PHYS-4007/5007
COMPUTATIONAL PHYSICS PROJECT:
Quantum Scattering and Tunneling

1 Introduction.

In the quantum world, as is the case in classical physics, some of the most interesting problems evolve from the collision of particles and the collision of particles with barriers. This program should outline the mathematical and computational methods used to solve problems of quantum scattering and tunneling in one dimension. This program should explore the case of a collision between a beam of particles with energy $\boldsymbol{E}$ and a barrier with energy of $\boldsymbol{V}$.

Start with Schrödinger's equation which describes the "wave functions" of particles on a microscopic particles:

$$\imath\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi. \tag{1}$$

Use this equation to investigate the scattering and tunneling of a particles off of a boundary in one dimension. To begin, you must still obey the Law of Conservation of Energy. The total energy before and after the collision must be equal. Since you know energy of the particle beam ($\boldsymbol{E}$) and the energy of the potential barrier ($\boldsymbol{V}$), you must find a wave function Ψ that will satisfy Schrödinger's equation. Secondly, you are dealing with states of well-defined energies.

For this project, assume stationery states. A stationary state is one where the probability density, (the probability of finding the wave in a given area), of the wave function is independent of time. With this being the case, we can now use a different form of Schrödinger's equation — the *Time Independent Schrödinger's Equation* (TISE):

$$E\,\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\,\psi, \tag{2}$$

where

$$E = \imath\hbar\frac{\partial\Psi}{\partial t}, \tag{3}$$

and through a separation of variables, we find

$$\Psi(x,t) = \psi(x)e^{\frac{-\imath Et}{\hbar}}. \tag{4}$$

2 Traveling Waves and the Finite Square Barrier.

The wave function for **traveling waves** can always be described by

$$\psi(x) = A\,e^{-i\alpha x} + B\,e^{i\alpha x}. \tag{5}$$

One can easily see that this function has an oscillatory form from the trigonometric expression

$$e^{\pm i\,\alpha} = \cos\alpha \pm i\,\sin\alpha\ . \tag{6}$$

If the expression in the exponent of Eq. (5) is *positive*, the traveling wave moves from the *left* to the *right* $\Longrightarrow$ as such, at negative x, $A\,e^{-i\alpha x}$ corresponds to a wave traveling from the left towards the right, meanwhile, at positive x, $B\,e^{i\alpha x}$ corresponds to such a wave. If the expression in the exponent is *negative*, the traveling wave moves from the *right* to the *left* $\Longrightarrow$ as such, at negative x, $B\,e^{i\alpha x}$ corresponds to a wave traveling from the right towards the left, meanwhile, at positive x, $A\,e^{-i\alpha x}$ corresponds to such a wave.

Meanwhile, a **standing wave** is characterized by the following wave function:

$$\psi(x) = C\,\sin(\alpha x) + D\,\cos(\alpha x). \tag{7}$$

Here, the sine and the cosine terms do not have any specific directional information associated with them, which is easy to understand since we are talking about a standing wave. With this information in mind, consider the finite square barrier:

$$V(x) = \begin{cases} V_\circ, & \text{for } -a < x < a, \\ 0, & \text{for } |x| > a, \end{cases} \tag{8}$$

where $V_\circ$ is a (positive) constant as shown in Figure 1.

Reflection and tunneling states will occur when $0 < E < V_\circ$ (as indicated by Regions 1, 2, and 3 in Figure 1). Scattering states will occur when $E > V_\circ$ (as indicated by Regions 4, 5, and 6 in Figure 1).

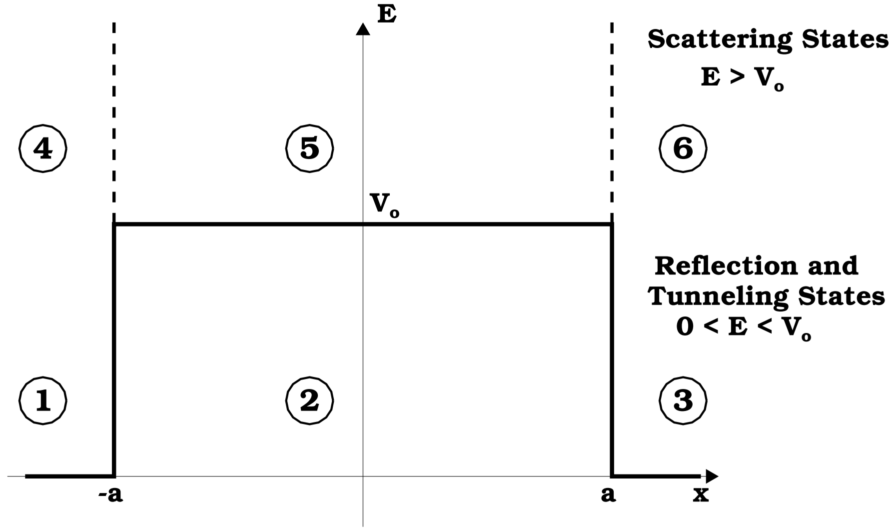

Figure 1: The finite square barrier potential (Eq. 8).

