Scattering and Bound States in One-Dimensional Potential*
Applications to Nanophysics

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We analyze a quantum particle under the influence of simple one-dimensional potentials. First, we develop qualitative techniques to determine whether the system will have bound or scattering states for a given energy. These techniques also help in asserting the shape of the wave function. We then provide a complete mathematical treatment of the wave function of a particle under the influence of three different potentials: (i) infinite well, (ii) finite well, and (iii) barrier potential. For all the cases, we exploit the symmetric nature of the potentials to calculate the bound states. We also provide examples demonstrating the usage of these models in nano-physical systems.

1. Introduction

Newton’s second law or Hamiltonian mechanics predicts a classical particle’s future once the particle’s position and momentum are known. Similarly, in quantum mechanics, Schrödinger’s equation describes the time evolution of the wave function, which contains information about the state of the particle. The Schrödinger equation is mathematically described as a linear partial differential equation, and its derivation was considered one of the significant developments in the theory of quantum mechanics. One of the topics encountered in undergraduate quantum mechanics course is solving the Schrödinger equation for a particle in different potentials.

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Figure 1. Suppose a student wants to reach his house situated beyond a hill. In the classical world, he must ride through the top of the hill to reach his destination. However, in the quantum world, a strange thing can happen. A quantum particle can tunnel through such a potential hill rather than going over it.

A practical application of these studies is in nanophysics which deals with physical systems whose at least one of three dimensions is of the order of nanometers. For designing a nanosystem, theoretical modeling before a real experiment is advantageous. Fortunately, most encountered nanosystems like quantum dots or quantum wires can be modelled using simple potentials.

Given the recent developments in nanophysics, it becomes necessary to comprehend the subtleties of quantum physics. To this end, we first provide a qualitative analysis of the general properties of the solutions of the Schrödinger equation. We then discuss quantitative results of the Schrödinger equation for different simple one-dimensional potentials.

2. Time-dependent Schrödinger Equation

We consider a system with a single spatial degree of freedom under the effect of a time-independent potential. The time-dependent Schrödinger equation\(^1\) can be written as

\[
\frac{i\hbar}{\partial t}\Psi(x, t) = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \Psi(x, t).
\]  

(1)

Here, \(\hbar = h/2\pi\) is the reduced Planck constant, \(m\) is the mass of the particle, \(V(x)\) is the potential energy and \(\Psi(x, t)\) is the time-dependent wave function of the particle. Square of the modulus of the wave function \(|\Psi(x, t)|^2\) represents the probability of finding
the particle at position \( x \), and time \( t \). A normalized wave function satisfies

\[
\int_{-\infty}^{\infty} dx \left| \Psi(x, t) \right|^2 = 1. \tag{2}
\]

The condition above is generally known as the normalization condition, meaning that the particle has to be located somewhere between \( x = -\infty \) and \( x = \infty \) at all times.

Since the potential \( V(x) \) is independent of time, the total wave function can be expressed as a product of time-dependent part and spatial coordinate dependent part,

\[
\Psi(x, t) = \psi(x) \phi(t). \tag{3}
\]

Substituting (3) in (1) and dividing by \( \Psi(x, t) \) yields

\[
-\frac{\hbar^2}{2m} \frac{1}{\psi(x)} \frac{d^2 \psi(x)}{dx^2} + V(x) = i\hbar \frac{1}{\phi(t)} \frac{d\phi(t)}{dt}. \tag{4}
\]

Since \( x \) and \( t \) are independent variables, the above expression can be true only if both sides of the equality are independently equal to a constant \( E \), which we call as the separation constant. Consequently, we obtain two ordinary differential equations which can be written as,

\[
\frac{d\phi}{dt} = -\frac{iE}{\hbar} \phi, \tag{5}
\]

and

\[
-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V\psi = E\psi. \tag{6}
\]

Integration of first differential equation (5) yields \( \phi(t) = Ce^{-iEt/\hbar} \),

Since \( C \) is a constant, it can be included in \( \psi(x) \) and consequently \( \phi(t) \) can be rewritten as

\[
\phi(t) = e^{-iEt/\hbar}. \tag{7}
\]

The other differential equation (6) is known as the time-independent Schrödinger equation and can be solved for various forms of the potential \( V(x) \). Since (6) can also be written as \( \hat{H}\psi = E\psi \) with \( \hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V \), it is also known as energy eigenvalue equation.

