

# Waves and Particles: Basic Concepts of Quantum Mechanics

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This part of the course is based on Refs. [1] – [4].

## 1. Mathematical description of waves

Let us begin with a brief reminder of waves and some of their basic properties. The purpose of this section is to remind the basic definitions and mathematical formulation, to be used in the following discussion.

### 1.1. Definition

A **wave** is an (oscillatory) perturbation of a medium, which is accompanied by transfer of energy. Since the disturbance is moving, it must be a function of both position and time:

$$\psi = f(x, t) \tag{1}$$

(here, we restrict ourself to 1-dimensional waves). The function  $f(x, t)$  is the **shape** of the wave. We will currently limit the discussion to waves that do not change their shape as they progress in space.

Assume that the perturbation propagates at constant velocity  $v$  (we will normally encounter  $v = c$ , but we keep using  $v$  for now) in the positive  $x$  direction. If at time  $t = 0$  the peak of the perturbation was at  $x$ , it is now at  $x + vt$ . We can transform to a new coordinate system  $S'$  that moves at the same speed,  $v$ . In this new system, the wave is stationary (having the same shape as in the old system at  $t = 0$ ), and its shape is thus  $\psi = f(x')$ . Using  $x' = x - vt$  we thus find

$$\psi(x, t) = f(x - vt, t = 0) \tag{2}$$

Let us for now restrict the discussion to **harmonic waves**, which can be described by a sin or cos functions:

$$\psi(x, t = 0) \equiv \psi(x) = A \sin(kx). \tag{3}$$

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Here,  $A$  is called the **amplitude** of the wave, and  $k$  is called the **wavenumber** (in 3-d,  $\vec{k}$  is also called **wavevector**).

The **spatial period** is known as the **wavelength**, and denoted by  $\lambda$  (see Figure 1). Clearly,  $\lambda$  has units of [length]. An increase of  $x$  by  $\lambda$  leaves the wave unaltered,

$$\psi(x, t) = \psi(x + \lambda, t), \quad (4)$$

which implies, via Equation 3 that

$$k = \frac{2\pi}{\lambda}. \quad (5)$$

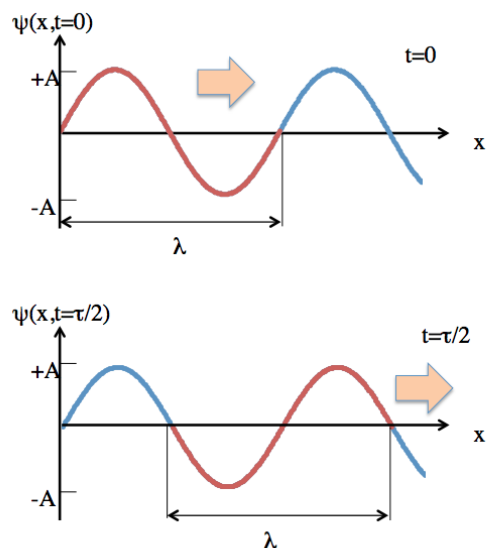


Fig. 1.— Simple, infinite sinusoidal wave propagating to the right, as seen at  $t = 0$  and  $t = \tau/2$ .

Using Equation 2, after some time  $t$ , the wave is

$$\psi(x, t) = A \sin k(x - vt). \quad (6)$$

Similar to the discussion above, after time  $\tau = 2\pi/kv$ , one complete wave cycle passes through a stationary observer, and therefore

$$\psi(x, t) = \psi(x, t + \tau). \quad (7)$$

The time  $\tau$  is known as the **temporal period** of the wave. Using Equation 5, it follows that

$$\tau = \frac{\lambda}{v}. \quad (8)$$

The inverse of  $\tau$  is known as the **frequency** of the wave, and is denoted by  $\nu$ ,

$$\nu \equiv \frac{1}{\tau} = \frac{v}{\lambda}, \quad (9)$$

and has units of [cycles / s], or [Hertz].

Another useful quantity is the **angular frequency**,  $\omega$  defined by

$$\omega \equiv \frac{2\pi}{\tau} = 2\pi\nu. \quad (10)$$

Using it, Equation 6 can be written as

$$\psi(x, t) = A \sin(kx - \omega t). \quad (11)$$

## 1.2. Phase and phase velocity

The argument of the sin function is known as the **phase** of the wave,

$$\phi = kx - \omega t. \quad (12)$$

For the wave presented above, at  $x = t = 0$ , we have  $\phi = 0$ . This is obviously a special case, which can be generalized to write

$$\psi(x, t) = A \sin(kx - \omega t + \phi_0), \quad (13)$$

where  $\phi_0$  is the **initial phase** of the wave.

Obviously, the rate of change of the phase with time (at constant  $x$ ) is

$$\left| \left( \frac{\partial \phi}{\partial t} \right)_x \right| = \omega, \quad (14)$$

and the rate of change of phase with distance (at constant time) is

$$\left| \left( \frac{\partial \phi}{\partial x} \right)_t \right| = k. \quad (15)$$

Using these two relations, one can write the propagation velocity at constant phase,

$$\left( \frac{\partial x}{\partial t} \right)_\phi = \frac{-(\partial \phi / \partial t)_x}{(\partial \phi / \partial x)_t} = \frac{\omega}{k} = v. \quad (16)$$

Thus, the velocity  $v$  is the **phase velocity** of the wave, also denoted by  $v_\phi$ .

### 1.3. Complex representation of simple waves

Using Euler's formula,

$$e^{i\theta} = \cos \theta + i \sin \theta, \quad (17)$$

it is often very convenient to write a simple wave in the form

$$\psi(x, t) = Ae^{i(kx - \omega t)}. \quad (18)$$

This enables quick computations with waves. Using this notation, it is understood that at the end of the calculation,  $\psi(x, t)$  is the real part of the complex formula, namely

$$\psi(x, t) = \text{Re} (Ae^{i(kx - \omega t)}) = A \cos(kx - \omega t). \quad (19)$$

### 1.4. Wave packets and group velocity

When dealing with simple waves as is done so far, there is no need to introduce another velocity. However, often one encounters more complicated waves, such as waves that are composed by superposition of several simple waves. When superposition of simple waves occur in a localized position in space, the result is known as **wave packet**.

As we will see shortly, wave packets are of particular importance in quantum mechanics. They are not difficult to analyze, due to the principle of superposition, from which it follows that every wave - regardless of how complicated its shape is, can be written as a superposition of simple (plane) waves,

$$\psi(x, t) = \int A(k)e^{i(kx - \omega(k)t)} dk. \quad (20)$$

Note that we assume an explicit dependence of the angular frequency  $\omega$  on the wavenumber  $k$ ,  $\omega = \omega(k)$ .

When treating wave packets, in addition to the phase velocity of individual waves defined above, one can define the velocity of the overall shape of the wave's amplitude (also known as the *envelope* of the wave). This is known as the **group velocity**, defined by

$$v_g \equiv \left( \frac{d\omega}{dk} \right)_{k=k_0}, \quad (21)$$

where  $k_0$  is the wavenumber at the center of the wavepacket.

Note that for a simple wave,  $v_g = v_\phi$ . Consider, however, the simple example of two waves having slightly different wavenumbers and angular frequencies that travel together as

a wavepacket:

$$\begin{aligned}\psi_1 &= A \sin((k + \Delta k)x - (\omega + \Delta\omega)t), \\ \psi_2 &= A \sin((k - \Delta k)x - (\omega - \Delta\omega)t).\end{aligned}\tag{22}$$

We have

$$\psi_1 + \psi_2 = 2A \sin(kx - \omega t) \cos(\Delta kx - \Delta\omega t),\tag{23}$$

which can be thought of as a simple wave, with varying amplitude,  $2A \cos(\Delta kx - \Delta\omega t)$ . In the limit  $\Delta\omega, \Delta k \rightarrow 0$ , one retrieves the group velocity (Equation 21), which is the velocity in which the “envelope” propagates (see Figure 2). The group velocity is the velocity in which information travels, and is always  $v_g \leq c$ , for any physical wave packet.

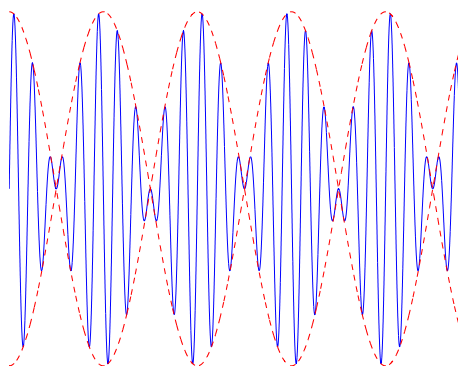


Fig. 2.— Spatial variation of the superposition of two simple waves with the same amplitude and slightly different wavenumbers reveals an “envelope” wave (red dotted curve) on top of the carrier wave (blue line). The envelope travels at the group velocity.

