

# Quantum Mechanics in One Dimension, Part II

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# No Degeneracy Theorem

**Theorem:** There is no degeneracy in one-dimensional bound states.

**Proof:** Suppose, there are two TISE solutions corresponding to the same energy:

$$\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \psi_1(x) = E \psi_1(x) \quad (1)$$

$$\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \psi_2(x) = E \psi_2(x) \quad (2)$$

Multiply Eq. 1 by  $\psi_2(x)$ , multiply Eq. 2 by  $\psi_1(x)$ , and then subtract Eq. 2 from Eq. 1. Obtain

$$\begin{aligned} \psi_1(x) \frac{d^2}{dx^2} \psi_2(x) - \psi_2(x) \frac{d^2}{dx^2} \psi_1(x) &= 0 \\ \frac{d}{dx} \left( \psi_1(x) \frac{d}{dx} \psi_2(x) - \psi_2(x) \frac{d}{dx} \psi_1(x) \right) &= 0 \\ \psi_1(x) \frac{d}{dx} \psi_2(x) - \psi_2(x) \frac{d}{dx} \psi_1(x) &= c \end{aligned}$$

# No Degeneracy Theorem (Cont'd)

For bound states,  $\psi_1(x)$  and  $\psi_2(x)$  vanish as  $x \rightarrow \infty$ , so  $c = 0$ . Therefore, we must have

$$\begin{aligned}\psi_1(x) \frac{d}{dx} \psi_2(x) &= \psi_2(x) \frac{d}{dx} \psi_1(x) \\ \frac{1}{\psi_2(x)} \frac{d}{dx} \psi_2(x) &= \frac{1}{\psi_1(x)} \frac{d}{dx} \psi_1(x) \\ \ln \psi_2(x) &= \ln \psi_1(x) + c' \\ \psi_2(x) &= A\psi_1(x)\end{aligned}$$

However, states described by  $\psi_1(x)$  and  $A\psi_1(x)$  are physically equivalent. Q.E.D.

Note that this theorem works *for bound states only*. It is manifestly false for the free particle.

# Real Eigenfunctions Theorem

**Theorem:** The eigenfunctions of  $H$  corresponding to one-dimensional bound states can always be chosen pure real in the coordinate basis.

**Proof:** If  $\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)\right) \psi(x) = E\psi(x)$  then, by conjugation,  $\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)\right) \psi^*(x) = E\psi^*(x)$ . Averaging these two equations,  $\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)\right) \frac{\psi(x) + \psi^*(x)}{2} = E \frac{\psi(x) + \psi^*(x)}{2}$ . Note that the wavefunction  $\frac{\psi(x) + \psi^*(x)}{2}$  is manifestly real and, according to the “no degeneracy theorem”, represents a unique state corresponding to energy  $E$ .

# Existence of a Bound State Theorem

**Theorem:** Every “attractive” potential in one dimension has at least one bound state.

**Proof:** Note that  $\langle E \rangle = \langle H \rangle \geq E_0$ , where  $E_0$  is the lowest possible eigenvalue of the TISE. Consider  $H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$ . Suppose,  $\psi(x)$  is real and  $\lim_{|x| \rightarrow \infty} \psi(x) = 0$ . Then

$$\begin{aligned} \left\langle -\frac{d^2}{dx^2} \right\rangle &= -\int_{-\infty}^{\infty} \psi(x) \frac{d^2}{dx^2} \psi(x) dx = -\psi(x) \psi'(x) \Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \left( \frac{d\psi(x)}{dx} \right)^2 dx \\ &= \int_{-\infty}^{\infty} \left( \frac{d\psi(x)}{dx} \right)^2 dx \end{aligned}$$

Now, consider  $\psi_{\kappa}(x) = \sqrt{\kappa} e^{-\kappa|x|}$ . For this function,

$$\left\langle -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right\rangle = \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \left( \frac{d\psi_{\kappa}(x)}{dx} \right)^2 dx = \frac{\hbar^2 \kappa^2}{2m} \quad (3)$$

# Existence of a Bound State Theorem (Cont'd)

At the same time,

$$\langle V(x) \rangle = \kappa \int_{-\infty}^{\infty} e^{-2\kappa|x|} V(x) dx \quad (4)$$

Combining together Eqs. 3 and 4,

$$\langle H \rangle = \frac{\hbar^2 \kappa^2}{2m} + \kappa \int_{-\infty}^{\infty} e^{-2\kappa|x|} V(x) dx$$