Different values of \( E \) satisfying \( \hat{H}\psi = E\psi \) are known as energy eigenvalues and the corresponding \( \psi \) are called energy eigenfunctions.
**Figure 2.** Condition on particle’s energy $E$ for bound states: $V_{\text{min}} < E < V(-\infty)$ and $V(+\infty)$, and scattering states: $E > V(-\infty)$ or $V(+\infty)$.

3. Qualitative Analysis

Before solving the time-independent Schrödinger equation, we digress a little and analyze the general properties of an arbitrary potential. This analysis will help us in predicting the possibility of bound or scattering states and the broad nature of the wave functions, which will enable us to verify quantitative results.

3.1 Bound and Scattering States

Consider a particle with energy $E$ interacting with a one-dimensional potential with $V(\infty) = V_1$, $V(-\infty) = V_2$ and minimum of $V_{\text{min}}$ as shown in Figure 2. We consider different cases where different outcomes are possible depending on the magnitude of particle’s energy.

(i) $V_{\text{min}} < E < V_1$
Suppose $E = V(x_1) = V(x_2)$. In this case, a classical particle moves back and forth between $x_1$ and $x_2$. Hence, the particle is localized and this situation in quantum mechanics leads to bound states.

(ii) $V_1 < E < V_2$
Suppose $E = V(x_3)$. A classical particle approaches from $x = +\infty$ side, reaches $x_3$ and then returns to $x = +\infty$.
side. Such situation in quantum mechanics leads to scattering states.

(iii) \( E > V_2 \)

Here the particle can approach the potential from either \( x = +\infty \) or \( x = -\infty \) side and continue its journey to \( x = -\infty \) or \( x = +\infty \) side, respectively. This situation in quantum mechanics also leads to scattering states.

3.2 Shape of the Wave Function

To study the shape of the wave function, we consider (6) written in a slightly different form as

\[
\frac{d^2 \psi}{dx^2} = \frac{2m}{\hbar^2} (V(x) - E)\psi. \tag{8}
\]

Depending on the sign of \( V(x) - E \) and \( \psi(x) \), \( d^2 \psi/dx^2 \) can be positive or negative, and thus wave functions will be concave up or concave down respectively. This is depicted in the top row of Figure 3.

As a demonstration of the concept mentioned above, we plot the ground state wave function of the finite potential well, as illustrated in the bottom of Figure 3. Inside the well where \( V(x) < E \), wave function curves towards the axis and is normalizable. However, outside the well where \( V(x) > E \), the wave function curves away from the axis and is non-normalizable. For the wavefunction to be concave upward and yet normalizable, we require that the wave function in the region \( V(x) > E \) decreases smoothly such that it touches the \( x \) axis in the limit \( x \to \pm \infty \).

3.3 Symmetric Potential

For symmetric potentials \( V(x) = V(-x) \), Schrödinger equation (6) leads to the conclusion \( \psi(x) = \pm \psi(-x) \), i.e., the wave functions are either even or odd. The reason that the wave functions are either even or odd for symmetric potentials can be understood intuitively as follows. Since the potential is symmetric, probability

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2 If the second derivative \( d^2 f/dx^2 \) of a function \( f \) is positive (negative), the graph is concave up (down).

3 Wavefunction \( \psi(x) \) is normalizable if \( \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx < \infty \). If the above integral is infinite, the wavefunction is non-normalizable.
Figure 3.

**Top Left:** \((V(x) < E)\)

Depending on \(\psi > 0\) or \(\psi < 0\), \(\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(V(x) - E)\psi\) is negative or positive and thus \(\psi\) is concave down or concave up respectively.

**Top Right:** \((V(x) > E)\)

Similar arguments lead to wave function concave up or concave down when \(\psi > 0\) or \(\psi < 0\) respectively.

**Bottom:** Plotting ground state wave function of finite potential well.

Inside the well \((V(x) < E)\), wave function curves towards the axis. However, outside the well \((V(x) > E)\), the wave function curves away from the axis and is non-normalizable (dashed).