### 1.5. Standing waves

The general solution of a (1-d) wave equation enables the existence of waves that propagate in both directions,  $+x$  and  $-x$ . Consider two such simple waves, having the same amplitude:

$$\psi(x, t) = A \sin(kx - \omega t) + A \sin(kx + \omega t).\tag{24}$$

Using sum of sin functions, we find

$$\psi(x, t) = 2A \sin(kx) \cos(\omega t).\tag{25}$$

This is an equation of a **standing**, or **stationary** wave. At certain points, namely  $x = 0, \lambda/2, \lambda, 3\lambda/2, \dots$ , the amplitude of this wave is always 0. These are therefore the waves that can be obtained in a medium (e.g., a string) whose boundaries are held fixed.

Consider a string of length  $L$ , whose two edges, at  $x = 0$  and  $x = L$  are held fixed. According to Equation 25, such a string could maintain stationary waves as long as  $kL = n\pi$ , where  $n$  is an integer number. Using  $k = 2\pi/\lambda$ , the stationary wavelengths are

$$\lambda = \frac{2L}{n} \tag{26}$$

(see Figure 3).

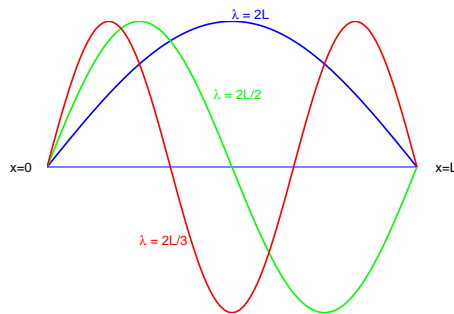


Fig. 3.— Standing waves on a string of length  $L$  have wavenumbers  $\lambda_n = 2L/n$ , where  $n = 1, 2, 3, \dots$  (shown are  $n = 1, 2, 3$ ).

## 2. Analysis of Young’s experiment: wave-particle duality of light

After this short mathematical bypass, let us now return to Young’s double slit experiment, and analyze it from a modern point of view. Recall that Young’s inevitable conclusion from seeing the diffraction pattern was that light is a wave. However, Einstein considered light as particles. Let us see how these two approaches live together.

The first thing we do is block one of the slits. (see Figure 4). We obtain the light intensity distribution  $I_1(x)$ , the diffraction pattern of slit 1. Similar, if we block the second slit, we obtain  $I_2(x)$ .

We note that when both slits are open, the obtained intensity  $I(x)$  is

$$I(x) \neq I_1(x) + I_2(x). \tag{27}$$

This result seem to be in contradiction to the particle theory. However, it can easily be explained in the framework of the wave theory. If  $E_1(x)$  and  $E_2(x)$  represent, in complex notation, the electric fields produced at point  $x$  by the two slits, then when both slits are open, the total electric field at this point is

$$E(x) = E_1(x) + E_2(x).$$

Since  $I(x) \propto |E(x)|^2$ , where  $|E(x)|$  is the amplitude of the electric field, we have

$$I(x) \propto |E(x)|^2 = |E_1(x) + E_2(x)|^2 \neq |E_1(x)|^2 + |E_2(x)|^2. \quad (28)$$

(The difference, of course, is the interference term).

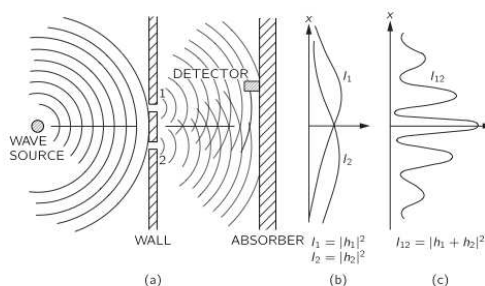


Fig. 1-2. Interference experiment with water waves.

Fig. 4.— Interference pattern through a double slit experiment (the one shown here is done with water waves, though the results with light are identical). Figure taken from Feynman lectures on physics, Vol. 3.

Now, let us conduct a second experiment: keeping both slits open, we dim the source of light, until the emitted photons strike the screen practically one by one. In this case, the interference must diminish, and the fringes should disappear.

When conducting the experiment, we find the following:

1. When looking at the screen for a short time, we observe that each photon produces a **localized impact**, rather than a (weak) interference pattern.

**The wave interpretation must be rejected.**

2. When taking a long exposure, we find that **the fringes reappear**.

Therefore, **the purely corpuscular interpretation must be rejected as well.**

What we see is that **while a single photon seem to impact the screen in an individual, random manner, when we collect many individual photons, interference pattern appears.**

We seem to encounter a paradox: if we treat each photon individually, how does the photon “know” if both slits or only one of them is open? Classically, the photon should pass through only one slit! The resulting pattern from two open slits should therefore be a simple sum of the pattern we get when only one slit is open - **but it isn't !**

We could try and put a detector behind one slit, to examine if the photon passed through this slit. We could detect photons; but the photons passing through the other slit, will not show the interference pattern. This leads to the first conceptual issue:

**A measurement disturbs the system in a fundamental way.**

The fact that the photons gradually build an interference pattern also implies that we do not know in advanced where they will end up on the screen; despite the fact that all the photons are emitted under the same conditions. Thus, the second conceptual issue is that contrary to classical mechanics,

**The initial conditions do not fully determine the (classical) motion of a particle.**

(In fact, as we will shortly see, in quantum mechanics there is no motion at all!).

The gradual build up of interference pattern by individual, distinctive photons leads to a very surprising, yet an inevitable conclusion from this experiment:

**Each individual photon passes through both slits.**

Namely, in some sense the photon 'interfere with itself'.

How can a photon be described then? We use the analogy with the classical theory of waves introduced above (which we cannot use directly, since it does not consider the particle nature of light). In describing a photon (any particle, in fact), we introduce a **wave function**  $\psi(x, y, z, t)$ . The wave function contains all the possible information about the particle (photon, in our case).

The wave function  $\psi(\vec{r}, t)$  is interpreted as a **probability amplitude of the particle's presence**, namely: *if we measure the particle's location*, we have some probability  $P$  of finding it in a particular location  $\vec{r} = (x, y, z)$  at time  $t$  (**Max Born**). This probability is

$$P(x, y, z, t) \propto |\psi(x, y, z, t)|^2 \tag{29}$$

In general (from reasons which will become clear later) the wave function  $\psi$  is complex. However, clearly,  $P$  is a real, positive number.

Let  $\psi_A, \psi_B$  be the wavefunctions of the photon corresponding to waves spreading from slits A and B, respectively. These correspond to an experiment done when only one slit is



open. The probability distributions are  $P_A \propto |\psi_A|^2$ , and  $P_B \propto |\psi_B|^2$ . When both slits are open, then the wave function  $\psi = \psi_A + \psi_B$ , and the corresponding probability distribution is

$$P \propto |\psi_A + \psi_B|^2. \quad (30)$$

Clearly,  $P \neq P_A + P_B$ . **The concept of wavefunction therefore enables to capture both key results:** (1) the fact that the location of each individual photon on the screen is random (but has a finite probability, different for each location), and (2) the fact that the interference pattern is different when the two slits are open than the pattern obtained as a sum of two single open slits.

**Important note.** Mathematically, wave functions are treated similarly to ‘regular’ waves. However, physically, they have a very different interpretation. Waves describe a physical perturbation in a medium. As such, their shape must be real. **Wave functions**, on the other hand, tell us the probability of finding the particle in a given location *if we make a measurement*. Since this probability is  $\propto |\psi|^2$ , wave functions don’t have to be real (and indeed, they are not), but imaginary functions. Note that we do not measure  $\psi$  directly, but can only measure  $P \propto |\psi|^2$  !

### 3. Matter particles and matter waves

#### 3.1. De Broglie relations

Recall that de-Broglie postulated that material particles have wave-like aspect. For a particle with energy  $E$  and momentum  $\vec{p}$ , the associate frequency  $\nu$ , angular frequency,  $\omega = 2\pi\nu$ , wavelength,  $\lambda$  and wave vector,  $\vec{k}$  ( $|\vec{k}| = 2\pi/\lambda$ ) are

$$\begin{aligned} E &= h\nu = \hbar\omega, \\ \lambda &\equiv \frac{2\pi}{|\vec{k}|} = \frac{h}{|\vec{p}|}, \\ \vec{p} &= \hbar\vec{k}. \end{aligned} \quad (31)$$

We made use of the convention

$$\hbar \equiv \frac{h}{2\pi}. \quad (32)$$

### 3.2. Matter wave functions

We apply the idea of wave functions introduced above to matter particles. This means the following:

- Instead of particle’s *trajectory* discussed in classical physics, we introduce the concept of (time-varying) **quantum state**. This quantum state is described by the **wave function**,  $\psi(\vec{r}, t)$ , which contain all possible information on the particle.
- The wave function is interpreted as **probability amplitude of the particle’s presence (when measured)**. The probability of the particle to be, at time  $t$ , in a volume element  $d^3r = dx dy dz$  around point  $\vec{r}$  is

$$dP(\vec{r}, t) = |\psi(\vec{r}, t)|^2 d^3r. \quad (33)$$

Since, close enough to  $\vec{r}$  (namely,  $d\vec{r} \rightarrow 0$ ) this probability  $\rightarrow 0$ , the function  $|\psi(\vec{r}, t)|^2$  is denoted as **probability density**.