For small values of  $\kappa$ ,

$$\langle H \rangle \approx \kappa \int_{-\infty}^{\infty} V(x) dx$$

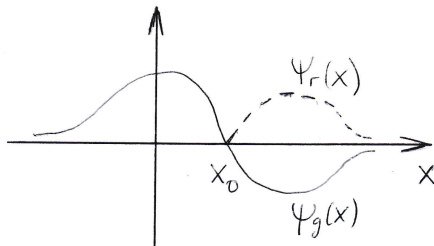
Therefore,  $\langle H \rangle$  can always be made negative as long as  $\int_{-\infty}^{\infty} V(x) dx < 0$ . As  $E_0 \leq \langle H \rangle$ ,  $E_0 < 0$ . If  $\lim_{|x| \rightarrow \infty} V(x) = 0$ , this is a bound state. Q.E.D.

Note that this theorem effectively *defines* an attractive potential as the potential for which  $\int_{-\infty}^{\infty} V(x) dx < 0$  and  $\lim_{|x| \rightarrow \infty} V(x) = 0$ .

# No Nodes in the Ground State Theorem

**Theorem:** Wavefunction that corresponds to the lowest energy bound state (a.k.a. the ground state) of a 1-d system has no nodes in the coordinate representation.

**Proof:** The wavefunction that corresponds to the ground state,  $\psi_g(x)$ , must be unique and can be chosen pure real. Suppose, this function has a node. Then we can construct another function,  $\psi_r(x)$ , by reflecting a part of  $\psi_g(x)$  vertically, whenever  $\psi_g(x) < 0$  (see figure below). Note that  $\psi_r(x) \neq \alpha\psi_g(x)$  for any  $\alpha$ , so  $\psi_r(x)$  represents a distinct physical state.



# No Nodes in the Ground State Theorem (Cont'd)

The following assumes a single node at  $x_0$ , but the extension to multiple nodes is obvious. Consider  $\langle E_r \rangle = \langle \psi_r | H | \psi_r \rangle$ . As  $\psi_r$  represents a distinct physical state, we must have  $\langle E_r \rangle > E_0 = \langle \psi_g | H | \psi_g \rangle$ . On the other hand, in the coordinate basis,

$$\begin{aligned}\langle \psi_g | H | \psi_g \rangle &= \int_{-\infty}^{\infty} \psi_g(x) H \psi_g(x) dx \\ &= \int_{-\infty}^{x_0 - \varepsilon} \psi_g(x) H \psi_g(x) dx + \int_{x_0 - \varepsilon}^{x_0 + \varepsilon} \psi_g(x) H \psi_g(x) dx \\ &\quad + \int_{x_0 + \varepsilon}^{\infty} \psi_g(x) H \psi_g(x) dx,\end{aligned}$$

with a similar decomposition for  $\langle \psi_r | H | \psi_r \rangle$ . The following should be obvious:

$$\begin{aligned}\int_{-\infty}^{x_0 - \varepsilon} \psi_g(x) H \psi_g(x) dx &= \int_{-\infty}^{x_0 - \varepsilon} \psi_r(x) H \psi_r(x) dx \\ \int_{x_0 + \varepsilon}^{\infty} \psi_g(x) H \psi_g(x) dx &= \int_{x_0 + \varepsilon}^{\infty} \psi_r(x) H \psi_r(x) dx \\ \lim_{\varepsilon \rightarrow 0} \int_{x_0 - \varepsilon}^{x_0 + \varepsilon} \psi_g(x) H \psi_g(x) dx &= 0\end{aligned}$$



# No Nodes in the Ground State Theorem (Cont'd)

But what is  $\lim_{\varepsilon \rightarrow 0} \int_{x_0-\varepsilon}^{x_0+\varepsilon} \psi_r(x) H \psi_r(x) dx$ ? As  $\psi_r(x)$  has a discontinuous first derivative at  $x_0$  and an infinite second derivative, this is not immediately apparent. Consider, however

$$- \int_{x_0-\varepsilon}^{x_0+\varepsilon} \psi_r(x) \frac{d^2}{dx^2} \psi_r(x) dx = -\psi_r(x) \psi'_r(x) \Big|_{x_0-\varepsilon}^{x_0+\varepsilon} + \int_{x_0-\varepsilon}^{x_0+\varepsilon} \left( \frac{d\psi_r(x)}{dx} \right)^2 dx$$