To be normalizable, it should decrease in such a way that \(\psi(x) \to 0\) as \(x \to \pm \infty\) (solid).

density of finding the particle should be same on both sides, i.e., \(|\psi(x)|^2 = |\psi(-x)|^2\). Taking the square root, we get \(\psi(x) = \pm \psi(-x)\).

In this article, we consider symmetric potentials to simplify the calculations of bound states.

### 3.4 Boundary Conditions

Since the time-dependent part (5) of Schrödinger equation (1) is a first-order ordinary differential equation in time, the general solution has one unknown parameter. Hence, one condition is required to determine the unknown parameter. Generally, wave function at initial time \(\Psi(x, t_0)\) is provided.

Similarly, the \(x\) dependent part (6) is a second-order ordinary dif-
ferential equation, and thus the general solution contains two unknown parameters. To determine these parameters, two conditions involving $\psi(x)$ and/or its derivative $d\psi/dx$ at some points are required. These conditions are known as boundary conditions and can be written as

1. wave function $\psi(x)$ should be continuous and

2. the first derivative of the wave function $d\psi/dx$ should be continuous except for the case when the potential is infinite at the boundary.

If the particle is confined within an infinite potential, the wave function must vanish at the boundaries. Discontinuity in the wave function or its derivative leads to nonphysical results.

4. Quantitative Analysis

In this section, we solve the time-independent Schrödinger equation for a few simple potentials. We consider potential well or barrier extending from $-a$ to $a$, and since the potential is symmetric, we exploit its property to simplify the bound state solutions. Some of the textbooks consider well or barrier extending from 0 to $a$. While there is no physical difference, their mathematical expressions can be related to ours by suitable transformation.

4.1 Infinite Potential Well

Consider a particle of mass $m$ and energy $E$ interacting with the potential

$$V(x) = \begin{cases} 0 & |x| < a, \\ \infty & |x| \geq a. \end{cases} \quad (9)$$

Outside the well ($|x| \geq a$):

Since the potential is infinite, the particle cannot go there, and thus the wave function is

$$\psi(x) = 0. \quad (10)$$
**Figure 4.** First three eigenfunctions for an electron in an infinite potential well are shown. Since the potential is symmetric about the centre of the well, eigenfunctions are either even or odd about the centre of the well.

Optical absorption of beta-carotene, a molecule in carrot, can be explained using particle in an infinite potential well model.

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*Inside the well* (*|x| < a*):

Time-independent Schrödinger equation (8) becomes

\[
\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi, \quad (11)
\]

where \( k = \sqrt{2mE/\hbar} \). Here \( E \) is positive since negative values of \( E \) would not lead to normalizable solutions. Therefore, \( k \) is real.

The general solution to above differential equation is of the form \( \psi(x) = A \sin(kx) + B \cos(kx) \). But since, the potential is symmetric, the solution will be either even or odd. Even eigenfunction will have the form \( \psi_e(x) = B \cos(kx) \). Applying the boundary condition at \( x = a \), we obtain \( \psi_e(a) = B \cos(ka) = 0 \), which yields the condition

\[
ka = \frac{n\pi}{2} \Rightarrow k = \frac{n\pi}{2a}, \quad n = 1, 3, 5 \ldots \quad (12)
\]

Similarly, odd eigenfunction will have the form \( \psi_o(x) = A \sin(kx) \).

Applying the boundary condition at \( x = a \), we obtain \( \psi_o(a) = \)
A \sin(ka) = 0, which leads to the condition
\[ ka = \frac{n\pi}{2} \Rightarrow k = \frac{n\pi}{2a}, \quad n = 2, 4, 6 \ldots \quad (13) \]

Therefore, normalized even eigenfunctions can be written as
\[ \psi_n(x) = \frac{1}{\sqrt{a}} \cos \left( \frac{n\pi x}{2a} \right), \quad n = 1, 3, 5 \ldots \quad (14) \]

Similarly, normalized odd eigenfunctions can be expressed as
\[ \psi_n(x) = \frac{1}{\sqrt{a}} \sin \left( \frac{n\pi x}{2a} \right), \quad n = 2, 4, 6 \ldots \quad (15) \]

Since \( k = \sqrt{2mE}/\hbar \), energy of the \( n^{th} \) eigenfunction is
\[ E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2m(2a)^2}. \quad (16) \]

Figure 4 shows the first three energy eigenfunctions superimposed on infinite potential well. Since Schrödinger equation is a linear differential equation, any linear combination of the solutions is also a solution. Moreover, any wavefunction satisfying the infinite potential well boundary conditions can be expressed as a linear combination of all even (14) and odd (15) eigenfunctions, and hence the even and odd eigenfunctions form a complete basis for the infinite potential well. The above statements also hold for arbitrary potentials.