2.1 Reflection and Tunneling States ($0 < E < V_\circ$).

Region 1: For the states in the region $x < -a$, $V(x) = 0$ and the TISE becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi, \quad \text{or} \quad \frac{d^2\psi}{dx^2} = -k^2\psi, \tag{9}$$

where

$$k \equiv \frac{\sqrt{2mE}}{\hbar} \tag{10}$$

is real and positive. The general solution to the TISE is

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \quad \text{for } (x < -a), \tag{11}$$

where

$$k \equiv \frac{\sqrt{2mE}}{\hbar}. \tag{12}$$

Here, the A term is the incident wave (we will assume here that all incident particles are coming in from the left) and the B will represent reflected particles (*i.e.*, waves).

Region 2: In the region $-a < x < a$, $V(x) = V_\circ$ and the TISE becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_\circ\psi = E\psi, \quad \text{or} \quad \frac{d^2\psi}{dx^2} = \kappa^2\psi, \tag{13}$$

where

$$\kappa \equiv \frac{\sqrt{-2m(E - V_\circ)}}{\hbar}, \tag{14}$$

here, $E - V_\circ$ is negative since $V_\circ > E$ inside the barrier, so the parameter inside the square root will be positive. The general solution to this differential equation is

$$\psi(x) = Ce^{-\kappa x} + De^{\kappa x}, \quad \text{for } (-a < x < a), \tag{15}$$

where C and D are arbitrary constants. The C term will represent the incident particles traveling from left to right that penetrate the barrier, and the D term represent those incident particles that tunnel into the barrier and get reflected off of the back surface.

Region 3: For bound states in the region $x > a$, the potential is again zero and the general solution has the form of $\psi(x) = Fe^{ikx} + Ge^{-ikx}$, where the F term represents particles transmitted through the barrier (since the exponent is positive due to $x > 0$, hence moving left to right) and the G term represents incident particles coming in from the right (since the exponent is negative). Since we have already made the assumption that the incident particles are only coming in from the left, $G = 0$, and hence

$$\psi(x) = Fe^{ikx}, \quad \text{for } (x > a). \tag{16}$$

The final solution for the states ($0 < E < V_\circ$) of the finite square barrier: Imposing the standard boundary conditions, ψ and $d\psi/dx$ continuous at $-a$ and a, we can to determine the constants of our solution:

$$\psi(x) = \begin{cases} A\,e^{-ikx} + Be^{ikx}, & \text{for } (x < -a), \\ Ce^{-\kappa x} + De^{\kappa x} & \text{for } (-a < x < a), \\ Fe^{ikx}, & \text{for } (x > 0)\ . \end{cases} \tag{17}$$

The boundary conditions give:

- The continuity of $\psi(x)$, at $x = -a$, says

$$A\,e^{ika} + Be^{-ika} = Ce^{\kappa a} + De^{-\kappa a}\ . \tag{18}$$

- The continuity of $d\psi/dx$ at $x = -a$ says

$$-ikA\,e^{ika} + ikBe^{-ika} = -\kappa Ce^{\kappa a} + \kappa De^{-\kappa a}\ . \tag{19}$$

- The continuity of $\psi(x)$, at $x = a$, says

$$Ce^{-\kappa a} + De^{\kappa a} = Fe^{ika}\ . \tag{20}$$

- The continuity of $d\psi/dx$ at $x = a$ says

$$-\kappa Ce^{-\kappa a} + \kappa De^{\kappa a} = ikFe^{ika}\ . \tag{21}$$

The probability that a particle will be transmitted through the barrier is given by the **transmission coefficient**:

$$T = \frac{|F|^2}{|A|^2} \tag{22}$$

and the probability that a particle will be reflected back by the barrier is given by the **reflection coefficient**:

$$R = \frac{|B|^2}{|A|^2} \, . \tag{23}$$

Note that to conserve particle flux $T + R = 1$. Should $T > 0$, then those particles that are transmitted though the barrier are said to have **tunneled** their way through. You will need to analytically come up with an expression for both of these coefficients that depends only on the energy (and potential). (*Hint*: Solve F, A, and B in terms of only one of the other coefficients (say D) and carry out the division.)