We know that, when considering a single particle, the probability of finding the particle *somewhere* in space must be equal to 1. Thus, we have

$$\int_V dP(\vec{r}, t) dV = \int_V |\psi(\vec{r}, t)|^2 d^3r = 1. \quad (34)$$

A wave function which fulfills this condition (namely, for which the integral on the left hand side of equation 34 is finite), is called **square integrable**. When the right hand side is equal to 1, it is also **normalized** (though often we will absorb the term “normalized” into the “square integrable”).

## 4. The time-dependent Schrödinger equation

The next question is how the wave function of a particle evolves in time.

Consider a free particle of mass  $m$  moving non-relativistically in 1-d. The particle’s momentum is  $\vec{p} = p\hat{x}$ , and its kinetic energy is  $E = p^2/2m$ .

We associate with this particle a simple (plane) wave, namely its wavefunction is

$$\psi(x, t) = Ae^{i(kx - \omega t)}. \quad (35)$$

This plane wave obeys, of course, the wave equation:  $\partial^2\psi/\partial t^2 = v^2\partial^2\psi/\partial x^2$ , with  $v = \omega/k$ . Using de-Broglie relations (Equations 31), we can write this wavefunction as

$$\psi(x, t) = Ae^{i(px-Et)/\hbar} \quad (36)$$

If we differentiate Equation 36 with respect to time, we obtain

$$\frac{\partial\psi}{\partial t} = -i\frac{E}{\hbar}\psi \quad (37)$$

Furthermore, if we differentiate it twice with respect to  $x$ , we obtain

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{p^2}{\hbar^2}\psi \quad (38)$$

Substituting the relation  $E = p^2/2m$ , we obtain the *time dependent Schrödinger equation* for the evolution of  $\psi$ ,

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \quad (39)$$

The generalization from 1-d to 3-d is straightforward; instead of  $\frac{\partial^2}{\partial x^2}$  we write

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (40)$$

and obtain

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r}, t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}, t) \quad (41)$$

This result can be easily generalized to particles that move in field of force. If the force  $\vec{F}$  acting on a particle is derived from a potential,

$$\vec{F}(\vec{r}, t) = -\vec{\nabla}V(\vec{r}, t), \quad (42)$$

then, as  $E$  denotes the total particle's energy (kinetic + potential), the particle's momentum  $p$  is given by

$$\frac{p^2}{2m} = E - V. \quad (43)$$

Repeating the same steps, one concludes that when a potential is introduced,

$$\boxed{i\hbar\frac{\partial}{\partial t}\psi(\vec{r}, t) = \left[ -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}, t) \right] \psi(\vec{r}, t).} \quad (44)$$

This is the **time-dependent Schrödinger equation** for a (non-relativistic) particle moving in a potential. It is the basic equation of (non-relativistic) quantum mechanics, and was

introduced by Schrödinger in 1926. Note that, similar to Newton’s laws, it follows some basic postulates we made; No one can validate these assumptions (hence, Schrödinger equation). Its proof lies on its ability to provide accurate predictions to all experiments carried in the past 90 years or so.

Schrödinger equation is a **linear, differential equation**; this means that every superposition of plane waves that satisfy this equation will also satisfy it. Namely, if  $\psi_1$  and  $\psi_2$  are solutions of this equation, so will be  $c_1\psi_1 + c_2\psi_2$ , where  $c_1$  and  $c_2$  are complex numbers. This is important, because a single plane wave is *not* square-integrable; hence, it cannot represent a physical particle (more on that below).

The appearance of  $i$  in the left hand side implies that, as opposed to regular waves, **the wave function  $\psi$  must be complex**<sup>1</sup>. Thus,

$$|\psi|^2 = \psi^*\psi. \tag{45}$$

## 5. Wave packets

A pure plane wave function,

$$\psi(x, t) = Ae^{i(kx - \omega t)}$$

is **not** square integrable, namely  $|\psi(x, t)|^2 = \psi^*\psi = |A|^2$  (we consider here and below the 1-d case, for simplicity). This follows from the fact that

$$\int_x P(x, t)dx = \int_x |\psi(x, t)|^2 dx = |A|^2 \int_{-\infty}^{+\infty} dx, \tag{46}$$

which is infinite, and clearly  $\neq 1$ .

As we will see, there is a physical reason for this. For a pure plane wave,  $|\psi|^2 = |A|^2$ . This means, that if we represent a particle by a pure plane wave, there is an equal chance of finding the particle at any point in space. Thus, this is an “ideal” situation, in which the particle is completely *delocalized*. In this case, the particle’s momentum,  $p = \hbar k$  is perfectly well defined, as  $k$  is known.

The physical way out is to abandon the idea that the particle have a well defined momentum. Mathematically, we use the superposition principle, from which it follows that every linear combination of plane waves is also a solution to Schrödinger equation. We will

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<sup>1</sup>Note that this follows from the fact that  $E \propto p^2$ , and de-Broglie relations,  $E = \hbar\omega$  and  $|\vec{p}| = \hbar|\vec{k}|$ .

therefore superpose plane waves with different momenta, to form a **wave packet**. The probability amplitude of the wave packet could be normalized to unity.

Using the superposition principle, we define the 1-d wavepacket as a combination of plane waves with different wave vectors  $k$ ,

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} g(k) e^{i(kx - \omega(k)t)} dk \quad (47)$$

The function  $g(k)$  is simply the **Fourier transform** of  $\psi(x, t = 0)$ :

$$g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \psi(x, t = 0) e^{-ikx} dx \quad (48)$$

Since this is always true, it implies that the analysis is valid for any particle - not just free.

Consider the wave packet at  $t = 0$ :

$$\psi(x, t = 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} g(k) e^{ikx} dk. \quad (49)$$

The probability amplitude is maximal when the different plane waves interfere constructively. In order to quantify this, let us write  $g(k)$  in the form

$$g(k) = |g(k)| e^{i\alpha(k)}, \quad (50)$$

and assume that  $\alpha(k)$  varies smoothly within the interval  $[k_0 - \Delta k/2, k_0 + \Delta k/2]$ , where  $|g(k)|$  is non-negligible.

We can Taylor expand  $\alpha(k)$  around  $k = k_0$ ,

$$\alpha(k) = \alpha(k_0) + (k - k_0) \left( \frac{d\alpha}{dk} \right)_{k=k_0} + \dots \quad (51)$$

Equation 49 takes the form:

$$\begin{aligned} \psi(x, t = 0) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} |g(k)| e^{i(kx + \alpha(k))} dk \\ &\simeq \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} |g(k)| e^{i(kx + \alpha(k_0) - (k - k_0)x_0)} dk \\ &\simeq \frac{e^{i(k_0 x + \alpha(k_0))}}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} |g(k)| e^{i(k - k_0)(x - x_0)} dk \end{aligned} \quad (52)$$

where

$$x_0 \equiv - \left( \frac{d\alpha}{dk} \right)_{k=k_0} \quad (53)$$

Looking at the integrand, we see that when  $|x - x_0|$  is large, the exponent oscillates many times within the interval  $\Delta k$ . The contributions of these oscillations then cancel each other out, and the integral over  $k$  becomes negligible.

On the other hand, for  $x \simeq x_0$ , the integrand barely oscillates, and the wave function  $|\psi(x, 0)|$  gets its maximum value. Thus, the wave packet is centered at  $x_{\max} = x_0 = -\left(\frac{d\alpha}{dk}\right)_{k=k_0}$ .

An estimate of the domain in which  $\psi$  obtains its maximum value is found by setting

$$(k - k_0)(x - x_0) \simeq 1 \tag{54}$$

or

$$\Delta k \cdot \Delta x \gtrsim 1. \tag{55}$$

This is a classical relation between the widths of two functions which are Fourier transforms of each other.