This is in analogy to the case of a vector in three dimensions, which can be expressed as a linear combination of \( \hat{i} \), \( \hat{j} \) and \( \hat{k} \) unit vectors.

### 4.2 Example

Now, we consider an example where we show how to determine the wave function at any time \( t \) when the initial wave function at time \( t = 0 \) is given. Consider the initial wave function of a particle in a box as shown in Figure 5:
\[
\Psi(x, 0) = \begin{cases} 
N(a + x) & -a < x < 0, \\
N(a - x) & 0 < x < a, \\
0 & |x| \geq a,
\end{cases} \quad (17)
\]
Figure 5. Left: Initial wave function $\Psi(x, 0)$ is even about $y$-axis ($x = 0$), and thus can be expanded as a linear combination of only the even eigenfunctions $\psi_n^e(x) = \sqrt{\frac{2}{a}} \cos \left( \frac{n\pi x}{a} \right)$ of the infinite well.

Right: Bar diagram of first few coefficients $c_n$ of even eigenfunctions.

where $N = \sqrt{3/2a^3}$ is the normalization constant.

Since $\Psi(x, 0)$ is even, it can be expressed as a linear combination of only even eigenfunctions $\psi_n^e(x)$. Mathematically, this can be written as

$$\Psi(x, 0) = \sum_{n=\text{odd}} c_n \psi_n^e(x).$$

Using Fourier analysis, the coefficients $c_n$ can be expressed as

$$c_n = \int_{-a}^{a} \psi_n^e(x) \Psi(x, 0) \frac{4\sqrt{6}}{n^2\pi^2}.$$  \hspace{1cm} (19)

Here, $|c_n|^2$ represents the probability of the particle being in state $\psi_n^e$. Further, the coefficients satisfy the equation $\sum_{n=\text{odd}} |c_n|^2 = 1$, which means that the probability of finding the particle in any of the eigenfunction adds up to one. According to (3) and (7), $\Psi(x, t)$ can be determined by multiplying a factor of $\exp(-iE_nt/\hbar)$ to $\psi_n^e(x)$ in (18) as follows:

$$\Psi(x, t) = \sum_{n=\text{odd}} \frac{4\sqrt{6}}{n^2\pi^2} \psi_n^e(x) \exp(-iE_nt/\hbar).$$ \hspace{1cm} (20)

4.3 Finite Potential Well

Consider a particle of mass $m$ interacting with a finite well potential as shown in Figure 6:

$$V(x) = \begin{cases} 0 & |x| < a, \\ V_0 & |x| \geq a. \end{cases}$$  \hspace{1cm} (21)

As we can see from the analysis of section 3.1, both bound states and scattering states are possible for this potential depending on particle’s energy. We first consider the bound states of the system.
Case I: $E < V_0$

Since the potential is symmetric about $x = 0$, bound states are either odd or even. First, we will calculate even bound states for this potential. In region I ($x \leq -a$), Eqn. (8) becomes

$$\frac{d^2 \psi_e}{dx^2} = \frac{2m}{\hbar^2} (V_0 - E) \psi_e = k^2 \psi_e.$$  \hspace{1cm} (22)

where $k = \sqrt{2m(V_0 - E)}/\hbar$. The general solution can be written as

$$\psi_e(x) = Ae^{kx} + Be^{-kx}. \hspace{1cm} (23)$$

Since $e^{-kx}$ blows up as $x \to -\infty$, the allowed solution is

$$\psi_e(x) = Ae^{kx}. \hspace{1cm} (24)$$

Similarly, in region III ($x \geq a$), the potential is $V_0$, and the general solution is the same as region I. However, this time $e^{kx}$ blows up as $x \to \infty$. Therefore, the allowed solution in this region is

$$\psi_e(x) = Ae^{-kx}. \hspace{1cm} (25)$$

Here, normalization constant is also $A$ as we are considering even bound state. Finally, in region II ($-a < x < a$), the potential is zero and (8) reads

$$\frac{d^2 \psi}{dx^2} = -\frac{2mE}{\hbar^2} \psi = -k^2 \psi.$$  \hspace{1cm} (26)
where \( k = \sqrt{2mE/h} \). General solution to above differential equation is of the form \( \psi(x) = C \sin(kx) + D \cos(kx) \), but since we are considering even bound state, \( \psi_e(x) = D \cos(kx) \).

