Quantum Mechanics in One Dimension, Part II

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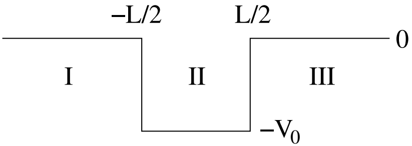
Quantum Mechanics I, September 17, 2020

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

$$A \cos \frac{kL}{2} = C e^{-\frac{\kappa L}{2}} \qquad \text{from the continuity of the wavefunction} \tag{1}$$

$$-kA \sin \frac{kL}{2} = -\kappa C e^{-\frac{\kappa L}{2}} \quad \text{from the continuity of the derivative} \tag{2}$$

Now, divide Eq. 2 by Eq. 1 and obtain

$$k \tan \frac{kL}{2} = \kappa \tag{3}$$

For the odd wavefunction similar reasoning generates the condition

$$k \cot \frac{kL}{2} = -\kappa \tag{4}$$

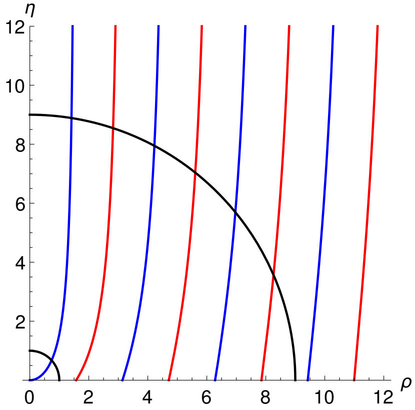
Solving the TISE for the Finite Depth Square Well (Cont'd)

- While Eqs. 3 and 4 can be used to define κ in terms of k, they are by themselves insufficient to pinpoint possible values of k and κ. 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. 3 or 4, this constraint gives us the ability to find k and κ.
- 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 η curves defined by these formulae as a function of ρ.

Graphical TISE Solution for the Finite Depth Square Well



$\eta = \rho \tan \rho$ — even eigenfunctions

$\eta = -\rho \cot \rho$ — odd eigenfunctions

$\rho^2 + \eta^2 = \frac{mV_0 L^2}{2\hbar^2}$ — constraint

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

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:

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

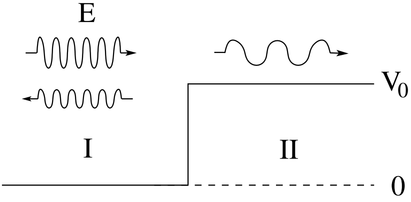
From this equation (check!),

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

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?

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 $j_{\rm II}/j_{\rm I,in}$.

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

$$\psi(x) = \begin{cases} Ae^{ik_1 x} + Be^{-ik_1 x}, & x < 0 \;\; \text{(region I)} \\ Ce^{ik_2 x} + De^{-ik_2 x}, & x > 0 \;\; \text{(region II)} \end{cases},$$

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:

$$\psi(x) = \begin{cases} e^{ik_1 x} + Be^{-ik_1 x}, & x < 0 \;\; \text{(region I)} \\ Ce^{ik_2 x}, & x > 0 \;\; \text{(region II)} \end{cases} \quad (5)$$

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 $\psi'(-0) = \psi'(+0)$.

$$\begin{aligned} 1 + B &= C && \text{from the continuity of the wavefunction} \\ ik_1(1 - B) &= ik_2 C && \text{from the continuity of the derivative} \end{aligned}$$

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

$$B = \frac{k_1 - k_2}{k_1 + k_2} = \frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}} \tag{6}$$

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

Transmission and Reflection Coefficients

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

$$T = \frac{j_{\text{II}}}{j_{\text{I,in}}} = \frac{|C|^2 v_{\text{II}}}{v_{\text{I}}} = \frac{|C|^2 \sqrt{E - V_0}}{\sqrt{E}} = \frac{4\sqrt{E}\sqrt{E - V_0}}{\left|\sqrt{E} + \sqrt{E - V_0}\right|^2} \tag{8}$$

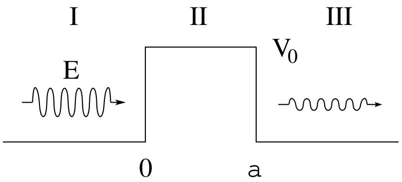
$$R = \frac{j_{\text{I,out}}}{j_{\text{I,in}}} = |B|^2 = \left|\frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}}\right|^2 \tag{9}$$

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

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?