The wave packet, thus centered around  $k_0$  moves at the *group velocity*,

$$v_g = \left(\frac{d\omega}{dk}\right)_{k=k_0} = \left(\frac{dE}{dp}\right)_{p=p_0} = \frac{p_0}{m}$$

(see Equation 21), where we used de-Broglie relations,  $p_0 = \hbar k_0$  and  $E = p^2/2m$ . This result should be of no surprise: this is the velocity that a particle have in the **classical limit**, where both  $\Delta x$  and  $\Delta p$  are too small to be measured.

Note that this velocity is different than the *phase velocity* of each individual wave, and in particular the phase velocity of the central frequency,

$$v_\psi = \frac{\omega}{k} = \frac{E}{p} = \frac{p_0}{2m} = \frac{v_g}{2}$$

by a factor 2.

## 6. Heisenberg uncertainty relation

<sup>2</sup> Return, for a moment to the plane wave,  $e^{i(kx-\omega t)}$ . We saw that it cannot represent a physical wavepacket, since this function is not square-integrable. Physically, it implies that

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<sup>2</sup>I am giving a very sketchy proof here. An exact proof will be given later, and/or in 4th year QM. An exact proof is based on the fact that for any two observables  $A$  and  $B$ , there exists an uncertainty of  $\Delta A \cdot \Delta B \geq \frac{1}{2}|\langle[A, B]\rangle|$ . The meaning of all this will become clear later.

the particle can be found anywhere in space with equal probability. However, its **momentum** ( $p = \hbar k$ ) is exactly known. We can think of a plane wave as a limiting case of equation 55, where  $\Delta p = \hbar \Delta k \rightarrow 0$ , while  $\Delta x \rightarrow \infty$ .

Returning now to the wave-packet representation (Equation 47),  $\psi(x, t)$  is a *linear superposition* of plane waves, each with different  $k$  (different momentum). For a particle represented by a wave packet, its position is known only up to uncertainty  $\Delta x$ , and its wave vector is also known, but only up to uncertainty  $\Delta k$ . The function  $|g(k)|^2$  then tells us the probability of the particle to have wave vector  $k$  (momentum  $p = \hbar k$ ).

This discussion leads to the following result. We can re-write Equation 55 as

$$\boxed{\Delta x \cdot \Delta p_x \gtrsim \hbar} \quad (56)$$

This is known as **Heisenberg uncertainty relation**. It implies that we cannot measure simultaneously both the position and momentum of a particle to accuracy better than  $\hbar$ . There is no classical analogue to this relation.

The wave function interpretation enables to expand Heisenberg uncertainty principle to the time-energy domain. Consider a particle that is described by a wave function of width  $\Delta x$ . It travels at group velocity  $v_g$ , and therefore the time it takes it to pass a certain point cannot be precisely determined, but only up to uncertainty

$$\Delta t \approx \frac{\Delta x}{v_g}.$$

Furthermore, this wave packet has a spread in momentum space, resulting in an uncertainty in the particle's energy,

$$\Delta E \approx \frac{\partial E}{\partial p} \Delta p = v_g \Delta p.$$

Overall, we get

$$\Delta E \cdot \Delta t \approx \Delta x \cdot \Delta p_x \gtrsim \hbar. \quad (57)$$

## 7. Conservation of probability and probability current density

**The basic interpretation of the wave function is *statistical in nature*.** Square of the wave functions are interpreted as the probability of finding a particle at position  $\vec{r}$  and time  $t$ ,

$$dP(\vec{r}, t) = |\psi(\vec{r}, t)|^2 d^3r$$

(see Equation 33).

When considering a single particle, since we know it must exist **somewhere**, the wavefunction must be normalized such that

$$\int_{\text{all space}} P(\vec{r}, t) dV = \int_{\text{all space}} |\psi(\vec{r}, t)|^2 d^3r = \int_{\text{all space}} \psi^* \psi d^3r = 1 \quad (58)$$

(see Equation 34).

As time changes, the total probability of finding the particle somewhere is still 1; therefore, we can write

$$\frac{\partial}{\partial t} \int_{\text{all space}} P(\vec{r}, t) dV = 0. \quad (59)$$

Consider now a **finite volume** in space,  $V$ . We have

$$\frac{\partial}{\partial t} \int_V P(\vec{r}, t) dV = \int_V \left[ \psi^* \left( \frac{\partial \psi}{\partial t} \right) + \left( \frac{\partial \psi^*}{\partial t} \right) \psi \right] d^3r. \quad (60)$$

The time dependence of  $\psi$  and  $\psi^*$  are not arbitrary, but are governed by the Schrödinger equation (Equation 44),

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}, t) \right] \psi(\vec{r}, t),$$

and its complex conjugate,

$$-i\hbar \frac{\partial}{\partial t} \psi^*(\vec{r}, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}, t) \right] \psi^*(\vec{r}, t). \quad (61)$$

(Note that the potential  $V(\vec{r}, t)$  is a real quantity). We thus get

$$\begin{aligned} \frac{\partial}{\partial t} \int_V P(\vec{r}, t) dV &= \frac{i\hbar}{2m} \int_V [\psi^*(\nabla^2 \psi) - (\nabla^2 \psi^*)\psi] d^3r \\ &= \frac{i\hbar}{2m} \int_V \vec{\nabla} \cdot [\psi^*(\vec{\nabla} \psi) - (\vec{\nabla} \psi^*)\psi] d^3r \\ &\equiv - \int_V \vec{\nabla} \cdot \vec{j} d^3r \end{aligned} \quad (62)$$

where in the last line we introduced the vector

$$\vec{j}(\vec{r}, t) \equiv \frac{\hbar}{2mi} [\psi^*(\vec{\nabla} \psi) - (\vec{\nabla} \psi^*)\psi]. \quad (63)$$

The vector  $\vec{j}$  is called **the probability current density**.

As a final step, we use Green's theorem (which is equivalent to the divergence theorem in 2-d)<sup>3</sup>, to write Equation 62 as

$$\frac{\partial}{\partial t} \int_V P(\vec{r}, t) dV = - \int_S \vec{j} \cdot d\vec{S}. \quad (64)$$

---

<sup>3</sup>The divergence theorem states that the outward flux of a vector field through a closed surface is equal to the volume integral of the divergence over the region inside the surface, or  $\int_V (\vec{\nabla} \cdot \vec{F}) dV = \int_S (\vec{F} \cdot \vec{n}) dS$ , where  $S$  is the surface enclosing  $V$  and  $n$  is a unit vector pointing outwards normal to  $S$ .



Note that equation 64 is valid for a finite volume,  $V$ . If we extend  $V$  to infinity, the surface  $S$  extends to infinity as well, and the surface integral (the right hand side of Equation 64) must vanish, in order for  $\psi$  to be square integrable. We thus proved that in this case

$$\frac{\partial}{\partial t} \int_{V \rightarrow \infty} P(\vec{r}, t) dV = 0, \quad (65)$$

namely that the **Schrödinger equation conserves the probability.**

We can further write Equation 62 in a differential form,

$$\frac{\partial}{\partial t} P(\vec{r}, t) + \vec{\nabla} \cdot \vec{j}(\vec{r}, t) = 0 \quad (66)$$

This equation has the same form as the *continuity equation*, which expresses conservation of charge/mass/particle number etc in hydrodynamics or electrodynamics. Here, the conserved quantity is the probability density  $P$ , thereby justifying the name “probability current density” for  $\vec{j}$ , as it represents the “rate of leak” (or current) of the probability (of finding the particle inside a volume) through the surface of  $V$ , for a system with no sources or sinks.

As a final comment, note that we may write the probability current density as

$$\vec{j}(\vec{r}, t) = \text{Re} \left[ \psi^* \frac{\hbar}{im} \vec{\nabla} \psi \right] \quad (67)$$

This further shows that for real  $\psi$ ,  $\vec{j}$  vanishes; non-zero probability current requires the wave function  $\psi$  to be complex !.

## 8. The time independent Schrödinger equation

Often in physics, one encounters problems in which the potential  $V$  is independent on time, so  $V = V(\vec{r})$ . When this is the case, Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right] \psi(\vec{r}, t)$$

(Equation 44) takes a particular simple form.

In this case, we can search for a solution of the form

$$\psi(\vec{r}, t) = \phi(\vec{r})\chi(t) \quad (68)$$

This is known as *separation of variables*, as  $\phi$  is only a function of space, and  $\chi$  is only a function of time.