Summarizing the above results, we write the even bound state wave function in all three regions:

\[
\psi_e(x) = \begin{cases} 
Ae^{kx} & x \leq -a, \\
D \cos(kx) & -a < x < a, \\
Ae^{-kx} & x \geq a.
\end{cases} 
\]  

(27)

Similarly, we can obtain the odd bound state wave function which can be written as

\[
\psi_o(x) = \begin{cases} 
A'e^{kx} & x \leq -a, \\
C \sin(kx) & -a < x < a, \\
-A'e^{-kx} & x \geq a.
\end{cases} 
\]  

(28)

Since, we are already considering even and odd bound states separately, applying boundary condition either at \( x = a \) or \( x = -a \) yields the quantization condition. Continuity of \( \psi(x) \) at \( x = a \) for even wave function (27) yields

\[
Ae^{-ka} = D \cos(ka),
\]  

(29)

and continuity of \( d\psi/dx \) at \( x = a \) results in

\[
-\kappa Ae^{-ka} = -kD \sin(ka).
\]  

(30)

Dividing (30) by (29), we obtain

\[
\kappa = k \tan(ka).
\]  

(31)

Similarly, application of boundary conditions on odd bound state (28) yields

\[
\kappa = -k \cot(ka).
\]  

(32)

To obtain solutions of implicit (31) and (32), we can use either a graphical solution method or a root-finding program, for example, Newton–Raphson method. Only a finite number of bound
eigenfunctions are possible for finite potential well. For example, if an electron is confined in a finite well of depth $V_0 = 4 \text{ eV}$ and width 1 nm, only four bound states are possible. These bound states are shown in Figure 7. According to classical mechanics, the probability of finding the particle outside the well is zero when the energy of the particle is less than the potential depth. However, in quantum mechanics, the particle has a nonzero probability of being outside the well, as we can see from Figure 7. This quantum-mechanical phenomenon is known as tunneling. 

**Case II: $E > V_0$**

In this case, a particle approaching the potential gets scattered, and thus only scattering states are possible.

We consider a beam of particles, each having energy $E$, travelling from left to right incident upon the well. We also assume that the incident beam has unit amplitude, and the reflected and transmitted beam amplitudes are set to be $r$ and $t$, respectively. The schematic is shown in Figure 8. In this case, $V(x) - E$ is negative in all three regions, and thus the general solution of the time-

\[ e^{ikx} \] represents particles travelling towards right and left respectively.
**Figure 8.** A beam of particles, each having energy $E$ is travelling from left to right. $e^{i\kappa x}$ represents the wave function of the incident beam, $re^{-i\kappa x}$ and $te^{i\kappa x}$ represent the wave function of the reflected and the transmitted beam respectively.

The independent Schrödinger equation is of the form $Ae^{ikx} + Be^{-ikx}$. We do not consider the alternate form of the solution $A \sin(kx) + B \cos(kx)$ as it does not simplify the calculations for scattering states.

Thus, solution to time-independent Schrödinger equation in all three regions can be written as

$$
\psi(x) = \begin{cases} 
e^{i\kappa x} + B e^{-i\kappa x} & x \leq -a, \\
A e^{i\kappa x} + B e^{-i\kappa x} & -a < x < a, \\
B e^{i\kappa x} & x \geq a,
\end{cases}
$$

where $k = \sqrt{2mE}/\hbar$ and $\kappa = \sqrt{2m(E - V_0)}/\hbar$. Now applying continuity of $\psi$ and $d\psi/dx$ at $x = -a$ and $x = a$ yield four equations in four unknowns $r$, $t$, $A$, and $B$. After a little algebra, one can find the quantity $t$ by eliminating $r$, $A$, and $B$. The transmission coefficient representing the probability that the particle gets transmitted across the well is given by

$$
T = |t|^2 = \frac{4E(E - V_0)}{4E(E - V_0) + V_0^2 \sin^2 \left(\frac{2a}{\hbar}\sqrt{2mE}\right)}
$$

Classically, the particle would have been transmitted through the well with unit probability. This happens in the current quantum-mechanical scenario when $\sin(2a \sqrt{2mE}/\hbar) = 0$. 