As  $\left( \frac{d\psi_r(x)}{dx} \right)^2 = \left( \frac{d\psi_g(x)}{dx} \right)^2$ ,  $\lim_{\varepsilon \rightarrow 0} \int_{x_0-\varepsilon}^{x_0+\varepsilon} \left( \frac{d\psi_r(x)}{dx} \right)^2 dx = 0$ . On the other hand,

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \left( -\psi_r(x) \psi'_r(x) \Big|_{x_0-\varepsilon}^{x_0+\varepsilon} \right) &= -\psi_r(x_0) (\psi'_r(x_0 + 0) - \psi'_r(x_0 - 0)) \\ &= 2\psi_g(x_0) \psi'_g(x_0) = 0 \end{aligned}$$

because  $x_0$  is a node. Therefore,  $\lim_{\varepsilon \rightarrow 0} \int_{x_0-\varepsilon}^{x_0+\varepsilon} \psi_r(x) H \psi_r(x) dx = 0$ , and we have  $\langle E_r \rangle = E_0$ . This is impossible, so the assumption about existence of the node must be incorrect. Q.E.D.

# No Nodes in the Ground State Theorem (Cont'd)

**Corollary:** The bound state eigenfunctions corresponding to TISE eigenvalues other than  $E_0$  must have at least one node.

**Proof:** This is obvious from the orthogonality condition  $\int_{-\infty}^{\infty} \psi_n(x)\psi_g(x)dx = 0$ . This condition can not be satisfied if both  $\psi_n(x)$  and  $\psi_g(x)$  have no nodes. In this case the integrand has the same sign everywhere, and  $\left| \int_{-\infty}^{\infty} \psi_n(x)\psi_g(x)dx \right| > 0$ .

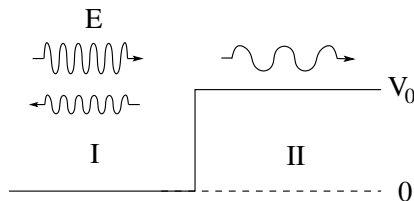
Note that, for 1-d bound states, the wavefunction corresponding to the  $n^{\text{th}}$  energy level (counting from  $n = 0$  for the ground state) has exactly  $n$  nodes. This powerful statement is known as the *oscillation theorem* or the *nodal theorem*. Proof of this theorem is beyond the scope of this course.

# Special Properties of 1-d Bound States (a Summary)

Please keep in mind the four theorems about 1-d bound states discussed above:

- No degeneracy
- Real eigenfunctions
- Existence of a bound state for an attractive potential
- No nodes in the ground state

# Scattering off a Single-Step Potential



- The single-step potential is

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

- Shankar performs a detailed treatment of a Gaussian packet scattering off the single-step potential. We will limit the discussion to a monochromatic wave. This example is already sufficient to illustrate all basic concepts.
- Our main goal will be to determine the *transmission* and *reflection coefficients*. These coefficients are defined as the ratios of the probability fluxes, e.g., the transmission coefficient  $T$  is  $j_{II}/j_{I,in}$ .

# Wavefunction for the Single-Step Potential

- The TISE for this problem is

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

Assuming that  $E > V_0$ , the general solution of this equation is

$$\psi(x) = \begin{cases} Ae^{ik_1x} + Be^{-ik_1x}, & x < 0 \text{ (region I)} \\ Ce^{ik_2x} + De^{-ik_2x}, & x > 0 \text{ (region II)} \end{cases},$$

where  $k_1 = \frac{\sqrt{2mE}}{\hbar}$  and  $k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$ . The coefficients  $k_1$  and  $k_2$  are sometimes called **wave numbers**.

- We can simplify the expression for  $\psi(x)$  using physics arguments:

$$\psi(x) = \begin{cases} e^{ik_1x} + Be^{-ik_1x}, & x < 0 \text{ (region I)} \\ Ce^{ik_2x}, & x > 0 \text{ (region II)} \end{cases} \quad (5)$$

# Solving the TISE for the Single-Step Potential

- The coefficients  $B$  and  $C$  are determined using the wavefunction continuity conditions at  $x = 0$ :  $\psi(-0) = \psi(+0)$  and  $\psi'(-0) = \psi'(+0)$ .

$$\begin{aligned} 1 + B &= C && \text{from the continuity of the wavefunction} \\ ik_1(1 - B) &= ik_2C && \text{from the continuity of the derivative} \end{aligned}$$