Substituting this solution in Schrödinger equation, we get

$$i\hbar\phi(\vec{r})\frac{d\chi(t)}{dt} = \chi(t) \left[ -\frac{\hbar^2}{2m}\nabla^2\phi(\vec{r}) + V(\vec{r})\phi(\vec{r}) \right] \quad (69)$$

Dividing both sides by  $\phi(\vec{r})\chi(t)$ , we get

$$\frac{i\hbar}{\chi(t)}\frac{d\chi(t)}{dt} = \frac{1}{\phi(\vec{r})} \left[ -\frac{\hbar^2}{2m}\nabla^2\phi(\vec{r}) + V(\vec{r})\phi(\vec{r}) \right] \quad (70)$$

We see that the left hand side depends only on time,  $t$ , while the right hand side depends only on  $\vec{r}$ . This is possible only if both sides are constants. This constant has the dimension of energy, so let us denote it  $E$ . We thus find

$$i\hbar\frac{d\chi(t)}{dt} = E\chi(t) \quad (71)$$

and

$$\boxed{\left[ -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}) \right] \phi(\vec{r}) = E\phi(\vec{r})} \quad (72)$$

Equation 72 is known as **time-independent Schrödinger equation**.

The solution to Equation 71 is straightforward,

$$\chi(t) = Ae^{-iEt/\hbar} = Ae^{-i\omega t} \quad (73)$$

where we will chose to set  $A = 1$  (we can absorb the constant  $A$  in  $\phi(\vec{r})$ ). Thus, the solution to the Schrödinger equation is given by

$$\psi(\vec{r}, t) = \phi(\vec{r})e^{-iEt/\hbar}, \quad (74)$$

if  $\phi(\vec{r})$  is a solution to the time-independent Schrödinger equation (Equation 72).

Solution of the form given by Equation 74 is known as a **stationary solution** of the Schrödinger equation. It leads to **time-independent probability density**, since

$$|\psi(\vec{r}, t)|^2 = |\phi(\vec{r})|^2, \quad (75)$$

which is constant in time. This is the origin of the name “stationary state”.

In a stationary state that solves the time-independent Schrödinger equation, only the energy  $E$  appears; thus, **a stationary state is a state with a well-defined energy**. Such states are known as **energy eigenstates**, which we will define properly later.

Recall that in classical mechanics, the energy is constant of motion; in quantum mechanics, there exist well-determined energy states.

### 8.1. Example 1: a free particle

Let us illustrate the discussion by considering few basic examples. Here and below, we will treat 1-d problems, for simplicity.

Let us begin by considering the case of constant potential,  $V(x) = V_0$ . The force acting on a particle  $F = -dV/dx = 0$ , and thus the particle is *free*. Without loss of generality, we take  $V_0 = 0$  - addition of constant simply shifts the energies (more accurately: energy eigenvalues)<sup>4</sup> of the time-independent Schrödinger equation.

The (1-d) time independent Schrödinger equation (Equation 72) takes the form

$$-\frac{\hbar^2}{2m} \frac{d^2\phi(x)}{dx^2} = E\phi(x) \quad (76)$$

We can write

$$k^2 = \frac{2m}{\hbar^2} E \quad (77)$$

and obtain two linearly-independent solutions to Equation 76 (note that this is the equation of classical simple harmonic oscillator)

$$\phi(x) = Ae^{ikx} + Be^{-ikx}, \quad (78)$$

where  $A$  and  $B$  are arbitrary constants.

Clearly, for the solution to be physical,  $k$  must be real; otherwise,  $\phi(x)$  would go to infinity as  $x \rightarrow \pm\infty$ . This translates, via Equation 77 to the condition  $E \geq 0$ . Note that currently, there is no other restriction on the value of  $E$ , which can obtain *continuous* values between  $0 \dots \infty$ . Each value of  $E$  is **doubly degenerated**, since there are two linearly independent wave functions,  $e^{ikx}$  and  $e^{-ikx}$  that correspond to the same positive energy.

With the use of Equation 74, we find that the general plane-wave solution of the Schrödinger equation is

$$\psi(x, t) = (Ae^{ikx} + Be^{-ikx}) e^{-iEt/\hbar} = Ae^{i(kx-\omega t)} + Be^{-i(kx+\omega t)}. \quad (79)$$

We can look at particular cases. If we set  $B = 0$ , we find that the first solution,  $Ae^{i(kx-\omega t)}$  represents a wave traveling to the right ( $+x$  direction). Similarly, setting  $A = 0$ , the second solution,  $Be^{-i(kx+\omega t)}$  represents a wave traveling in the negative ( $-x$ ) direction.

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<sup>4</sup>The concept of “eigenvalues” would be properly introduced below.

The probability density corresponding to the first solution,  $Ae^{i(kx-\omega t)}$ , is

$$P = |\psi(x, t)|^2 = |A|^2.$$

This is independent on both time and space; physically, we cannot say anything about the position of the particle on the  $x$  axis. (We do know precisely its momentum,  $p_x = \hbar k$  – in accordance to Heisenberg uncertainty principle).

The probability current density corresponding to the plane wave  $Ae^{i(kx)}$  is (see Equation 63,  $\vec{j}(\vec{r}, t) \equiv \frac{\hbar}{2mi} [\psi^*(\vec{\nabla}\psi) - (\vec{\nabla}\psi^*)\psi]$ ):

$$\begin{aligned} j &= \frac{\hbar}{2mi} [A^* e^{-ikx} A i k e^{ikx} - A e^{ikx} A^* (-ik) e^{-ikx}] \\ &= \frac{\hbar k}{m} |A|^2 = \frac{p}{m} |A|^2 = v_g |A|^2. \end{aligned} \quad (80)$$

We can also write this as  $j = v_g P$ ; this is a similar expression to the classical relation between flux, velocity and density in hydrodynamics.

Finally, repeating a similar calculation for the complete wavefunction in Equation 78,  $\phi(x) = Ae^{ikx} + Be^{-ikx}$  we obtain the associated current density,

$$j = \frac{\hbar k}{m} (|A|^2 - |B|^2) = v_g (|A|^2 - |B|^2). \quad (81)$$

## 8.2. Example 2. Infinite square well.

As we already saw (Section 5, Equation 46), the free (plane) wave solution cannot represent a physical particle, since the wave function is not square integrable, but is, in fact infinite:

$$\int_{-\infty}^{+\infty} |\psi(x, t)|^2 dx = |A|^2 \int_{-\infty}^{+\infty} dx.$$

In principle, this problem would be solved when we treat wavepackets.

Here, we consider another solution: we enclose the particle in a box, thereby imposing boundary conditions at the walls. We would set the (1d) box length to be  $L$ , a free parameter. After finding the solution, we could take the limit  $L \rightarrow \infty$ .

Let us assume that the potential is 0 inside the box, and infinite outside of it, namely

$$V(x) = \begin{cases} \infty & x < 0 \\ 0 & 0 \leq x \leq L \\ \infty & x > L \end{cases} \quad (82)$$

This sets boundary conditions at  $x = 0$  and  $x = L$ , as  $\psi(x = 0, t) = \psi(x = L, t) = \phi(x = 0) = \phi(x = L) = 0$ .

In the range  $0 \leq x \leq L$ , the potential is  $V = 0$ , and thus the solution given in Equations 77 and 78 hold. By imposing the boundary condition  $\phi(x = 0) = 0$  we find that  $A = -B$ , and thus

$$\phi(x) = A (e^{ikx} - e^{-ikx}) = 2iA \sin(kx). \quad (83)$$

By imposing the boundary condition  $\phi(x = L) = 0$ , we find  $\sin(kL) = 0$ ,

$$k = \frac{n\pi}{L}, \quad n = 1, 2, 3, \dots \quad (84)$$

from which (see Equation 77)

$$\boxed{E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \left( \frac{n^2 \pi^2}{L^2} \right)} \quad (85)$$

We see that in this case, **the energy levels are quantized**; obviously, as  $L$  increases, the spacing between the energy levels decreases, so in the macroscopic case where  $L \rightarrow \infty$ , the spectrum becomes continuous.

The wave function can now be made square integrable,

$$\begin{aligned} \int_0^L \phi^* \phi &= 4A^2 \int_0^L \sin^2 \left( \frac{n\pi x}{L} \right) dx = 2A^2 L = 1, \\ \rightarrow A &= \frac{1}{\sqrt{2L}} \end{aligned} \quad (86)$$

from which we find the stationary wavefunctions

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin \left( \frac{n\pi x}{L} \right). \quad (87)$$

(note that the  $i$  in Equation 83 can be absorbed into the normalization of  $A$ ). The subscript “ $n$ ” denotes the dependence of  $\phi$  on the integer  $n$ . The first three functions are plotted in Figure 5.

