 1$  V. So this uncertainty is substantial.

## Part 1. The Quantum Particle

Where  $\hat{V}$  is the potential energy operator.

$$\hat{V} = V(x, t). \quad (1.89)$$

We can rewrite Eq. (1.88) in even simpler form by defining the so called Hamiltonian operator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}. \quad (1.90)$$

Now,

$$\hat{E}|\psi\rangle = \hat{H}|\psi\rangle. \quad (1.91)$$

Or we could rewrite the expression as

$$i\hbar \frac{d}{dt} \psi(x, t) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x, t) + V(x, t) \psi(x, t). \quad (1.92)$$

All these equations are statements of Schrödinger's wave equation. We can employ whatever form is most convenient.

### A Summary of Operators

Note there is no operator for time.

Position	$\hat{x}$	$x$	Energy	$\hat{E}$	$i\hbar \frac{d}{dt}$
Wavenumber	$\hat{k}$	$-i \frac{d}{dx}$	Potential Energy	$\hat{V}$	$V$
Angular Frequency	$\hat{\omega}$	$i \frac{d}{dt}$	Kinetic Energy	$\hat{T}$	$\frac{\hat{p}^2}{2m}$
Momentum	$\hat{p}$	$-i\hbar \frac{d}{dx}$	Hamiltonian	$\hat{H}$	$\frac{\hat{p}^2}{2m} + \hat{V}$

**Table 1.2.** All the operators used in this class.

### The Time Independent Schrödinger Equation

When the potential energy is constant in time we can simplify the wave equation. We assume that the spatial and time dependencies of the solution can be separated, i.e.

$$\Psi(x, t) = \psi(x) \zeta(t) \quad (1.93)$$

Substituting this into Eq. (1.92) gives

$$i\hbar \psi(x) \frac{d}{dt} \zeta(t) = -\frac{\hbar^2}{2m} \zeta(t) \frac{d^2}{dx^2} \psi(x) + V(x) \psi(x) \zeta(t) \quad (1.94)$$

Dividing both sides by  $\psi(x) \zeta(t)$  yields

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$$i\hbar \frac{1}{\zeta(t)} \frac{d}{dt} \zeta(t) = -\frac{\hbar^2}{2m} \frac{1}{\psi(x)} \frac{d^2}{dx^2} \psi(x) + V(x). \quad (1.95)$$

Now the left side of the equation is a function only of time while the right side is a function only of position. These are equal for all values of time and position if each side equals a constant. That constant turns out to be the energy,  $E$ , and we get two coupled equations

$$E\zeta(t) = i\hbar \frac{d}{dt} \zeta(t) \quad (1.96)$$

and

$$E\psi(x) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x)\psi(x). \quad (1.97)$$

The solution to Eq. (1.96) is

$$\zeta(t) = \zeta(0) \exp\left[-i \frac{E}{\hbar} t\right] \quad (1.98)$$

Thus, the complete solution is

$$\Psi(x,t) = \psi(x) \exp\left[-i \frac{E}{\hbar} t\right] \quad (1.99)$$

By separating the wavefunction into time and spatial functions, we need only solve the simplified Eq. (1.97).

There is much more to be said about this equation, but first let's do some examples.

### Free Particles

In free space, the potential,  $V$ , is constant everywhere. For simplicity we will set  $V = 0$ .

Next we solve Eq. (1.97) with  $V = 0$ .

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) = E\psi(x) \quad (1.100)$$

Rearranging slightly gives the second order differential equation in slightly clearer form

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2} \psi \quad (1.101)$$

A general solution is

$$\psi(x) = \psi(0) \exp[ikx] \quad (1.102)$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad (1.103)$$

Inserting the time dependence (see Eq. (1.99)) gives

$$\psi(x,t) = \psi(0) \exp[i(kx - \omega t)] \quad (1.104)$$

where

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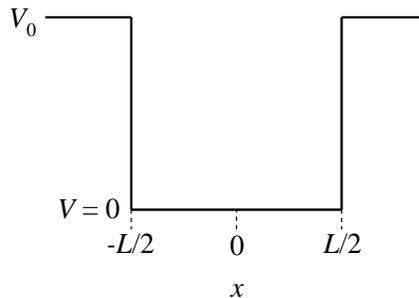
$$\omega = \frac{E}{\hbar} = \frac{\hbar k^2}{2m}. \quad (1.105)$$

Thus, as expected the solution in free space is a plane wave.