- This obviously results in  $ik_1(1 - B) = ik_2(1 + B)$  and then

$$B = \frac{k_1 - k_2}{k_1 + k_2} = \frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}} \quad (6)$$

$$C = \frac{2k_1}{k_1 + k_2} = \frac{2\sqrt{E}}{\sqrt{E} + \sqrt{E - V_0}} \quad (7)$$

# Transmission and Reflection Coefficients

Reminder: the probability flux for  $\psi(x) = Ae^{ikx}$  is  $j = |A|^2 \frac{k\hbar}{m} = |A|^2 v$ .

$$T = \frac{j_{II}}{j_{I,in}} = \frac{|C|^2 v_{II}}{v_I} = \frac{|C|^2 \sqrt{E - V_0}}{\sqrt{E}} = \frac{4\sqrt{E}\sqrt{E - V_0}}{|\sqrt{E} + \sqrt{E - V_0}|^2} \quad (8)$$

$$R = \frac{j_{I,out}}{j_{I,in}} = |B|^2 = \left| \frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}} \right|^2 \quad (9)$$

- The probability flux is conserved, i.e.,  $j_{II} + j_{I,out} = j_{I,in}$ . This means that we must have  $T + R = 1$ . Check that this is indeed the case!
- $\lim_{E \rightarrow \infty} T = \lim_{V_0 \rightarrow 0} T = 1$ .
- $\lim_{E \rightarrow V_0} T = 0$ .
- What happens if  $V_0 < 0$ ? What is  $\lim_{V_0 \rightarrow -\infty} T$ ?

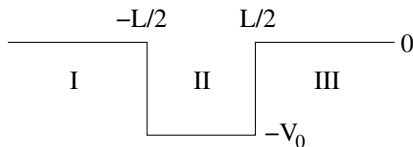
# Penetration Depth

- Consider the single-step potential problem with  $E < V_0$ . Do we have to solve it differently?
- It turns out that the solution given by Eqs. 5, 6, and 7 works just fine if we allow for imaginary  $k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$  (note that we need to choose the correct square root). The wavefunction in region II is now  $Ce^{-|k_2|x}$ . The probability density is then  $p(x) \propto |C|^2 e^{-2|k_2|x}$ .
- The quantity  $d = \frac{1}{2|k_2|}$  is called **penetration depth**. In terms of the penetration depth,  $p(x) \propto e^{-x/d}$ .
- The reflection coefficient from Eq. 9 becomes 1.
- The sum of the transmission coefficient from Eq. 8 and the reflection coefficient from Eq. 9 is no longer 1. What is going on? Is the probability flux still conserved?



# Going (Slightly) Beyond Shankar's Ch. 5

# Finite Depth Square Well



- The finite depth square well potential is

$$V(x) = \begin{cases} -V_0 & \text{if } |x| < L/2 \\ 0 & \text{if } |x| > L/2 \end{cases}$$

- We will be interested in the bound states of this system,  $E < 0$  case.
- Due to the parity argument, the TISE solutions must be even or odd:

$$\psi_{\text{even}}(x) = \begin{cases} Ce^{-\kappa|x|}, & |x| > \frac{L}{2} \quad (\text{regions I and III}) \\ A \cos kx, & |x| < \frac{L}{2} \quad (\text{region II}) \end{cases}$$

$$\psi_{\text{odd}}(x) = \begin{cases} -Ce^{\kappa x}, & x < -\frac{L}{2} \quad (\text{region I}) \\ B \sin kx, & |x| < \frac{L}{2} \quad (\text{region II}) \\ Ce^{-\kappa x}, & x > \frac{L}{2} \quad (\text{region III}) \end{cases}$$

# Solving the TISE for the Finite Depth Square Well

- To determine  $\psi(x)$ , we need to impose the wavefunction continuity conditions at  $x = \frac{L}{2}$ :  $\psi(\frac{L}{2} - 0) = \psi(\frac{L}{2} + 0)$  and  $\psi'(\frac{L}{2} - 0) = \psi'(\frac{L}{2} + 0)$ . The continuity conditions at  $x = -\frac{L}{2}$  will be satisfied automatically due to the wavefunction symmetry.
- For the even wavefunction the continuity conditions give

$$A \cos \frac{kL}{2} = Ce^{-\frac{\kappa L}{2}} \quad \text{from the continuity of the wavefunction} \quad (10)$$

$$-kA \sin \frac{kL}{2} = -\kappa Ce^{-\frac{\kappa L}{2}} \quad \text{from the continuity of the derivative} \quad (11)$$

