Schroedinger's Equation

Xin Wan (*Zhejiang Univ.*)

Lecture 23

Motivation

- A classical wave $\psi(x, y, z, t)$ satisfies the wave equation

$$\frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2} = \nabla^2\psi.$$

- In the quantum theory, a microscopic particle is described by a probability amplitude $\psi(x, y, z, t)$, and the probability of finding it is proportional to

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

- What is, then, the wave equation that governs the motion of the quantum particle?

Outline

- Schroedinger's Equation
- Wave Packet
- Reflection from a Potential Step
- Tunneling through a Potential Barrier
- Scanning Tunneling Microscope

Classical Particle

- Let us start with a pedagogical discussion on how to write down an equation that governs the quantum behavior of a free particle of mass m represented by a wave

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

- For a free classical one-dimensional particle, on the other hand, the energy is

$$E = \frac{p^2}{2m}$$

- According to the de Broglie's hypothesis, we expect

$$p = \frac{h}{\lambda} = \hbar k = -i\hbar \frac{1}{\psi(x,t)} \frac{\partial \psi(x,t)}{\partial x}$$

$$p^2 = \hbar^2 k^2 = -\hbar^2 \frac{1}{\psi(x,t)} \frac{\partial^2 \psi(x,t)}{\partial x^2}$$

- Similarly, we expect

$$E = h\nu = \hbar\omega = i\hbar \frac{1}{\psi(x,t)} \frac{\partial \psi(x,t)}{\partial t}$$

- So using wave function, the energy-momentum relation is

$$i\hbar\frac{1}{\psi(x,t)}\frac{\partial\psi(x,t)}{\partial t}=-\frac{\hbar^2}{2m}\frac{1}{\psi(x,t)}\frac{\partial^2\psi(x,t)}{\partial x^2}$$

- In the presence of potential, e.g. a harmonic potential $U(x)=ax^2/2$, the classical relation is modified to

$$E=\frac{p^2}{2m}+U(x)$$

  where E is a constant of motion, but p is not. In other words, a plane wave is not a solution any more.

Schroedinger's Equation (1926)

- Schroedinger proposed that the wave function $\psi(x,t)$ of a single particle moving around in 1D satisfies

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x,t)}{\partial x^2} + U(x,t)\psi(x,t),$$

  where $U(x,t)$ is the potential energy of the particle and m the mass of the particle.
- We can easily generalize it to higher dimensions.
- Note that **Schroedinger's equation** is a postulate of quantum mechanics, not derived from classical physics.

- In most cases we discuss, the potential energy $U = U(x)$ is independent of time. We can solve the Schroedinger equation by an ansatz $\psi(x,t) = \phi(x)e^{-iEt/\hbar}$.
- The wave function $\phi(x)$ satisfies

$$\frac{\partial^2 \phi(x)}{\partial x^2} + \frac{2m}{\hbar^2}[E - U(x)]\phi(x) = 0.$$

- In free space, $U(x) = 0$. The general solution is

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

where A and B are constants and $k = \sqrt{2mE}/\hbar$.

- The complete time-dependent wave function is

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

  where $\omega = E/\hbar$. The two terms correspond to right- and left-moving waves, respectively.
- Consider the right-moving wave $\psi(x,t) = Ae^{i(kx-\omega t)}$, the probability density is

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

  That means that if we make a measurement to locate the particle, the location could turn out to be at any x value.

Wave Packets

- What is the speed of a free quantum mechanical particle? The general solution of the particle is

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \quad k = \sqrt{2mE}/\hbar$$

or, with standard time dependence, $e^{-iEt/\hbar}$,

$$\psi(x,t) = Ae^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} + Be^{-i\left(kx + \frac{\hbar k^2}{2m}t\right)}.$$

- The formula represents a right- and a left-moving wave with speed (of the wavefront)

$$v_{\mathrm{ph}} = \frac{\hbar k}{2m} = \sqrt{\frac{E}{2m}}.$$

- On the other hand, the classical speed of a free particle with energy E is given by

$$v_{\mathrm{cl}} = \sqrt{\frac{2E}{m}} = 2v_{\mathrm{ph}}.$$

- Problem #1: The quantum mechanical wave function travels at half the speed of the particle it is supposed to represent!