### The Square Well

Next we consider a single electron within a square potential well as shown in Fig. 1.20. As mentioned in the discussion of the photoelectric effect, electrons within solids are bound by attractive nuclear forces.

By modeling the binding energy within a solid as a square well, we entirely ignore fine scale structure within the solid. Hence the square well, or *particle in a box*, as it is often known, is one of the crudest approximations for an electron within a solid. The simplicity of the square well approximation, however, makes it one of the most useful problems in all of quantum mechanics.



**Fig. 1.20.** The square well. Within the solid the potential is defined to be zero. In free space, outside the solid, the repulsive potential is  $V_0$ .

Since the potential changes abruptly, we treat each region of constant potential separately. Subsequently, we must connect up the solutions in the different regions. Tackling the problem this way is known as a *piecewise* solution.

Now, the Schrödinger Equation is a statement of the conservation of energy

$$\text{total energy } (E) = \text{kinetic energy } (KE) + \text{potential energy } (V) \quad (1.106)$$

In classical mechanics, one can never have a negative kinetic energy. Thus, classical mechanics requires that  $E > V$ . This is known as the *classically allowed* region.

But in our quantum analysis, we will find solutions for  $E < V$ . This is known as the *classically forbidden* regime.

#### (i) The classically allowed region

Rearranging Eq. (1.97) gives the second order differential equation:

$$\frac{d^2\psi}{dx^2} = -\frac{2m(E-V)}{\hbar^2}\psi \quad (1.107)$$

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In this region,  $E > V$ , solutions are of the form

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad (1.108)$$

or

$$\psi(x) = A \sin kx + B \cos kx \quad (1.109)$$

where

$$k = \sqrt{\frac{2m(E-V)}{\hbar^2}} \quad (1.110)$$

In the classically allowed region we have oscillating solutions.

### (ii) The classically forbidden region

In this region,  $E < V$ , and solutions are of the form

$$\psi(x) = Ae^{\alpha x} + Be^{-\alpha x} \quad (1.111)$$

i.e. they are either growing or decaying exponentials where

$$\alpha = \sqrt{\frac{2m(V-E)}{\hbar^2}}. \quad (1.112)$$

### Matching piecewise solutions

The Schrödinger Equation is a second order differential equation. From Eq. (1.107) we observe the second derivative of the wavefunction is finite unless either  $E$  or  $V$  is infinite.

Infinite energies are not physical, hence if the potential is finite we can conclude that  $\frac{d\psi}{dx}$

and  $\psi(x)$  are continuous everywhere.

That is, at the boundary ( $x = x_0$ ) between piecewise solutions, we require that

$$\psi_-(x_0) = \psi_+(x_0) \quad (1.113)$$

and

$$\frac{d}{dx}\psi_-(x_0) = \frac{d}{dx}\psi_+(x_0) \quad (1.114)$$

### Bound solutions

Electrons with energies within the well ( $0 < E < V_0$ ) are *bound*. The wavefunctions of the bound electrons are localized within the well and so they must be normalizable. Thus, the wavefunction of a bound electron in the classically forbidden region (outside the well) must decay exponentially with distance from the well.

A possible solution for the bound electrons is then

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$$\psi(x) = \begin{cases} Ce^{\alpha x} & \text{for } x \leq -L/2 \\ A \cos(kx) + B \sin(kx) & \text{for } -L/2 \leq x \leq L/2 \\ De^{-\alpha x} & \text{for } x \geq L/2 \end{cases} \quad (1.115)$$

where

$$\alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \quad (1.116)$$

and

$$k = \sqrt{\frac{2mE}{\hbar^2}}, \quad (1.117)$$

and  $A$ ,  $B$ ,  $C$  and  $D$  are constants.

### The limit that $V_0 \rightarrow \infty$ (the infinite square well)

At the walls where the potential is infinite, we see from Eq. (1.116) that the solutions decay immediately to zero since  $\alpha \rightarrow \infty$ . Thus, in the classically forbidden region of the infinite square well  $\psi = 0$ .