Now, divide Eq. 11 by Eq. 10 and obtain

$$k \tan \frac{kL}{2} = \kappa \quad (12)$$

For the odd wavefunction similar reasoning generates the condition

$$k \cot \frac{kL}{2} = -\kappa \quad (13)$$

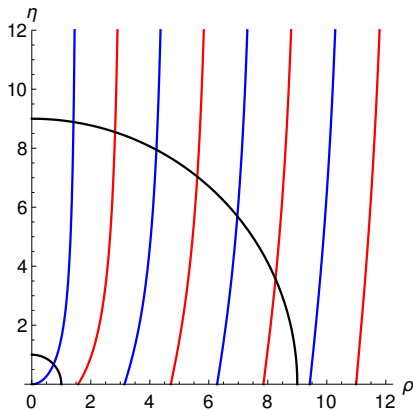
# Solving the TISE for the Finite Depth Square Well (Cont'd)

- While Eqs. 12 and 13 can be used to define  $\kappa$  in terms of  $k$ , they are by themselves insufficient to pinpoint possible values of  $k$  and  $\kappa$ . Note, however, that  $\kappa^2 = -\frac{2mE}{\hbar^2}$  while  $k^2 = \frac{2m(E+V_0)}{\hbar^2}$ . This means that  $\kappa^2 + k^2 = \frac{2mV_0}{\hbar^2}$ . In combination with Eq. 12 or 13, this constraint gives us the ability to find  $k$  and  $\kappa$ .
- It is more convenient to work with dimensionless variables  $\rho = \frac{kL}{2}$  and  $\eta = \frac{\kappa L}{2}$ . In terms of these variables, we have

$$\begin{aligned}\eta &= \rho \tan \rho && \text{for even eigenfunctions} \\ \eta &= -\rho \cot \rho && \text{for odd eigenfunctions} \\ \rho^2 + \eta^2 &= \frac{mV_0L^2}{2\hbar^2} && \text{for the constraint}\end{aligned}$$

- While these equations can not be solved in terms of simple algebraic functions, a pretty good idea about possible solutions can be obtained by plotting  $\eta$  curves defined by these formulae as a function of  $\rho$ .

# Graphical TISE Solution for the Finite Depth Square Well



$$\begin{aligned}\eta &= \rho \tan \rho && \text{even eigenfunctions} \\ \eta &= -\rho \cot \rho && \text{odd eigenfunctions} \\ \rho^2 + \eta^2 &= \frac{mV_0L^2}{2\hbar^2} && \text{constraint}\end{aligned}$$

The constraint equation is shown for couple different values of  $V_0$  (black line)

Are possible values of  $k$  consistent with the infinite square well as  $V_0 \rightarrow \infty$ ?

What is the smallest possible value of  $V_0$  that allows for two bound states in the square well potential? What is the energy of the second bound state in this case?

# Example Inverse Problem

## August 2020 Prelim problem D1P4

A particle of mass  $m$  is moving in one dimension in the potential  $V(x)$ . The particle is in an eigenstate of the Hamiltonian, with probability density for the position given by  $\rho(x) = \frac{2a^3}{\pi(x^2+a^2)^2}$ , where  $a$  is a positive parameter.

- (a) (30 points) Determine the wave function  $\psi(x)$  from  $\rho(x)$ . Argue that the solution is unique (up to an overall phase factor).
- (b) (20 points) Is the particle in the ground state? Explain your reasoning.
- (c) (50 points) Determine  $V(x)$ .

# Solution of the Example Inverse Problem

- Part (a). Assuming  $\psi(x)$  continuity,

$$\psi(x) = \sqrt{\rho(x)} = \sqrt{\frac{2a^3}{\pi} \frac{1}{x^2 + a^2}}$$

Why this solution is unique?

- Part (b). Is this the ground state?
- Part (c). Use the 1-d TISE:

$$\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \psi(x) = E_0 \psi(x)$$

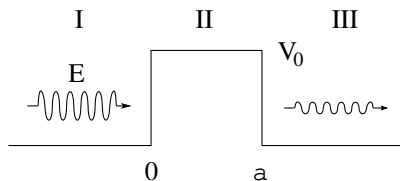
From this equation (check!),

$$V(x) = E_0 + \frac{1}{\psi(x)} \frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} = E_0 + \frac{\hbar^2}{m} \frac{3x^2 - a^2}{(x^2 + a^2)^2}$$

As  $E_0$  is arbitrary, this potential is defined up to an additive constant.