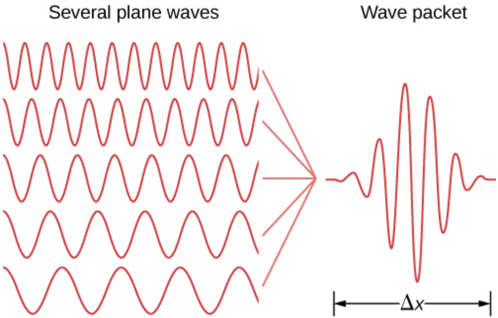
- How to normalize the wave function of the free particle, say, represented by Ae^{ikx}?

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = |A|^2 \int_{-\infty}^{\infty} 1 dx = |A|^2 \infty.$$

- Problem #2: This wave function is not normalizable!

- In fact, the stationary (separable) solutions do not represent physically realizable states; there is no such thing as a free particle with a definite energy.
- What is, then, the realistic solution to the Schroedinger equation for a free particle?

- In quantum theory, a localized particle is modeled by a linear superposition of these stationary free-particle (or plane-wave) states.

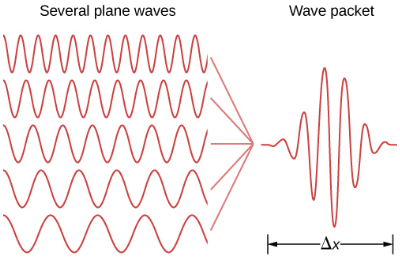


- In general, we can construct a linear combination (integral over continuous k)

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i\left(kx - \frac{\hbar k^2}{2m} t\right)} dk.$$

- This wave function can be normalized for appropriate $\phi(k)$, typically Gaussian. We call it a **wave packet**, which carries a range of k and, hence, a range of energies and speeds. In a general quantum problem, we are given $\Psi(x,0)$ and needed to find $\Psi(x,t)$.

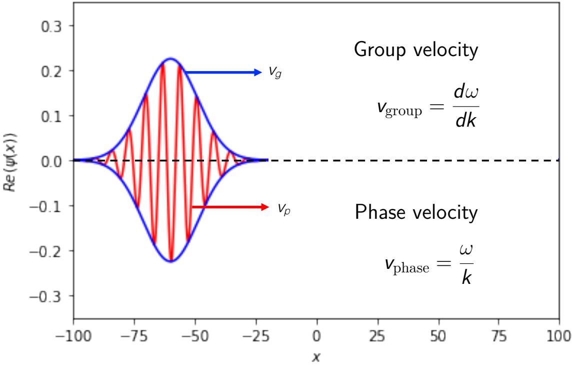
- The particle can be better localized (Δx can be decreased) if more plane-wave states of different wavelengths or momenta are added together in the right way (Δp is increased).



- According to Heisenberg, these uncertainties obey

$$\Delta x \Delta p \geq \hbar/2.$$

- It turns out that the group velocity of the wave packet, not the phase velocity of the stationary states, matches the classical particle velocity.



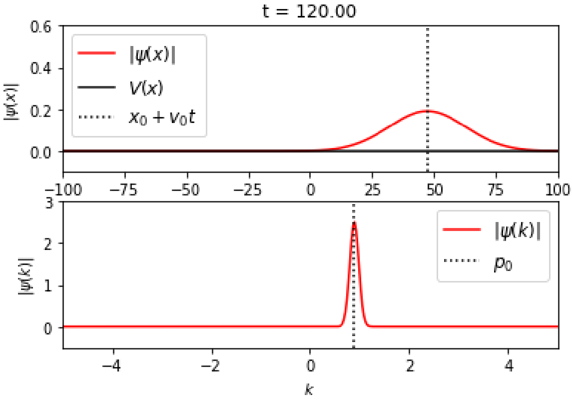
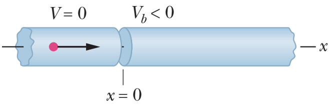


Figure 1: Propagation of a free particle.