The wavefunction is continuous, so it must approach zero at the walls. A possible solution with zeros at the left boundary is

$$\psi(x) = A \sin(k(x + L/2)) \quad (1.118)$$

where  $k$  is chosen such that  $\psi = 0$  at the right boundary also:

$$kL = n\pi \quad (1.119)$$

To normalize the wavefunction and determine  $A$ , we integrate:

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = \int_{-L/2}^{L/2} A^2 \cos^2(n\pi x/L + n\pi/2) dx \quad (1.120)$$

From which we determine that

$$A = \sqrt{2/L} \quad (1.121)$$

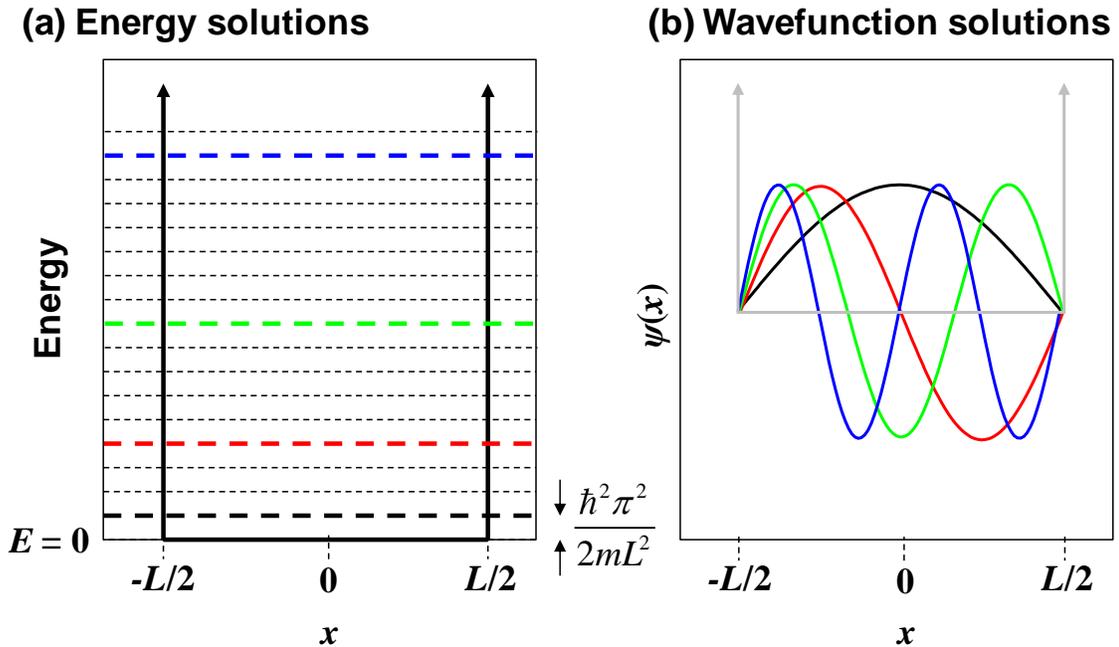
The energy is calculated from Eq. (1.117)

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2mL^2}. \quad (1.122)$$

The first few energies and wavefunctions of electrons in the well are plotted in Fig. 1.21.

Two characteristics of the solutions deserve comment:

1. The bound states in the well are quantized – only certain energy levels are allowed.
2. The energy levels scale inversely with  $L^2$ . As the box gets smaller each energy level and the gaps between the allowed energy levels get larger.



**Fig. 1.21.** The lowest four states for a single electron in an infinite square well. Note that we have plotted  $\psi(x)$  not  $|\psi(x)|^2$ .

### The Finite Square Well

When the confining potential is finite, we can no longer assume that the wavefunction is zero at the boundaries of the well. For a finite confining potential, the wavefunction penetrates into the barrier: the lower the confining potential, the greater the penetration.

From Eq. (1.115) the general solution for the wavefunction within the well was

$$\psi(x) = A \cos(kx) + B \sin(kx), \quad (1.123)$$

but from the solutions for the infinite well, we can see that, within the well, the wavefunction looks like

$$\psi(x) = A \cos(kx) \quad (1.124)$$

or

$$\psi(x) = A \sin(kx) \quad (1.125)$$

The simplification is possible because the well potential is symmetric around  $x = 0$ . Thus, the probability density  $|\psi(x)|^2$  should also be symmetric,<sup>†</sup> and indeed both  $\psi(x) = \sin(kx)$  and  $\psi(x) = \cos(kx)$  have symmetric probability distributions even though  $\psi(x) = \sin(kx)$  is an antisymmetric wavefunction.