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4.4 Finite Potential Barrier

We consider a particle of mass $m$ interacting with a finite potential barrier as shown in Figure 9:

$$V(x) = \begin{cases} V_0 & |x| < a, \\ 0 & |x| \geq a. \end{cases}$$  (35)

We can deduce from the analysis of section 3.1 that this potential cannot trap a particle, and thus can have only scattering states. Here also, we consider a beam of particles, each having energy $E$ incident upon the barrier and travelling from left to right. We also assume that the incident beam has a unit amplitude, and the reflected and the transmitted beam amplitudes are set to be $r$ and $t$, respectively. For a potential barrier, three different cases are possible, and we treat them one by one. In this section, we omit a few mathematical steps and directly write the final results.

**Case I: $E < V_0$**

Solving time-independent Schrödinger equation, we obtain the wave function in all three regions as

$$\psi(x) = \begin{cases} e^{ikx} + re^{-ikx} & x \leq -a, \\ Ae^{ikx} + Be^{-ikx} & -a < x < a, \\ te^{ikx} & x \geq a. \end{cases}$$  (36)
where \( k = \sqrt{2mE}/\hbar \) and \( \kappa = \sqrt{2m(V_0 - E)}/\hbar \). Here also we apply continuity of \( \psi \) and \( d\psi/dx \) at \( x = -a \) and \( x = a \) that yield four equations in four unknowns \( r, t, A, \text{and } B \). We can derive \( t \) by eliminating \( r, A \) and \( B \) from the four equations. The transmission coefficient can be expressed as

\[
T = |t|^2 = \frac{4E(V_0 - E)}{4E(V_0 - E) + V_0^2 \sinh^2 \left( \frac{2a}{\hbar} \sqrt{2m(V_0 - E)} \right)}, \quad (37)
\]

This expression shows that even though the particle energy is less than the barrier potential, it has a nonzero probability of passing through the potential barrier. This phenomenon is called tunneling (See Figure 9).

**Numerical example:**

To get a numerical estimate of tunneling probability, consider a particle with energy 1 eV incident on a barrier of height 2 eV and width 0.5 nm. Equation (37) yields \( T = 0.024 \), i.e., the probability of particle crossing the barrier is 2.4 %.

**Case II: \( E = V_0 \)**

In this case, \( V(x) - E \) is zero in region II and the solution is a linear function rather than an exponential in \( x \). The wave function in all three regions obtained after solving time-independent Schrödinger equation is

\[
\psi(x) = \begin{cases} 
e^{ikx} + re^{-ikx} & x \leq -a, \\ A + Bx & -a < x < a, \\ le^{ikx} & x \geq a, \end{cases} \quad (38)
\]

where \( k = \sqrt{2mE}/\hbar \).

Here also, we obtain four equations in four unknowns after applying the boundary conditions, and \( t \) can be derived after eliminating the other unknown quantities. The transmission coefficient, in this case, is

\[
T = |t|^2 = \frac{1}{\frac{2mE}{\hbar^2} a^2 + 1}, \quad (39)
\]
Case III: $E > V_0$

This case is almost similar to finite well scattering, and thus the solution of time-independent Schrödinger equation is almost identical in both cases. Here, we have

$$\psi(x) = \begin{cases} 
e^{ikx} + re^{-ikx} & x \leq -a, \\ Ae^{ikx} + Be^{-ikx} & -a < x < a, \\ te^{ikx} & x \geq a, \end{cases} \quad (40)$$

where $k = \sqrt{2mE}/\hbar$ and $\kappa = \sqrt{2m(E - V_0)}/\hbar$. In this case, wave number increases in region I and III and decreases in region II as compared to finite well scattering. The expression for transmission coefficient can be written as

$$T = |\gamma|^2 = \frac{4E(E - V_0)}{4E(E - V_0) + V_0^2 \sin^2 \left( \frac{a}{\hbar} \sqrt{2m(E - V_0)} \right)} \quad (41)$$

The barrier becomes totally transparent, that is, transmission coefficient $T$ becomes one when $\sin(2a \sqrt{2m(E - V_0)}/\hbar) = 0$. On the other hand, transmission coefficient $T$ never becomes one for the case $E < V_0$ as we can see from (37). This is because $\sinh \left( 2a \sqrt{2m(V_0 - E)}/\hbar \right) = 0$ only when $E = V_0$, since $a$ is the barrier width and cannot be equal to zero. In the next section, we consider symmetric double barrier where transmission coefficient $T$ can become one for $E < V_0$ as well as $E > V_0$.