Reflection from a Potential Step

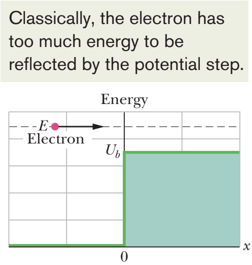
- Consider a beam of nonrelativistic electrons, each of total energy E, along an x axis through a narrow tube. They experience a negative electric potential step of height $V_b < 0$ at $x = 0$.

Can the electron be reflected by the region of negative potential?



- We consider the situation where $E > qV_b$. Classically, electrons should all pass through the boundary. Their total energy should be conserved, so their kinetic energy, hence speed, decreases when their potential energy increases. What happens quantum mechanically?

- We apply Schroedinger's equation to the two regions separately. However, the wave functions should be consistent with each other at $x = 0$, both in value and in slope (**boundary conditions**).



- Region 1 ($x < 0$): $k = \sqrt{2mE}/\hbar$

$$\psi_1 = Ae^{ikx} + Be^{-ikx}$$

- Region 2 ($x > 0$): $k_b = \sqrt{2m(E - qV_b)}/\hbar$

$$\psi_2 = Ce^{ik_b x} + De^{-ik_b x}$$

- We can first set $D = 0$, because there is no electron source off to the right, and there can be no electrons moving to the left in region 2.
- We now consider boundary conditions at $x = 0$:

$$A + B = C \ (\text{matching of values})$$

$$Ak - Bk = Ck_b \ (\text{matching of slopes})$$

- We should be able to solve B/A and C/A, but not A, B, and C. Note that the absolute values are not important for our purpose (it can be related to the beam intensities, though).

Reflection and Transmission Coefficients

- Indeed, to find the probability that electrons reflect from the step, we need to relate the probability density of the reflected wave (Be^{-ikx}) to that of the incident wave (Ae^{ikx}). We thus define a reflection coefficient R:

$$R = \frac{|B|^2}{|A|^2} = \left| \frac{k - k_b}{k + k_b} \right|^2 .$$

- Quantum mechanically, electrons are reflected from the boundary, but only with a probability.
- What happens if $E < qV_b$?

- Similarly, the transmission coefficient (the probability of transmission) is

$$T = 1 - R = \frac{4kk_b}{|k + k_b|^2}.$$

- What inspires us to define T in this way?
- Well, one can consider an alternative quantity

$$\frac{|C|^2}{|A|^2} = \frac{4k^2}{|k + k_b|^2} = T\frac{k}{k_b}.$$

- Recall current density $J = nqv$. Not surprisingly, one finds

$$T = \frac{|C|^2 k_b}{|A|^2 k} = \frac{|C|^2 q(\hbar k_b/m)}{|A|^2 q(\hbar k/m)} = \frac{J_{\text{transmitted}}}{J_{\text{incident}}}.$$

- One can also write

$$R = \frac{J_{\text{reflected}}}{J_{\text{incident}}}.$$

- Therefore, $T = 1 - R$ is nothing but the conservation of current

$$J_{\text{transmitted}} = J_{\text{incident}} - J_{\text{reflected}}.$$

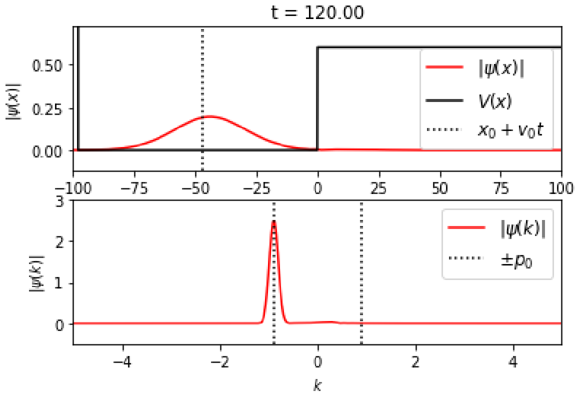
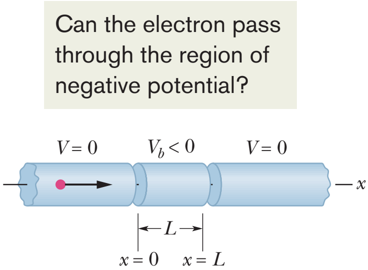


Figure 2: Particle reflected from a potential barrier.