We'll consider the symmetric ( $\cos(kx)$ ) and antisymmetric ( $\sin(kx)$ ) wavefunction solutions separately.

<sup>†</sup> After all, if the potential is the same in both left and right halves of the well, there is no reason for the electron to be more probable in one side of the well.

## Part 1. The Quantum Particle

(i) Symmetric wavefunction

We can assume a solution of the form:

$$\psi(x) = \begin{cases} e^{\alpha x} & \text{for } x \leq -L/2 \\ A \cos(kx) & \text{for } -L/2 \leq x \leq L/2 \\ e^{-\alpha x} & \text{for } x \geq L/2 \end{cases} \quad (1.126)$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad (1.127)$$

and

$$\alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \quad (1.128)$$

Note the solution as written is not normalized. We can normalize it later.

The next step is to evaluate the constant  $A$  by matching the piecewise solutions at the edge of the well. We need only consider one edge, because we have already fixed the symmetry of the solution.

At the right edge, equating the amplitude of the wavefunction gives

$$\psi(L/2) = A \cos(kL/2) = \exp[-\alpha L/2] \quad (1.129)$$

Equating the slope of the wavefunction gives

$$\psi'(L/2) = -kA \sin(kL/2) = -\alpha \exp[-\alpha L/2] \quad (1.130)$$

Dividing Eq. (1.130) by Eq. (1.129) to eliminate  $A$  gives

$$\tan(kL/2) = \alpha/k. \quad (1.131)$$

But  $\alpha$  and  $k$  are both functions of energy

$$\tan\left(\frac{\pi}{2} \sqrt{\frac{E}{E_L}}\right) = \sqrt{\frac{V_0 - E}{E}} \quad (1.132)$$

where we have defined the infinite square well ground state energy

$$E_L = \frac{\hbar^2 \pi^2}{2mL^2}. \quad (1.133)$$

As in the infinite square well case, we find that only certain, discrete, values of energy give a solution. Once again, the energies of electron states in the well are quantized. To obtain the energies we need to solve Eq. (1.132). Unfortunately, this is a transcendental equation, and must be solved numerically or graphically. We plot the solutions in Fig. 1.22.

(ii) Antisymmetric wavefunction

Antisymmetric solutions are found in a similar manner to the symmetric solutions. We first assume an antisymmetric solution of the form:

$$\psi(x) = \begin{cases} e^{\alpha x} & \text{for } x \leq -L/2 \\ A \sin(kx) & \text{for } -L/2 \leq x \leq L/2 \\ -e^{-\alpha x} & \text{for } x \geq L/2 \end{cases} \quad (1.134)$$

Then, we evaluate the constant  $A$  by matching the piecewise solutions at the edge of the well. Again, we need only consider one edge, because we have already fixed the symmetry of the solution.

At the right edge, equating the amplitude of the wavefunction gives

$$\psi(L/2) = A \sin(kL/2) = -\exp[-\alpha L/2] \quad (1.135)$$

Equating the slope of the wavefunction gives

$$\psi'(L/2) = kA \cos(kL/2) = \alpha \exp[-\alpha L/2] \quad (1.136)$$

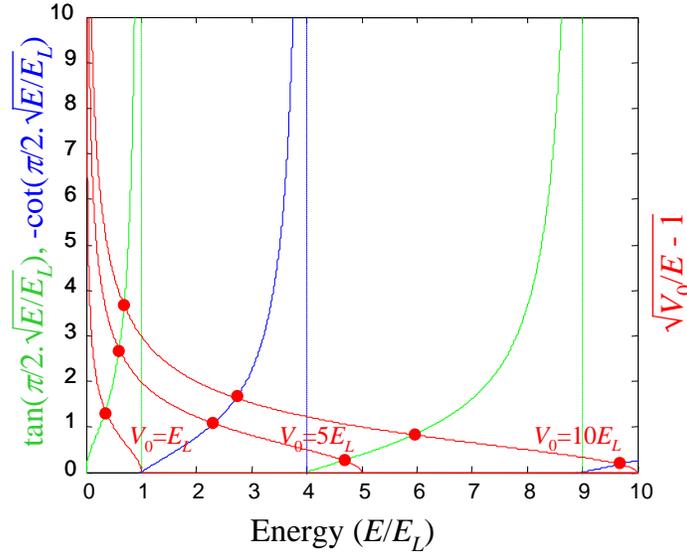
Dividing Eq. (1.130) by Eq. (1.129) to eliminate  $A$  gives