4.5 Symmetric Double Potential Barrier

The symmetric double potential barrier (Figure 10) is given by

$$V(x) = \begin{cases} 0 & x < -a, \\ V_0 & -a \leq x \leq a, \\ 0 & a < x < a + b, \\ V_0 & a + b \leq x \leq 3a + b, \\ 0 & x > 3a + b. \end{cases} \quad (42)$$

For a particle with energy $E > 0$, this potential always satisfies $E > V(\infty)$ or $V(-\infty)$, and thus only scattering states are possible. In what follows we present a brief calculation of the transmission coefficient $T$ for symmetric double potential barrier and
show that it can indeed become totally transparent for $E < V_0$. Solving time-independent Schrödinger equation in all the five regions yields the wave function as

$$
\psi(x) = \begin{cases} 
  e^{ikx} + re^{-ikx} & x < -a, \\
  A_1e^{kx} + B_1e^{-kx} & -a \leq x \leq a, \\
  A_2e^{ikx} + B_2e^{-ikx} & a < x < a + b, \\
  A_3e^{kx} + B_3e^{-kx} & a + b \leq x \leq 3a + b, \\
  re^{ikx} & x > 3a + b,
\end{cases}
$$

(43)

where $k = \sqrt{2mE}/\hbar$ and $\kappa = \sqrt{2m(V_0 - E)}/\hbar$. Continuity of $\psi$ and $d\psi/dx$ at $x = -a$, $x = a$, $x = a + b$, and $x = 3a + b$ yield eight equations in eight unknowns. We can obtain $t$ by eliminating other unknown variables from the eight equations. The transmission coefficient $T$ can be written in a compact form as [1]

$$
T = |t|^2 = \left[1 + R^2(\cosh(4\kappa a) - 1)\left(1 + \frac{R^2}{2}(\cosh(4\kappa a) - 1)\right)
\right]
\times (1 + \sin(2kb + \delta))^2,
$$

(44)

where

$$
\tan \delta = \frac{\cosh(4\kappa a) - \frac{R^2}{2}(\cosh(4\kappa a) - 1)}{S \sinh(4\kappa a)},
$$

(45)
We see from (44) that transmission coefficient $T$ becomes one when $\sin(2kb + \delta) = -1$. We plot the transmission coefficient $T$ for both single and double barrier potential as a function of scaled energy $E/V_0$ in Figure 11. Thus, the double barrier has a peculiar feature; for specific energy values in the range $0 < E/V_0 < 1$, the tunneling probability becomes one leading to the barrier becoming completely transparent. No such energy values exist for a single potential barrier, where for particle energies less than barrier energy, the tunneling probability is unity.

The scattering states associated with unit transmission probability in the region $E < V_0$ are called resonant states or quasi-bound states. Resonant tunneling diodes, which can be modeled as double, triple, or multiple potential barriers, are based on the occurrence of unit transmission probability in these structures.

5. Conclusion

Several 1D, 2D, and 3D structures in nanophysics are modeled using simple potentials. For instance, quantum wires are approximated as a sum of two independent finite well potentials, whereas
quantum dots are approximated as a sum of three independent finite well potentials. In these studies, we first obtain the energy levels by solving the Schrödinger equation and then calculate the electrical and absorption properties. Further, one can also do statistical mechanics and theoretically calculate various thermodynamic quantities, for instance, average energy, entropy, and heat capacity.

Qualitative techniques may be applied to gain insights into potentials that are not exactly solvable, such as the double Gaussian barrier. Interested readers should consult references [2, 3] for a detailed analysis of qualitative plots of the wave function. We hope that the tools and techniques provided in this article will prove useful in studying different models of a system of interest and derive new and interesting results.

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Suggested Reading