Tunneling through a Potential Barrier

- Now consider a potential energy barrier, which is a region of thickness L where the electric potential is V_b (< 0) and the barrier height is U_b $(= qV_b)$.

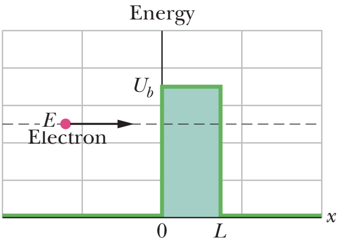


- We consider the situation where $E < qV_b$. Classically, electrons are forbidden in the barrier region, hence all reflected. However, a matter wave, has a finite probability of leaking (or, better, tunneling) through the barrier and materializing on the other side.

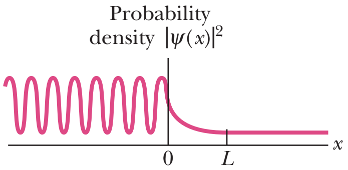
We are interested in the probability of the electron appearing on the other side of the barrier. Thus, we want the transmission coefficient T. The general procedure is the following.

1. Separate the space into three regions and solve Schroedinger's equation in each region ($3 \times 2 - 1 = 5$ unknowns).
2. Apply boundary conditions at the two boundaries ($2 \times 2 = 4$ equations).
3. Calculate the tunneling coefficient.

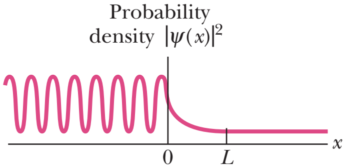
Classically, the electron lacks the energy to pass through the barrier region.



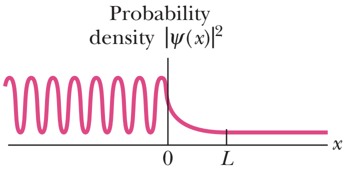
- We shall just examine the general results.



- The oscillating curve to the left of the barrier (for $x < 0$) is a combination of the incident matter wave and the reflected matter wave (which has a smaller amplitude than the incident wave). The oscillations occur because these two waves, traveling in opposite directions, interfere with each other, setting up a standing wave pattern.



- Within the barrier (for $0 < x < L$) the probability density decreases exponentially with x. However, if L is small, the probability density is not quite zero at $x = L$.
- To the right of the barrier (for $x > L$), the probability density plot describes a transmitted wave (through the barrier) with low but constant amplitude.



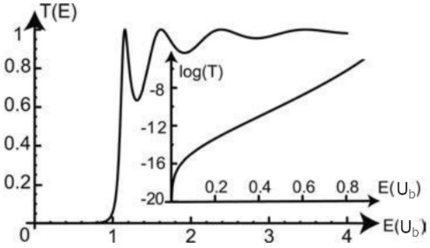
- We can assign a transmission coefficient T to the incident matter wave and the barrier. The transmission coefficient T is approximately

$$T \approx e^{-2\kappa L},$$

where

$$\kappa = \frac{\sqrt{2m(qV_b - E)}}{\hbar}.$$

- The exact result can be obtained for any U_b $(= qV_b)$ and L.



- In general, we speak of tunneling if $E < U_b$. In this regime, $T(E)$ increases approximately exponentially with energy, as shown in the inset.
- For $E \gg U_b$, $T(E) = 1$ as expected classically.