$$\cot(kL/2) = -\alpha/k. \quad (1.137)$$

Expanding  $\alpha$  and  $k$  in terms of energy

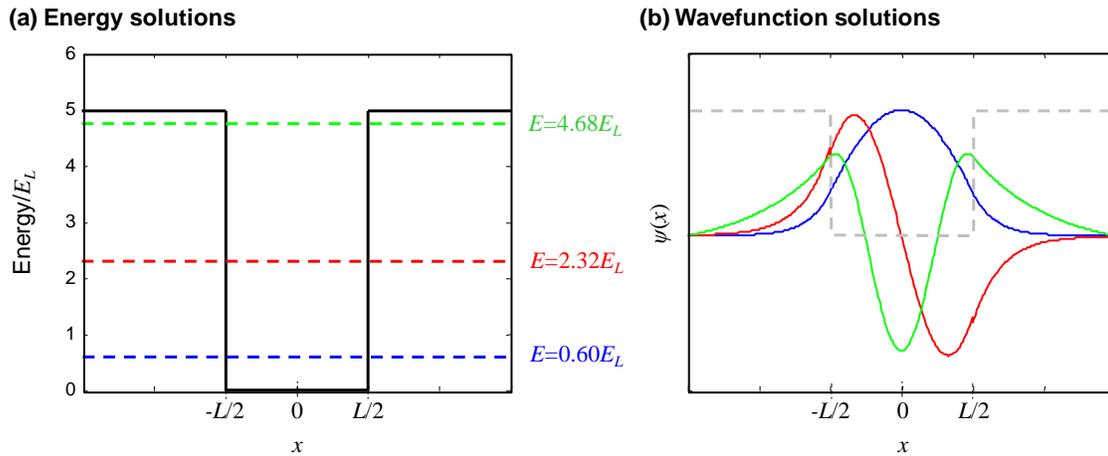
$$-\cot\left(\frac{\pi}{2} \sqrt{\frac{E}{E_L}}\right) = \sqrt{\frac{V_0 - E}{E}}. \quad (1.138)$$

In Fig. 1.22, we solve for the energy. Note that there is always at least one bound solution no matter how shallow the well. In Fig. 1.23 we plot the solutions for a confining potential  $V_0 = 5.E_L$ .



**Fig. 1.22.** A graphical solution for the energy in the finite quantum well. The green and blue curves are the LHS of Eqs. (1.132) and (1.138), respectively. The red curves are the RHS for different values of the confining potential  $V_0$ . Solutions correspond to the intersections between the red lines and the green or blue curves.

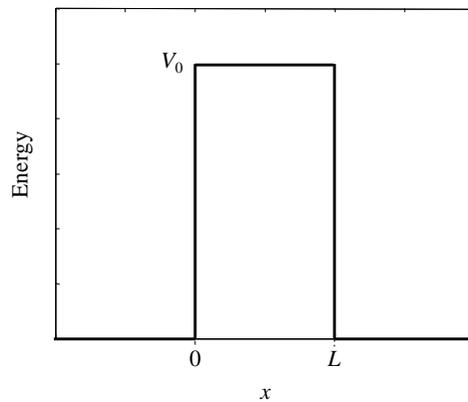
## Part 1. The Quantum Particle



**Fig. 1.23.** The three bound states for electrons in a well with confining potential  $V_0 = 5.E_L$ . Note that the higher the energy, the lower the effective confining potential, and the greater the penetration into the barriers.

### Potential barriers and Tunneling

Next we consider electrons incident on a potential barrier, as shown in Fig. 1.24.



**Fig. 1.24.** A potential barrier.

We will assume that the particle is incident on the barrier from the left. It has some probability of being reflected by the barrier. But it also has some probability of being transmitted even though its energy may be less than the barrier height. Transmission through a barrier is known as *tunneling*. There is no equivalent process in classical physics – the electron would need sufficient energy to jump over the barrier.