### 8.3. Example 3: the potential step

Consider a potential step, namely

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x > 0 \end{cases} \quad (88)$$

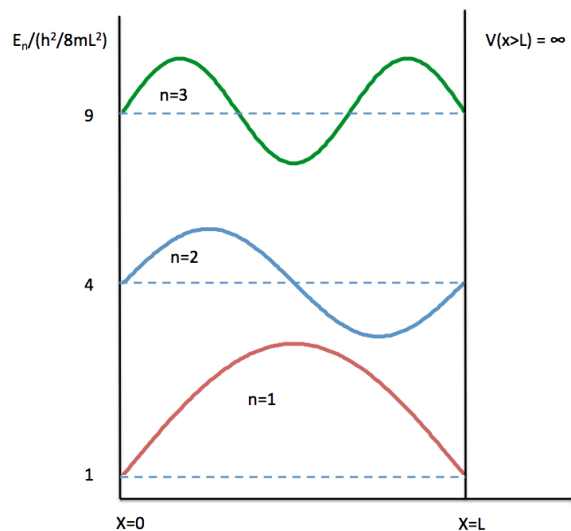


Fig. 5.— The first 3 stationary wavefunctions obtained in an infinite square well between  $x = 0$  and  $x = L$ .

In this case, the total energy  $E$  of the particle is important, as one needs to discriminate between two scenarios: (I)  $E < V_0$  and (II)  $E > V_0$ .

Classically, if  $E < V_0$ , then a particle incidenting from the left will reach the barrier at  $x = 0$  and would not be able to cross it, as it does not have sufficient kinetic energy; instead, it would always be **reflected** by the barrier.

On the other hand, if  $E > V_0$ , as the particle reaches the barrier it will always be **transmitted** (see Figure 6).

Let us now consider this problem quantum mechanically. We first extend the discussion on stationary states to the case of non-zero potential. The time-independent Schrödinger equation (72) takes the form (see also Equation 76):

$$-\frac{\hbar^2}{2m} \frac{d^2\phi(x)}{dx^2} = (E - V)\phi(x) \quad (89)$$

There are three cases:

1.  $E > V$ .

In this case, the analysis that led to Equation 78 holds, and the solution is

$$\phi(x) = Ae^{ikx} + Be^{-ikx}, \quad (90)$$

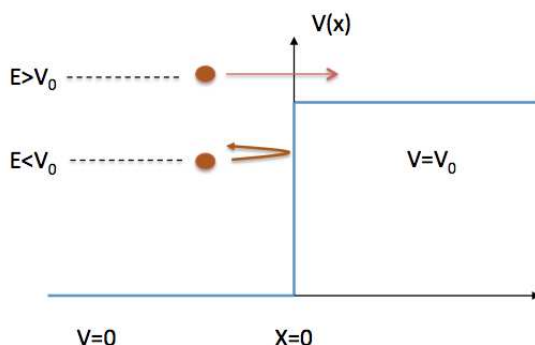


Fig. 6.— Finite potential barrier. Classically, if a particle that emerges from the left has energy  $E > V_0$  it will cross the barrier, while if  $E < V_0$  it will be reflected.

where now

$$k^2 = \frac{2m}{\hbar^2}(E - V). \quad (91)$$

2.  $E < V$ .

The solution to Equation 89 is

$$\phi(x) = Ce^{\rho x} + De^{-\rho x}, \quad (92)$$

where

$$\rho^2 = \frac{2m}{\hbar^2}(V - E). \quad (93)$$

3.  $E = V$ .

In this special case,  $\phi(x)$  is a linear function of  $x$ .

Before solving the problem, we note the following: **At the boundary**, where  $V(x)$  is discontinuous, both the wavefunction  $\phi(x)$  and its first derivative,  $d\phi(x)/dx$  are continuous. (The second derivative,  $d^2\phi/dx^2$  does not have to be continuous). This follows from the fact that the probability current density,  $\vec{j} \propto \psi^*(\vec{\nabla}\psi) - (\vec{\nabla}\psi^*)\psi$  (Equation 63) must be continuous everywhere.

Armed with this information, let us now consider the potential step problem.

1.  $E > V_0$ .

The solution to the Schrödinger equation in the two regimes ( $x < 0$  and  $x > 0$ ) can be written as

$$\begin{aligned} \phi_1(x) &= Ae^{ik_1x} + Be^{-ik_1x}, & (x < 0) \\ \phi_2(x) &= Ce^{ik_2x} + De^{-ik_2x}, & (x > 0) \end{aligned} \quad (94)$$

where

$$\begin{aligned} k_1 &= \left(\frac{2m}{\hbar^2}E\right)^{1/2}, \\ k_2 &= \left[\frac{2m}{\hbar^2}(E - V_0)\right]^{1/2}. \end{aligned} \quad (95)$$

In order to make progress, we must consider a physical scenario. Assume a particle coming from the left ( $x = -\infty$ ). This implies  $D = 0$ , since the last term in Equation 94 correspond to a reflected particle in the  $+x$  region that travels to the left - and there is nothing in the region of positive  $x$  that can cause such reflection.

We are left with

$$\phi(x) = \begin{cases} Ae^{ik_1x} + Be^{-ik_1x}, & (x < 0) \\ Ce^{ik_2x} & (x > 0) \end{cases} \quad (96)$$

Clearly, the physical situation is of **incident** wave (of amplitude  $A$ ), a **reflected** wave (of amplitude  $B$ ) - both in the region  $x < 0$ , and a **transmitted** wave (of amplitude  $C$ ) in the region  $x > 0$ .

We already see a **key difference** from classical physics, as the incoming particle has a non-zero probability of being reflected, despite the fact that  $E > V_0$ .

The values of  $A$ ,  $B$  and  $C$  are found by the continuity of  $\phi$  and  $d\phi/dx$  at  $x = 0$ . The continuity of  $\phi(x)$  gives

$$A + B = C \quad (97)$$

and the continuity of  $d\phi(x)/dx$  gives

$$k_1(A - B) = k_2C \quad (98)$$

from which

$$\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2} \quad (99)$$

and

$$\frac{C}{A} = \frac{2k_1}{k_1 + k_2}. \quad (100)$$

We define the **reflection coefficient**,  $R$  as the ratio of the reflected current (=intensity of the reflected probability current density) to the incident current. Using Equation 81,  $j = v_g(|A|^2 - |B|^2)$ , the reflected current is  $v_g|B|^2$ , while the incident current is  $v_g|A|^2$ . Their ratio is therefore

$$R = \frac{v_g|B|^2}{v_g|A|^2} = \frac{|B|^2}{|A|^2} = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} = \frac{\left[1 - \left(1 - \frac{V_0}{E}\right)^{1/2}\right]^2}{\left[1 + \left(1 - \frac{V_0}{E}\right)^{1/2}\right]^2} \quad (101)$$



Similarly, the current density for the transmitted wave is  $j = \frac{\hbar k_2}{m} |C|^2$  (see Equation 81). The transmission coefficient  $T$ , defined in a similar way to the reflection coefficient, is

$$T = \frac{k_2 |C|^2}{k_1 |A|^2} = \frac{4k_1 k_2}{(k_1 + k_2)^2} = \frac{4 \left(1 - \frac{V_0}{E}\right)^{1/2}}{\left[1 + \left(1 - \frac{V_0}{E}\right)^{1/2}\right]^2} \quad (102)$$

Clearly, both  $R$  and  $T$  depend only on the ratio  $V_0/E$ . It is easy to verify that  $R+T = 1$ : physically, the particle is either transmitted or reflected.

It is important not to get confused: the particle is **either transmitted or reflected, but not both**. Equations 101, 102 tells us the **probability** of the particle to be transmitted / reflected, when encountering a potential barrier  $V_0$ . **As opposed to classical mechanics, there is some probability that the particle will be reflected, even though  $E > V_0$ .**

The reflection coefficient (Equations 101, 109) is plotted in Figure 7.

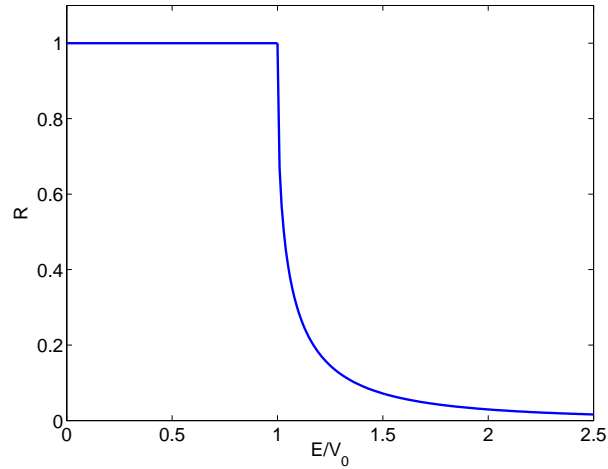


Fig. 7.— Reflection coefficient,  $R$ , as a function of the particle energy,  $E/V_0$ .