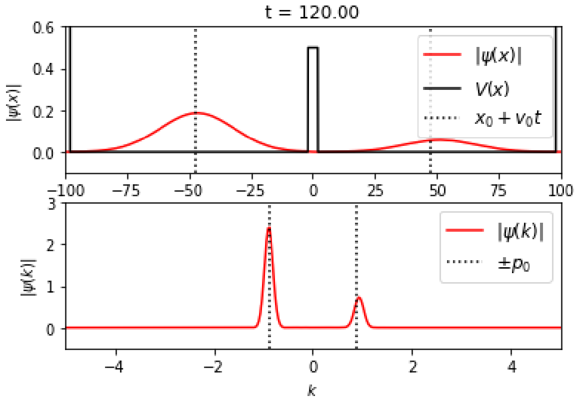
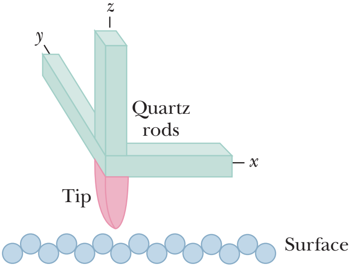


Figure 3: Particle tunneling through and reflected from a square barrier.

Scanning Tunneling Microscope (STM)

- The size of details that can be seen in an optical microscope is limited by the wavelength of the light the microscope uses (about 300 nm for ultraviolet light). We use electron matter waves (tunneling through potential barriers) to create images on the atomic scale.
- A fine metallic tip, mounted on quartz rods, is placed close to the surface to be examined. The space between the surface and the tip forms a potential energy barrier.



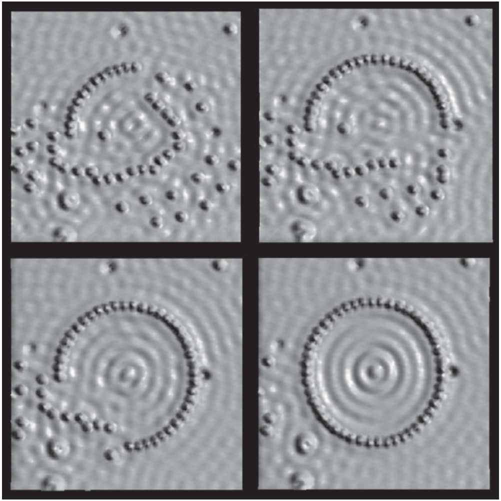


Figure 4: An STM not only can provide an image of a static surface, it can also be used to manipulate atoms and molecules on a surface.

Summary

- Understand the form of Schroedinger's equation and how to solve it. Understand how through Schroedinger's equation the wave-particle duality is realized quantitatively.
- Potential step: Compare this case to light being reflected and refracted at an interface. How to solve Schroedinger's equation and calculate the probability of reflection and transmission?

- Barrier tunneling: How to calculate the probability of tunneling through a barrier? Compare to the classical picture. How does the transmission coefficient for a given particle of mass m and energy E depend on the barrier height and thickness?

Reading

Halliday, Resnick & Krane:

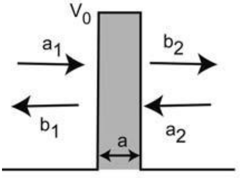
- Chapter 46: The Nature of Matter
- Chapter 47: Electrons in Potential Wells

Appendix 23A: S-Matrix

- Let us revisit the problem of tunneling through a square potential barrier and rewrite, for $k = \sqrt{2mE}/\hbar$,

$$\text{Left}: \quad \psi_1 = a_1 e^{ikx} + b_1 e^{-ikx}$$

$$\text{Right}: \quad \psi_2 = b_2 e^{ikx} + a_2 e^{-ikx}$$



- We can express the outgoing amplitudes as a linear map of the incoming amplitudes,

$$\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} r_{11} & t_{12} \\ t_{21} & r_{22} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

- The reflection symmetry and charge conservation require

$$r_{11} = r_{22} = r, \qquad t_{12} = t_{21} = t,$$

  and $|r|^2 + |t|^2 = 1$.

- The S-matrix can be calculated from elementary quantum mechanics as we discussed in the previous examples. In fact, we outlined how to solve the case with $a_2 = 0$.*

- With the S-matrix formalism, we can easily treat problems with multiple barriers (or scatterers).