Once again, we solve the time-independent Schrödinger Equation. To the left and right of the barrier, the electron is in a classically allowed region. We model the electron in these regions by a plane wave; see Eq. (1.108) and the associated discussion. On the other hand, within the barrier, if the energy,  $E$ , of the electron is below the barrier potential,  $V_0$ ,

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the barrier is a classically forbidden region. The solution in this region is described by expanding and decaying exponentials; see Eq. (1.111) and the associated discussion.

Analyzing the potential piece by piece, we assume a solution of the form

$$\psi(x) = \begin{cases} e^{ikx} + re^{-ikx} & \text{for } x \leq 0 \\ ae^{\alpha x} + be^{-\alpha x} & \text{for } 0 \leq x \leq L \\ te^{ikx} & \text{for } x \geq L \end{cases} \quad (1.139)$$

where once again

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad (1.140)$$

and

$$\alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \quad (1.141)$$

The intensity of the incoming plane wave is unity. Hence the amplitude of the reflected wave,  $r$ , is the reflection coefficient and the amplitude of the transmitted wave,  $t$ , is the transmission coefficient. (The reflectivity and transmissivity is  $|r|^2$  and  $|t|^2$ , respectively).

Next we match the piecewise solutions at the left edge of the barrier. Equating the amplitude of the wavefunction gives

$$\psi(0) = 1 + r = a + b \quad (1.142)$$

Equating the slope of the wavefunction gives

$$\psi'(0) = ik - ikr = \alpha a - \alpha b. \quad (1.143)$$

At the right edge of the barrier, we have

$$\psi(L) = ae^{\alpha L} + be^{-\alpha L} = te^{ikL} \quad (1.144)$$

and

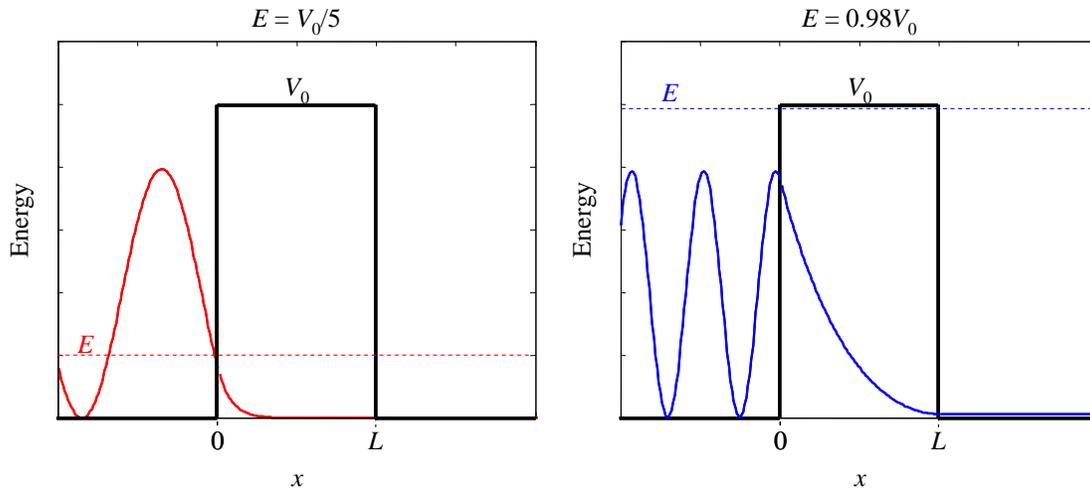
$$\psi'(L) = a\alpha e^{\alpha L} - b\alpha e^{-\alpha L} = ikte^{ikL}. \quad (1.145)$$

Thus, we have four simultaneous equations. But these are a pain to solve analytically. In Fig. 1.25 we plot solutions for energy much less than the barrier, and energy close to the barrier. It is observed that the tunneling probability is greatly enhanced when the incident electron has energy close to the barrier height. Note that the wavefunction decay within the barrier is much shallower when the energy of the electron is large. Note also that the reflection from the barrier interferes with the incident electron creating an interference pattern.