- Is this an attractive potential? Note that  $\int_{-\infty}^{\infty} \frac{3x^2 - 1}{(x^2 + 1)^2} dx = \pi$ . Is there a contradiction with the “existence of a bound state” theorem?

# Tunneling Through a Potential Barrier



- Consider the rectangular potential:

$$V(x) = \begin{cases} 0, & x < 0 \text{ or } x > a \\ V_0, & 0 < x < a \end{cases}$$

We will be interested in the transmission coefficient.

- What are some possible physical realizations of this potential?
- If we shift the potential to the interval  $[-a/2, a/2]$ , can parity be useful?



# Solving the TISE for the Rectangular Barrier

- Unlike the case of finite depth square well, here we are interested in the solutions with  $E > 0$ .
- Even though  $[\Pi, H] = 0$  for the shifted potential, parity is not useful in this problem because the conditions at  $x \rightarrow -\infty$  and  $x \rightarrow \infty$  are physically different. Both incoming and reflected waves propagate at  $x \rightarrow -\infty$ , while at  $x \rightarrow \infty$  only the transmitted wave exists.
- We will search for the TISE solution in the form

$$\psi(x) = \begin{cases} e^{ikx} + Ae^{-ikx}, & x < 0 & \text{(region I)} \\ Be^{i\kappa x} + Ce^{-i\kappa x}, & 0 < x < a & \text{(region II)} \\ De^{ik(x-a)}, & x > a & \text{(region III)} \end{cases}$$

where  $k = \frac{\sqrt{2mE}}{\hbar}$  and  $\kappa = \frac{\sqrt{2m(E-V_0)}}{\hbar}$ , allowing for pure imaginary  $\kappa$ .

- The transmission coefficient  $T = |D|^2$  (velocities are the same in region I and region III).

# Solving the TISE for the Rectangular Barrier (Cont'd)

- The wavefunction continuity conditions at  $x = 0$ :

$$1 + A = B + C \quad (14)$$

$$k(1 - A) = \kappa(B - C) \quad (15)$$

The wavefunction continuity conditions at  $x = a$ :

$$Be^{i\kappa a} + Ce^{-i\kappa a} = D \quad (16)$$

$$\kappa(Be^{i\kappa a} - Ce^{-i\kappa a}) = kD \quad (17)$$

- Eliminate  $D$  by multiplying Eq. 16 with  $k$  and subtracting Eq. 17. This gives

$$k(Be^{i\kappa a} + Ce^{-i\kappa a}) = \kappa(Be^{i\kappa a} - Ce^{-i\kappa a}) \quad (18)$$

- Solve Eq. 18 for  $C$  in terms of  $B$ . Obtain  $C = \frac{\kappa - k}{\kappa + k} e^{2i\kappa a} B$ . We can now say that

$$C = \alpha B, \quad (19)$$

where  $\alpha = \frac{\kappa - k}{\kappa + k} e^{2i\kappa a}$ .

# Solving the TISE for the Rectangular Barrier (Cont'd)

- Substitute Eq. 19 into Eqs. 14 and 15. Obtain

$$1 + A = (1 + \alpha)B \quad (20)$$

$$k(1 - A) = \kappa(1 - \alpha)B \quad (21)$$

- Divide Eq. 21 by Eq. 20. Obtain

$$k \frac{1 - A}{1 + A} = \kappa \frac{1 - \alpha}{1 + \alpha} \quad (22)$$

- Solve Eq. 22 for A. Obtain

$$A = \frac{1 - \frac{\kappa}{k} \frac{1 - \alpha}{1 + \alpha}}{1 + \frac{\kappa}{k} \frac{1 - \alpha}{1 + \alpha}} \quad (23)$$