2.2 Scattering States ($E > V_\circ$).

Region 4: For the scattering ($E > V_\circ$) states, to the left, where $V(x) = 0$, we have

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \quad \text{for } (x < -a), \tag{24}$$

where

$$k \equiv \frac{\sqrt{2mE}}{\hbar}. \tag{25}$$

Region 5: Over the barrier, where $V(x) = V_\circ$, we have

$$\psi(x) = C\sin(\ell x) + D\cos(\ell x), \quad \text{for } (-a < x < a), \tag{26}$$

where

$$\ell \equiv \frac{\sqrt{2m(E - V_\circ)}}{\hbar}, \tag{27}$$

where $E > V_\circ$ in this case.

Region 6: To the right, assuming no incoming wave from that region, we have

$$\psi(x) = Fe^{ikx}, \quad \text{for } (x > a). \tag{28}$$

As described at the beginning of this subsection, in Equations (24) and (28), A is the incident amplitude, B is the reflected amplitude, and F is the transmitted amplitude of a wave traveling in the vicinity of this finite square potential. There are 4 boundary conditions for these three equations (Eqs. 24, 26, and 28):

- Continuity of $\psi(x)$ at $-a$ says

$$Ae^{-ika} + Be^{ika} = -C\sin(\ell a) + D\cos(\ell a). \tag{29}$$

- Continuity of $d\psi/dx$ at $-a$ says

$$ik[Ae^{-ika} - Be^{ika}] = \ell[C\cos(\ell a) + D\sin(\ell a)]. \tag{30}$$

- Continuity of $\psi(x)$ at $+a$ says

$$C\sin(\ell a) + D\cos(\ell a) = Fe^{ika}. \tag{31}$$

- Continuity of $d\psi/dx$ at $+a$ says

$$\ell[C\cos(\ell a) - D\sin(\ell a)] = ikFe^{ika}. \tag{32}$$

We can use two of these to eliminate C and D, and solve the remaining two for B and F:

$$B = i\frac{\sin(2\ell a)}{2k\ell}\left(\ell^2 - k^2\right)F, \tag{33}$$

$$F = \frac{e^{-2ika}\,A}{\cos(2\ell a) - i[\sin(2\ell a)/2k\ell]\,(k^2 - \ell^2)}. \tag{34}$$

The transmission coefficient ($T = |F|^2/|A|^2$) is then

$$T^{-1} = 1 + \frac{V_\circ^2}{4E(E + V_\circ)}\,\sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E + V_\circ)}\right). \tag{35}$$

Notice that $T = 1$ (*i.e.*, the well becomes *transparent*) whenever the argument of the sine is zero, or

$$\frac{2a}{\hbar}\sqrt{2m(E + V_\circ)} = n\pi, \tag{36}$$

where n is any integer. The energies for perfect transmission are given by

$$E_n + V_\circ = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}. \tag{37}$$

Meanwhile, the reflection coefficient is once again $R = |B|^2/|A|^2$. I leave it to you to come up with an expression for this coefficient.

3 Graduate Student Component.

Numerically check how the wave functions $\psi(x)$ and the transmission and reflection coefficients behave as $E \to V_\circ$ for both cases described above (*i.e.*, $0 < E < V_\circ$ and $E > V_\circ$). Come up with an analytic solution for these parameters and compare them with your numeric solutions.

4 Analysis and Goals of the Project.

The problem now boils down to solving a second order differential equation. There are two linearly independent solutions to a second order differential equation. The general solution to the problem can thus be constructed as a linear combination of the two solutions. At this point you must look at how you set up the problem. For your project, you are **numerically** to solve the Schrödinger equation (see Eq. 2) for a square potential barrier as shown in Figure 1. You also are to make comparisons between your numerical solution and the analytic solutions described above. Your code also needs to calculate the transmission and reflection probabilities for both cases where $E > V_\circ$ and $E < V_\circ$ for an incident beam of particles on your barrier. Tabulate your numerical results and the analytic results. You must also graphically display what your wave functions look like in the different regions of the potential as shown in Figure 1. How are the scattering states both similar and different to the reflection/tunneling states?

The final computer project report must be written in LaTeX! I have a LaTeX template file called template.tex on the course web page.