When the electron energy is much less than the barrier height we can model the wavefunction within the barrier as simply a decaying exponential. The transmission probability is then approximately

$$T \approx \exp[-2\alpha L]. \quad (1.146)$$

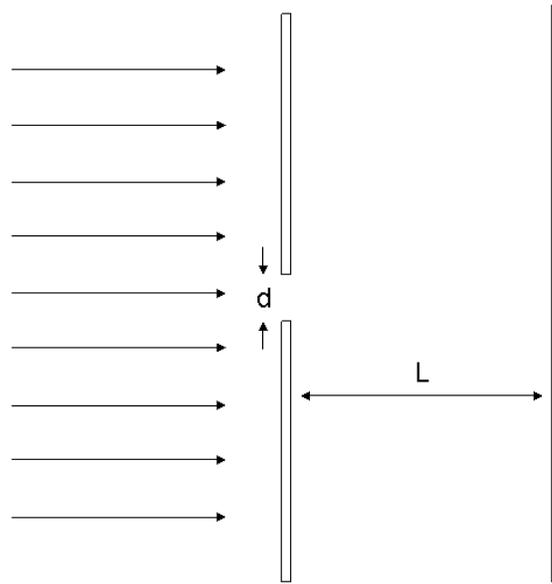
## Part 1. The Quantum Particle



**Fig. 1.25.** Plots of the wavefunction for an electron incident from the left. **(a)** When the electron energy is substantially below the barrier height, tunneling is negligible. **(b)** For an electron energy 98% of the barrier height, however, note the non-zero transmission probability to the right of the barrier.

## Problems

1. Suppose we fire electrons through a single slit with width  $d$ . At the viewing screen behind the aperture, the electrons will form a pattern. Derive and sketch the expression for the intensity at the viewing screen. State all necessary assumptions.



**Fig. 1.26.** The geometry of a single slit diffraction experiment.

How does this pattern differ from the pattern with two slits discussed in class?

2. Compare the different patterns at the viewing screen with  $d = 20\text{\AA}$  and  $L = 100\text{nm}$  for fired electrons with wavelengths of  $10\text{\AA}$ ,  $100\text{\AA}$ , and  $1000\text{\AA}$ . Explain.
3. Show that a shift in the position of a wavepacket by  $x_0$  is equivalent to multiplying the k-space representation by  $\exp[-ikx_0]$ . Also, show that a shift in the k-space representation by  $k_0$  is equivalent to multiplying the position of the wavepacket by  $\exp[ik_0x]$ . Show that similar relations hold for shifts in time and frequency.

4. Find  $|F(\omega)|^2$  where  $F(\omega)$  is the Fourier Transform of an exponential decay:

$$F(\omega) = \mathcal{F}[e^{-at}u(t)]$$

where  $u(t)$  is the unit step function.

5. Show that if

$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2$$

then

$$\Delta x = \sigma$$

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where

$$\psi(x) = \exp\left[-\frac{1}{4} \frac{(x-x_0)^2}{\sigma^2}\right]$$

6. Show the following:

$$(a) \quad \langle k \rangle = \frac{\langle A | k | A \rangle}{\langle A | A \rangle} = \frac{\langle \psi | -i \frac{d}{dx} | \psi \rangle}{\langle \psi | \psi \rangle}$$

$$(b) \quad \langle \omega \rangle = \frac{\langle A | \omega | A \rangle}{\langle A | A \rangle} = \frac{\langle \psi | i \frac{d}{dt} | \psi \rangle}{\langle \psi | \psi \rangle}$$

7. A free particle is confined to move along the x-axis. At time  $t=0$  the wave function is given by

$$\psi(x, t=0) = \begin{cases} \frac{1}{\sqrt{L}} e^{ik_0 x} & -\frac{L}{2} \leq x \leq \frac{L}{2} \\ 0 & \text{otherwise} \end{cases}$$

- What is the *most* probable value of momentum?
- What are the *least* probable values of momentum?
- Make a rough sketch of the wave function in  $k$ -space,  $A(k, t=0)$ .

8. The commutator of two operators  $\hat{A}$  and  $\hat{B}$  is defined as

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

Evaluate the following commutators:

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- (a)  $[\hat{x}, \hat{x}^2]$    (b)  $[\hat{p}, \hat{p}^2]$    (c)  $[\hat{x}^2, \hat{p}^2]$    (d)  $[\hat{x}\hat{p}, \hat{p}\hat{x}]$