## 2. $E < V_0$ .

In this case, the solution to Schrödinger equation is

$$\begin{aligned} \phi_1(x) &= Ae^{ik_1x} + Be^{-ik_1x}, & (x < 0) \\ \phi_2(x) &= Ce^{\rho x} + De^{-\rho x}, & (x > 0) \end{aligned} \quad (103)$$

where

$$\begin{aligned} k_1 &= \left(\frac{2m}{\hbar^2} E\right)^{1/2}, \\ \rho &= \left[\frac{2m}{\hbar^2} (V_0 - E)\right]^{1/2}. \end{aligned} \quad (104)$$

(see equations 92, 93).

In order for the solution to remain finite at  $+x \rightarrow \infty$ , we must demand  $C = 0$ .

The continuity of  $\phi$  at  $x = 0$  gives

$$A + B = D \quad (105)$$

and the continuity of  $d\phi/dx$  gives

$$ik_1(A - B) = -\rho D. \quad (106)$$

Simple algebra now gives

$$\frac{B}{A} = \frac{k_1 - i\rho}{k_1 + i\rho} = \frac{1 - i\left(\frac{V_0}{E} - 1\right)^{1/2}}{1 + i\left(\frac{V_0}{E} - 1\right)^{1/2}} \quad (107)$$

and

$$\frac{D}{A} = \frac{2k_1}{k_1 + i\rho} = \frac{2}{1 + i\left(\frac{V_0}{E} - 1\right)^{1/2}} \quad (108)$$

The reflection coefficient is

$$R = \frac{|B|^2}{|A|^2} = \frac{|k_1 - i\rho|^2}{|k_1 + i\rho|^2} = 1 \quad (109)$$

Thus, similar to classical mechanics, the particle is always reflected.

However, note a crucial different between quantum mechanics and classical mechanics. The region  $x > 0$  is classically forbidden. However, quantum mechanically, there is a probability

$$P(x) = |D|^2 e^{-2\rho x} \quad (110)$$

of finding the particle in this region.

Thus, **a particle can penetrate classically forbidden region**. Its typical penetration length is

$$\Delta x \sim \frac{1}{2\rho} \propto (V_0 - E)^{-1/2}, \quad (111)$$

and it has an exponentially decaying probability of being found in regions of large  $x$ .

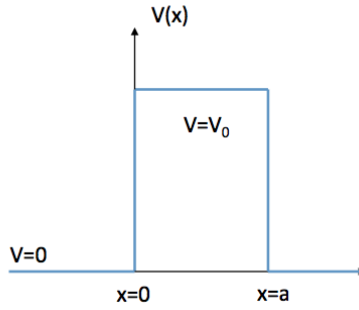


Fig. 8.— Potential barrier of width  $a$ .

#### 8.4. Example 4: the potential barrier

Consider next a potential barrier, of height  $V_0$  and width  $a$  (see Figure 8):

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 < x < a \\ 0 & x > a \end{cases} \quad (112)$$

In the external region,  $x < 0$  and  $x > a$  the particle is free, and therefore the solution to Schrödinger equation is

$$\begin{aligned} \phi(x) &= Ae^{ikx} + Be^{-ikx}, & x < 0 \\ \phi(x) &= Ce^{ikx} + De^{-ikx}, & x > a \end{aligned} \quad (113)$$

where  $k = (2mE/\hbar^2)^{1/2}$  (see Equation 77).

We again assume that the particle approaches the barrier from the left; thus, there is nothing in the  $+x$  ( $x > a$ ) that can cause a reflection, so we set  $D = 0$ . We encounter a similar situation to the potential step considered above, when  $A$  represents the amplitude of the **incident** wave,  $B$  the amplitude of the **reflected** wave, and  $C$  the amplitude of the **transmitted** wave.

The reflection and transmission coefficients,  $R$  and  $T$  are therefore defined similar to Equations 101 and 102,  $R = |B|^2/|A|^2$  and  $T = |C|^2/|A|^2$ .

Similar to the former analysis, we discriminate between the two scenarios:  $E < V_0$  and  $E > V_0$ .

1.  $E < V_0$

The wave function in the region  $0 < x < a$  is given by

$$\phi(x) = Fe^{\rho x} + Ge^{-\rho x},$$

with  $\rho = [2m(V_0 - E)/\hbar^2]^{1/2}$  (see Equations 103, 104).

Continuity of  $\phi$  and  $d\phi/dx$  at  $x = 0$  leads to

$$\begin{aligned} A + B &= F + G; \\ ik(A - B) &= \rho(F - G). \end{aligned} \quad (114)$$

Similarly, continuity of  $\phi$  and  $d\phi/dx$  at  $x = a$  leads to

$$\begin{aligned} Fe^{\rho a} + Ge^{-\rho a} &= Ce^{ika}; \\ \rho(Fe^{\rho a} - Ge^{-\rho a}) &= ikCe^{ika}. \end{aligned} \quad (115)$$

Using these equations, one can eliminate  $F$  and  $G$ , and find the reflection and transmission coefficients,

$$R = \frac{|B|^2}{|A|^2} = \left[ 1 + \frac{4k^2\rho^2}{(k^2 + \rho^2)\sinh^2(\rho a)} \right]^{-1} = \frac{V_0^2 \sinh^2(\rho a)}{4E(V_0 - E) + V_0^2 \sinh^2(\rho a)}, \quad (116)$$

and

$$T = \frac{|C|^2}{|A|^2} = \left[ 1 + \frac{(k^2 + \rho^2)^2 \sinh^2(\rho a)}{4k^2\rho^2} \right]^{-1} = \frac{4E(V_0 - E)}{4E(V_0 - E) + V_0^2 \sinh^2(\rho a)}. \quad (117)$$

Clearly,  $T + R = 1$ .

The result in Equation 117 is striking: **a particle can cross a potential barrier that is classically forbidden**. This is known as **tunnel effect**. It is fundamental in explaining a wide range of phenomena on the atomic scale.

In the limit  $\rho a \gg 1$ , we have  $\sinh(\rho a) \approx e^{\rho a}/2$ , and

$$T \simeq \frac{16E(V_0 - E)}{V_0^2} e^{-2\rho a}$$

is exponentially small, but non-zero.

This formula has an important implication in the *scanning tunneling microscope*. A sharp metal needle is brought very close to a metal surface. There exists a potential barrier, and therefore electrons can tunnel between the needle and the surface. When a voltage is applied, the magnitude of the resulting current, which depends on  $T$  will be very sensitive to the height, due to the exponent. Height of surfaces were measured to accuracy of  $10^{-11}$  m.

2.  $E > V_0$

In this case, the solution of the Schrödinger equation in the region  $0 < x < a$  is

$$\phi(x) = Fe^{ik_2x} + Ge^{-ik_2x},$$

where  $k_2 = [2m(E - V_0)/\hbar^2]^{1/2}$ . Repeating the same calculation as above (or simply replacing  $\rho \rightarrow ik_2$ ), one finds

$$R = \frac{|B|^2}{|A|^2} = \left[ 1 + \frac{4k^2k_2^2}{(k^2 - k_2^2) \sin^2(k_2a)} \right]^{-1} = \frac{V_0^2 \sin^2(k_2a)}{4E(E - V_0) + V_0^2 \sin^2(k_2a)}, \quad (118)$$

and

$$T = \frac{|C|^2}{|A|^2} = \left[ 1 + \frac{(k^2 - k_2^2)^2 \sin^2(k_2a)}{4k^2k_2^2} \right]^{-1} = \frac{4E(E - V_0)}{4E(E - V_0) + V_0^2 \sin^2(k_2a)}. \quad (119)$$

Again,  $T + R = 1$ .

The most important feature of this result is that **contrary to the classical result, the transmission coefficient,  $T$ , is in general  $T < 1$ .**

Full transmission ( $T = 1$ ) is obtained only if  $\sin(k_2a) = 0$ , namely when  $k_2a = n\pi$  ( $n = 1, 2, 3, \dots$ ). Alternatively when the de-Broglie wavelength inside the barrier,  $\lambda_2 \equiv 2\pi/k_2 = 2a/n$  (see Figure 9).

This can be understood as due to destructive interference between the reflections of the wave function inside the barrier at the two points,  $x = 0$  and  $x = a$ . This is analogue to *Febry-Perot interferometer* in optics (for those who know what it is).

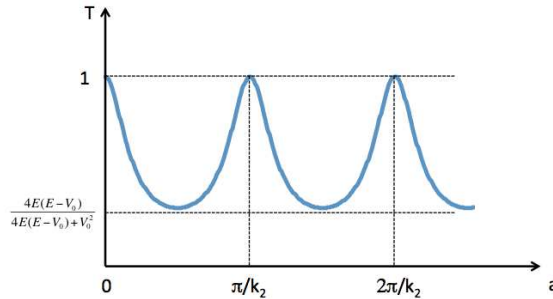


Fig. 9.— Transmission coefficient,  $T$ , as a function of barrier width,  $a$ .