Tunneling Through a Potential Barrier



- Consider the rectangular potential:

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

- What are some possible physical realizations of this potential?
- 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 κ.
- We will be interested in the transmission coefficient $T = |D|^2$.

Solving the TISE for the Rectangular Potential

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

$$1 + A = B + C \tag{10}$$

$$k(1 - A) = \kappa(B - C) \tag{11}$$

The wavefunction continuity conditions at $x = a$:

$$Be^{i\kappa a} + Ce^{-i\kappa a} = D \tag{12}$$

$$\kappa(Be^{i\kappa a} - Ce^{-i\kappa a}) = kD \tag{13}$$

- Eliminate D by multiplying Eq. 12 with k and subtracting Eq. 13. This gives

$$k(Be^{i\kappa a} + Ce^{-i\kappa a}) = \kappa(Be^{i\kappa a} - Ce^{-i\kappa a}) \tag{14}$$

- Solve Eq. 14 for C in terms of B. Obtain $C = \frac{\kappa - k}{\kappa + k} e^{2i\kappa a} B$. We can now say that

$$C = \alpha B, \tag{15}$$

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

Solving the TISE for the Rectangular Potential (Cont'd)

- Substitute Eq. 15 into Eqs. 10 and 11. Obtain

$$1 + A = (1 + \alpha)B \tag{16}$$

$$k(1 - A) = \kappa(1 - \alpha)B \tag{17}$$

- Divide Eq. 17 by Eq. 16. Obtain

$$k\frac{1 - A}{1 + A} = \kappa\frac{1 - \alpha}{1 + \alpha} \tag{18}$$

- Solve Eq. 18 for A. Obtain

$$A = \frac{1 - \frac{\kappa}{k}\frac{1-\alpha}{1+\alpha}}{1 + \frac{\kappa}{k}\frac{1-\alpha}{1+\alpha}} \tag{19}$$

Solving the TISE for the Rectangular Potential (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

$$\begin{aligned} \frac{1-\alpha}{1+\alpha} &= \frac{\beta + 1 - (\beta - 1)e^{2i\kappa a}}{\beta + 1 + (\beta - 1)e^{2i\kappa a}} = \frac{(\beta + 1)e^{-i\kappa a} - (\beta - 1)e^{i\kappa a}}{(\beta + 1)e^{-i\kappa a} + (\beta - 1)e^{i\kappa a}} \\ &= \frac{\cos \kappa a - i\beta \sin \kappa a}{\beta \cos \kappa a - i \sin \kappa a} \end{aligned} \tag{20}$$

- Substitute Eq. 20 into Eq. 19. 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 $\cos ix = \operatorname{ch} x$, $\sin ix = i \operatorname{sh} x$, $ch^2 x - sh^2 x = 1$.
- 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,

$$T = \begin{cases} \frac{4E(E-V_0)}{4E(E-V_0) + V_0^2 \sin^2\left(\frac{\sqrt{2m(E-V_0)}}{\hbar} a\right)}, & E > V_0 \\ \frac{4E(V_0-E)}{4E(V_0-E) + V_0^2 \operatorname{sh}^2\left(\frac{\sqrt{2m(V_0-E)}}{\hbar} a\right)}, & E < V_0 \end{cases} \tag{21}$$

Properties of the Transmission Coefficient

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

$$T \approx \frac{16E(V_0 - E)}{V_0^2} \exp\left(-2\frac{\sqrt{2m(V_0 - E)}}{\hbar} a\right) \tag{22}$$

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

$$T \approx \frac{16E}{V_0} \exp\left(-2\frac{\sqrt{2mV_0}}{\hbar} a\right) \tag{23}$$

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