9. Consider the wavefunction

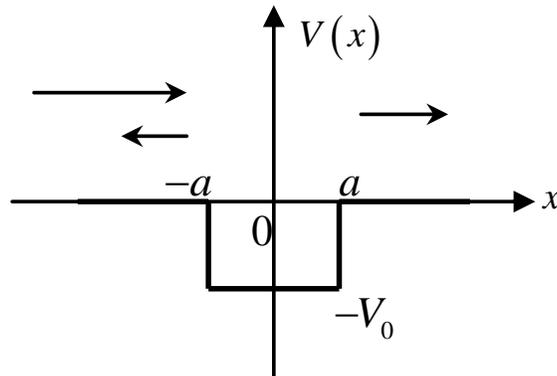
$$\psi(x) = \exp\left[-\frac{1}{2} \frac{x^2}{\sigma^2} (1+iC)\right]$$

Show that

$$|\sigma_x| |\sigma_k| \geq \frac{1}{2} \sqrt{1+C^2}$$

(Hint: Show that  $|\sigma_k|^2 = \frac{\langle \psi | -\frac{d^2}{dx^2} | \psi \rangle}{\langle \psi | \psi \rangle}$ )

10. For the finite square well shown below, calculate the reflection and transmission coefficients ( $E > 0$ ).



**Fig. 1.27.** A finite potential well.

11. Consider an electron in the ground state of an infinite square well of width  $L$ . What is the expectation value of its velocity? What is the expectation value of its kinetic energy? Is there a conflict between your results?

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12. Derive the reflection and transmission coefficients for the potential  $V(x) = A\delta(x)$ , where  $A > 0$ .

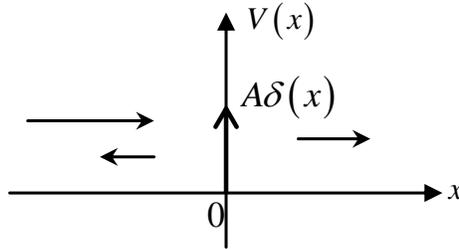


Fig. 1.28. A delta function potential.

One method to solve is by taking the Schrödinger equation with  $V(x) = A\delta(x)$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + A\delta(x)\psi(x) = E\psi(x)$$

and integrating both sides from  $-\varepsilon$  to  $\varepsilon$  for  $\varepsilon$  very small to get the constraint

$$-\frac{\hbar^2}{2m} \int_{-\varepsilon}^{+\varepsilon} \frac{\partial^2 \psi(x)}{\partial x^2} dx + A\psi(0) \approx 2\varepsilon E\psi(0) \approx 0$$

$$\Rightarrow \left. \frac{d\psi}{dx} \right|_{x=\varepsilon} - \left. \frac{d\psi}{dx} \right|_{x=-\varepsilon} = \frac{2mA}{\hbar^2} \psi(0)$$

13. Consider two quantum wells each with width  $w$  separated by distance  $d$ .

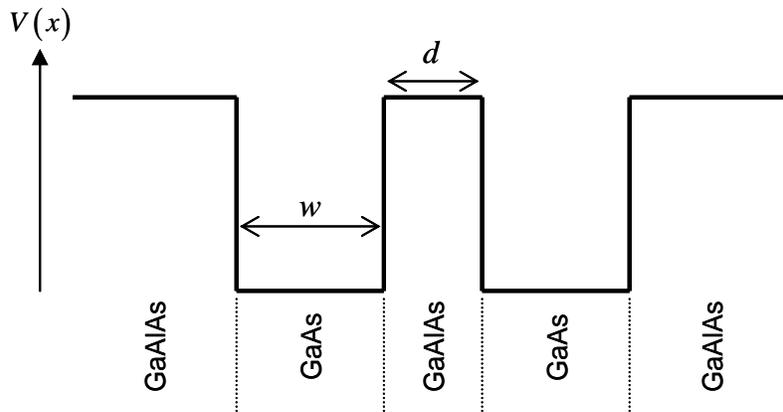


Fig. 1.29. The structure of the quantum wells.

- From your understanding of wavefunctions for a particle in a box, plot the approximate probability density for each of the two lowest energy modes for this system when the two quantum wells are isolated from each other.
- Plot the two lowest energy modes when the two quantum wells are brought close to each other such that  $d \ll w$ ?

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- (c) Next we wish to take a thin slice of another material and insert it in the structure above (where  $d \ll w$ ) to kill one of the two modes of part (b) but leave the other unaffected. How would you choose the material (compared to the materials already present in the structure), and where should this new material be placed?

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