# Solving the TISE for the Rectangular Barrier (Cont'd)

- It is convenient to introduce  $\beta = \frac{\kappa}{k}$ . Note that  $\alpha = \frac{\beta-1}{\beta+1}e^{2i\kappa a}$  and that

$$\begin{aligned}\frac{1-\alpha}{1+\alpha} &= \frac{\beta+1 - (\beta-1)e^{2i\kappa a}}{\beta+1 + (\beta-1)e^{2i\kappa a}} = \frac{(\beta+1)e^{-i\kappa a} - (\beta-1)e^{i\kappa a}}{(\beta+1)e^{-i\kappa a} + (\beta-1)e^{i\kappa a}} \\ &= \frac{\cos \kappa a - i\beta \sin \kappa a}{\beta \cos \kappa a - i \sin \kappa a}\end{aligned}\quad (24)$$

- Substitute Eq. 24 into Eq. 23. Obtain

$$A = \frac{(1 - \beta^2) \sin \kappa a}{(1 + \beta^2) \sin \kappa a + 2i\beta \cos \kappa a} = \frac{(k^2 - \kappa^2) \sin \kappa a}{(k^2 + \kappa^2) \sin \kappa a + 2ik\kappa \cos \kappa a}$$

- We can now calculate  $B = \frac{1+A}{1+\alpha}$ ,  $C = \alpha B$ , etc, and solve for the complete  $\psi(x)$ . However, knowledge of  $A$  is already sufficient for determination of transmission and reflection coefficients.

# Transmission Coefficient for the Rectangular Barrier

- Note that  $\cos ix = \operatorname{ch} x$ ,  $\sin ix = i \operatorname{sh} x$ ,  $\operatorname{ch}^2 x - \operatorname{sh}^2 x = 1$ .
- The reflection coefficient is

$$R = |A|^2 = \begin{cases} \frac{(k^2 - \kappa^2)^2 \sin^2 \kappa a}{(k^2 + \kappa^2)^2 \sin^2 \kappa a + 4k^2 \kappa^2 \cos^2 \kappa a}, & E > V_0, \text{ real } \kappa \\ \frac{(k^2 + |\kappa|^2)^2 \operatorname{sh}^2 |\kappa| a}{(k^2 - |\kappa|^2)^2 \operatorname{sh}^2 |\kappa| a + 4k^2 |\kappa|^2 \operatorname{ch}^2 |\kappa| a}, & E < V_0, \text{ imaginary } \kappa \end{cases}$$

- The transmission coefficient is

$$T = 1 - R = \begin{cases} \frac{4k^2 \kappa^2}{(k^2 + \kappa^2)^2 \sin^2 \kappa a + 4k^2 \kappa^2 \cos^2 \kappa a}, & E > V_0 \\ \frac{4k^2 |\kappa|^2}{(k^2 - |\kappa|^2)^2 \operatorname{sh}^2 |\kappa| a + 4k^2 |\kappa|^2 \operatorname{ch}^2 |\kappa| a}, & E < V_0 \end{cases}$$

Finally, in terms of  $E$  and  $V_0$ ,

$$T = \begin{cases} \frac{4E(E - V_0)}{4E(E - V_0) + V_0^2 \sin^2 \left( \frac{\sqrt{2m(E - V_0)}}{\hbar} a \right)}, & E > V_0 \\ \frac{4E(V_0 - E)}{4E(V_0 - E) + V_0^2 \operatorname{sh}^2 \left( \frac{\sqrt{2m(V_0 - E)}}{\hbar} a \right)}, & E < V_0 \end{cases} \quad (25)$$

# Properties of the Transmission Coefficient

- $\lim_{E \rightarrow \infty} T = \lim_{V_0 \rightarrow 0} T = 1$ .
- Note that  $T = 1$  also for the case  $E > V_0$ ,  $\kappa a = n\pi$ .
- $\lim_{E \rightarrow V_0} T = \frac{1}{1 + \frac{ma^2 V_0}{2\hbar^2}}$ .
- Consider tunneling through a wide barrier,  $E < V_0$  and  $\frac{\sqrt{2m(V_0 - E)}}{\hbar} a \gg 1$ . For  $x \gg 1$ ,  $\text{sh } x \approx \frac{1}{2}e^x$  and  $\text{sh}^2 x \approx \frac{1}{4}e^{2x}$ . Then

$$T \approx \frac{16E(V_0 - E)}{V_0^2} \exp\left(-2\frac{\sqrt{2m(V_0 - E)}}{\hbar} a\right) \quad (26)$$

If, in addition,  $E \ll V_0$  then

$$T \approx \frac{16E}{V_0} \exp\left(-2\frac{\sqrt{2mV_0}}{\hbar} a\right) \quad (27)$$

Exponential suppression of the transmission coefficient with barrier width is typical for many barrier types.