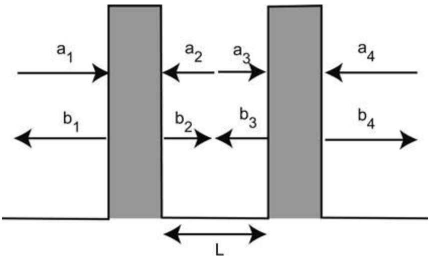
*Note when $a_1 = 1$, $a_2 = 0$, we have $b_1 = r$, $b_2 = t$.

Resonant Tunneling

- Now we consider the transmission of a double barrier structure within the S-matrix formalism

$$\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} r_1 & t_1 \\ t_1 & r_1 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

$$\begin{pmatrix} b_3 \\ b_4 \end{pmatrix} = \begin{pmatrix} r_2 & t_2 \\ t_2 & r_2 \end{pmatrix} \begin{pmatrix} a_3 \\ a_4 \end{pmatrix}$$



- For a single barrier,

$$T_{1,2} = t_{1,2}^* t_{1,2}$$

$$R_{1,2} = r_{1,2}^* r_{1,2}$$

- Suppose the transport between the barriers is completely coherent, and the electrons collect a phase θ as they travel between the barriers. That is,

$$a_2 = b_3 e^{i\theta}$$

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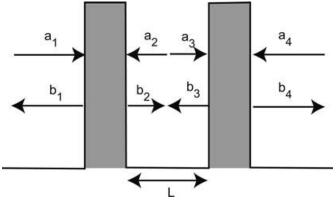

- If we set $a_1 = 1$ and $a_4 = 0$, we obtain

$$b_4 = \frac{t_1 t_2 e^{i\theta}}{1 - r_1 r_2 e^{2i\theta}}$$

- The result can also be obtained by summing up the interference paths, as each time a wave hits barrier j, a fraction r_j gets reflected and t_j gets transmitted.

$$
\begin{aligned}
b_4 &= t_1 e^{i\theta} t_2 + t_1 e^{i\theta} r_2 e^{i\theta} r_1 e^{i\theta} t_2 + \cdots \\
&= t_1 e^{i\theta} \left[\sum_{n=0}^{\infty} \left(r_2 e^{i\theta} r_1 e^{i\theta} \right)^n \right] t_2
\end{aligned}
$$

- The transmission probability is

$$
T = b_4^* b_4 = \frac{T_1 T_2}{1 + R_1 R_2 - 2\sqrt{R_1 R_2} \cos\Theta},
$$

where $\Theta = 2\theta + \arg(r_1 r_2)$ is the phase shift acquired in one round trip between the two barriers.

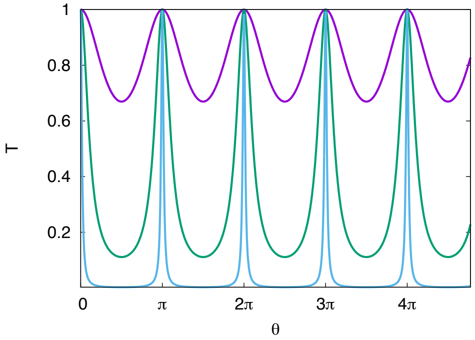

Figure 5: Coherent transmission of a double barrier as a function of the phase collected during one round trip between the barriers, shown for equal individual barrier transmissions $T_i = 0.9$, 0.5, and 0.1, respectively.

- Notice there are a series of θ values at which the tunneling probability is 1. Surprising?
- For simplicity, we assume $\arg(r_1 r_2) = 0$. The total transmission happens when $\theta = kL = n\pi$ (i.e., $\cos 2\theta = 1$), where L is the distance between the barriers. Hence,

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \theta^2}{2mL^2} = \frac{\hbar^2 n^2 \pi^2}{2mL^2} = \frac{n^2 h^2}{8mL^2}$$

- Therefore, the double barrier can be thought of as an electron interferometer. A resonance occurs when the wavelength is commensurable with L, i.e. $n\lambda/2 = L$. Have you encountered this condition before?