When the particle's energy,  $E$  increases,  $T$  approaches 1 asymptotically; though it only reaches it exactly only if the barrier has the correct width (see Figure 10).

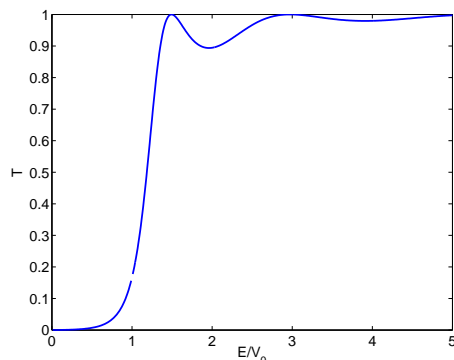


Fig. 10.— Transmission coefficient,  $T$ , as a function of the particle energy,  $E$  (normalized to  $V_0$ ). In making this figure,  $mV_0a^2/\hbar^2 = 10$  assumed.

### 8.5. Example 5: The finite square well

As a final example, let us consider the finite square potential well,

$$V(x) = \begin{cases} V_0 & |x| > a \\ 0 & |x| < a \end{cases} \quad (120)$$

(see Figure 11).

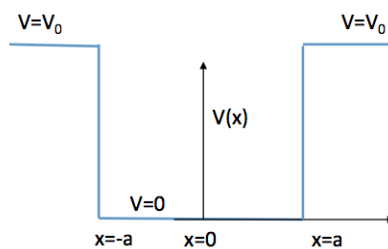


Fig. 11.— Square potential well.

Let us focus on the case  $0 < E < V_0$ , as the case  $E > V_0$  is similar to the scenarios discussed above.

While we can repeat the calculations along the same lines carried above, we can use an insight: we assume that the potential is symmetric with respect to  $x$ . Therefore, the probability of the particle to be at  $+x$ , is identical to its probability of being at  $-x$ , namely

$$|\phi(x)|^2 = |\phi(-x)|^2 \quad (121)$$

which is true for a state that is non-degenerated.

We can therefore classify the states as **even**, namely

$$\phi(x) = \phi(-x)$$

and **odd**,

$$\phi(x) = -\phi(-x).$$

This saves us a lot of work, since we can look only at the  $x > 0$  regime.

Inside the well ( $|x| < a$ ), the solutions to Schrödinger equation,

$$\frac{d^2\phi(x)}{dx^2} + \alpha^2\phi(x) = 0, \quad \alpha = \left[ \frac{2m}{\hbar^2} E \right]^{1/2}$$

(see Equations 76, 78) can be written as

$$\phi(x) = A \cos(\alpha x) + B \sin(\alpha x), \tag{122}$$

where  $A$  and  $B$  are independent. Therefore the **even** solution is clearly  $\phi(x) = A \cos(\alpha x)$  and the odd solution is  $B \sin(\alpha x)$ .

Outside the well, we have

$$\frac{d^2\phi(x)}{dx^2} - \beta^2\phi(x) = 0, \quad \beta = \left[ \frac{2m}{\hbar^2} (V_0 - E) \right]^{1/2}$$

(see, e.g., Equation 103). Using again the insight that  $\phi(x)$  cannot be infinite when  $x \rightarrow \infty$ , we find that the only acceptable solution at  $x > a$  must be  $Ce^{-\beta x}$ .

Looking first at the **even** solutions, and equating  $\phi$  and  $d\phi/dx$  at  $x = a$ , one finds

$$\begin{aligned} A \cos(\alpha a) &= Ce^{-\beta a} \\ -\alpha A \sin(\alpha a) &= -\beta C e^{-\beta a}. \end{aligned} \tag{123}$$

Dividing, we get

$$\alpha \tan(\alpha a) = \beta. \tag{124}$$

Similarly, if we look at the **odd** solutions,  $\phi(x) = B \sin(\alpha x)$  (at  $|x| < a$ ), we obtain the equation

$$\alpha \cot(\alpha a) = -\beta. \tag{125}$$

Equations 124, 125 are equation of the type known as *transcendental* equations. Unfortunately, there is no known analytic solution to these equations. However, these can be easily solved numerically or graphically, so that one could find the energy levels of the bound states.

The graphical method is straightforward. We note that

$$\alpha^2 + \beta^2 = \frac{2m}{\hbar^2}E + \frac{2m}{\hbar^2}(V_0 - E) = \frac{2m}{\hbar^2}V_0, \quad (126)$$

namely constant (independent on  $E$ ). We then multiply both sides of Equations 124 and 125 by  $a$ , and transform to new variables:  $\xi \equiv \alpha a$  and  $\eta \equiv \beta a$ , to get

$$\begin{aligned} \xi \tan \xi &= \eta & (\text{even solutions}) \\ \xi \cot \xi &= \eta & (\text{odd solutions}). \end{aligned} \quad (127)$$

With this transformation, Equation 126 becomes

$$\xi^2 + \eta^2 = R_0^2 \equiv \frac{2mV_0}{\hbar^2}a^2. \quad (128)$$

The solution of  $\xi$  and  $\eta$  can now be found by drawing Equations 127 and 128 in the  $\xi$ - $\eta$  plane, and finding the intersection points (see Figure 12). Note that Equation 128 is the equation of a circle, whose radius  $R_0$  depends on  $V_0 a^2$  (as well as on the particle's mass,  $m$ ).

Once the value of  $\xi$  is known, one can calculate  $\alpha$  and hence the energy,  $E = \hbar^2 \alpha^2 / 2m$ .

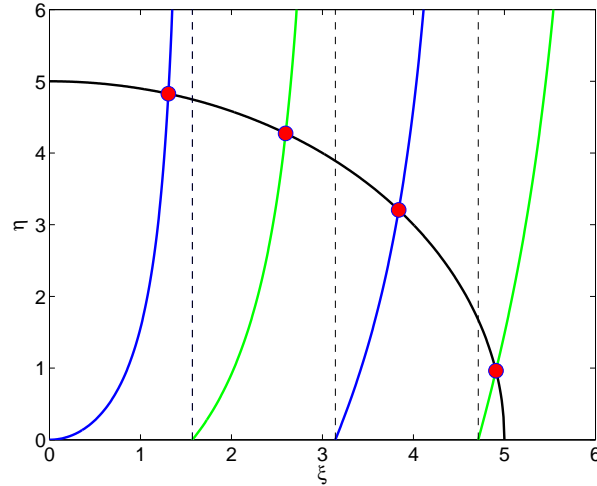


Fig. 12.— The functions  $\eta = \xi \tan(\xi)$  (blue) and  $\eta = -\xi \cot(\xi)$  (green) are plotted in the  $\xi$ - $\eta$  plane, along with the (quarter) circle,  $\xi^2 + \eta^2 = R_0^2$  (Equation 128). The intersection points are the solutions to  $\xi$  and  $\eta$  for a given  $V_0$ ,  $a$ .

As a final check, let's see what happens in the limit of infinite potential well, namely  $V_0 \rightarrow \infty$ . In this case,  $R_0 \rightarrow \infty$ , namely, the intersecting circle has infinite radius.



For the **even** solutions, we use the fact that  $\tan[\pi(n + 1/2)] = \pm\infty$  ( $n = 0, 1, 2, \dots$ ); namely, when  $\xi = \pi(n + 1/2)$ ,  $\eta \rightarrow \infty$ , and intersect the infinite circle. Similarly, for the **odd** solutions, we use  $\cot(n\pi) = \pm\infty$ , to find that  $\eta$  intersects the infinite circle as well. We can thus conclude that a solution in this case is given once

$$\xi = n\frac{\pi}{2} \quad n = 0, 1, 2, \dots$$

and since  $\xi = a\alpha = a(2mE/\hbar^2)^{1/2}$ , we get the energies

$$E_n = \frac{\hbar^2}{2m} \left( \frac{n\pi}{2a} \right)^2 \quad (129)$$

Not surprising, this is the same result as we obtained earlier, in Equation 85 (note that in deriving equation 85 we assumed that the potential is  $V_0 = 0$  in the region  $0 < x < L$ , while here this region is doubled in size,  $-a < x < a$ ).

## REFERENCES

- [1] E. Hecht, *Optics*, chapter 2
- [2] B.H. Bransden & C.J. Joachain, *Quantum Mechanics* (Second edition), chapter 2, 3, 4.
- [3] C. Cohen-Tannoudji, B. Diu & F. Laloe, *Quantum Mechanics*, Vol. 1., chapter 1.
- [4] R. Feynman, *The Feynman Lectures on Physics*, Vol. 3., Chapter 1.