A. Part I (Theory)

I. Introduction

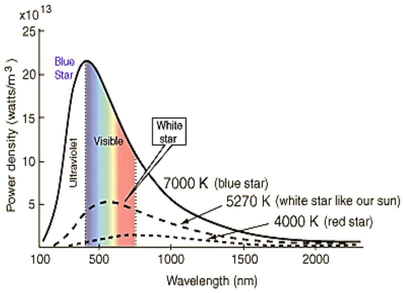
Quantum Mechanics is the physics of matter at scales much smaller than we are able to observe of feel. In another definition, a Quantum Mechanics is one of the more sophisticated field in physics that has affected our understanding of Nano-meter length scale systems important for chemistry, materials, optics, and electronics. The existence of orbitals and energy levels in atoms can only be explained by quantum mechanics. Quantum mechanics can explain the behaviors of insulators, conductors, semi-conductors, and giant magneto-resistance. It can explain the quantization of light and its particle nature in addition to its wave nature. Quantum mechanics can also explain the radiation of hot body, and its change of color with respect to temperature. It explains the presence of holes and the transport of holes and electrons in electronic devices. Quantum mechanics has played an important role in photonics, quantum electronics, and micro-electronics.

II. Principles of Quantum Mechanics

i. Energy quanta

- In 1900. Planck postulated that thermal radiation emitted from a heated surface is in a form of discrete packets of energy called quanta.

$$E = h\upsilon$$



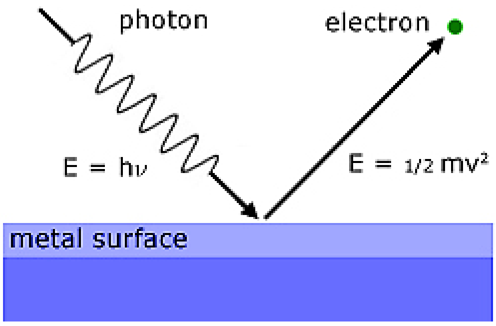
ii. Einstein interpretation for photoelectric effect:

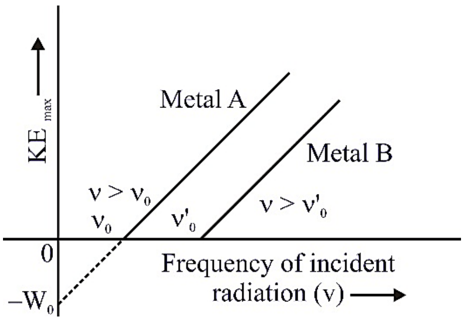
- In 1905, Einstein suggested the energy in a light wave is also contained in discrete packets or bundles.
- The particle -like packet of energy is called photon, whose energy is given by

$$E = h\upsilon$$

- The minimum energy required to remove an electron is called the work function of the material and any access photon energy goes into kinetic energy of the photoelectron.

$$T_{max} = \frac{1}{2}mv^2 = h\upsilon - h\upsilon_o. \quad Work\ function = h\upsilon_o$$





III. Wave particle duality

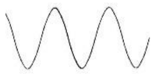
- The light wave in the photoelectric effect behave as if they are particle.
- In 1924, De Broglie postulated the existence of matter wave. Since wave exhibit particle-wave behavior, then particle should be expected to show particle-wave properties.

Energy $E = \frac{1}{2}mv^2$

Momentum $\vec{p} = m\vec{v}$

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

Force $F = ma = m\frac{d^2}{dt^2}$



Energy $E = hv = \hbar w$

Wavelength $\lambda = \frac{c}{v}$

Wavelength of particle $\lambda = \frac{h}{\sqrt{2mE}}$

Wave equation $\frac{\partial^2}{\partial x^2}\Psi(x.t) = \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\Psi(x.t)$

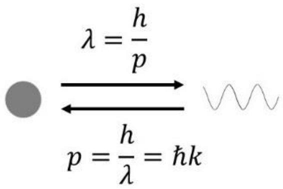
- Wave particle duality principle

Particle: momentum ⇒ wavelength

Wave: wavelength ⇒ momentum

The momentum of photon $p = \frac{h}{\lambda} = \hbar k.$ $\left(\hbar = \frac{h}{2\pi}.\ k = \frac{2\pi}{\lambda}\right)$.

The wavelength of particle $\lambda = \frac{h}{p}$, (*De Broglie wavelength*).



i. De Broglie Hypothesis

The reasoning that led de Broglie to put forward his revolutionary hypothesis runs as follows. The entire physical universe is composed of matter and radiation. In quantum theory of radiation, a fragment or quantum of energy E is assigned a frequency, $\omega\ (= 2\pi v)$ such that $E = hv$. Although there is no physical sense of frequency, nevertheless the theory based on this assumption works well. From this notion de Broglie speculated that material particles, which are also fragment of energy (e.g.,$E = mc^2$), might be assigned some characteristic frequency. A material particle of rest mass m_o is equivalent to energy $m_o c^2$, therefore, according to de Broglie idea we can write

$$m_o c^2 = \hbar\omega$$

Where $\omega,$ is the frequency of some intrinsic periodic process that associated with the material particle; Let us see what this periodic process appears to an observer with respect to which it is moving.

ii. Total Relativistic Energy

The relativistic energy expression is the tool used to calculate binding energies of nuclei and the energy yields of nuclear fission and fusion.

The famous Einstein relationship for energy

$$E = mc^2$$

includes both the kinetic energy and rest mass energy for a particle. The kinetic energy of a high speed particle can be calculated from

$$KE = mc^2 - m_o c^2$$

In other manner, it can be blended with the relativistic momentum expression

$$p = \frac{m_o v}{\sqrt{1 - \frac{v^2}{c^2}}}$$

to give an alternative expression for energy. The combination pc shows up often in relativistic mechanics. It can be manipulated as follows:

$$p^2c^2 = \frac{m_o^2 v^2 c^2}{1 - \frac{v^2}{c^2}} = \frac{m_o^2 \frac{v^2}{c^2} c^4}{1 - \frac{v^2}{c^2}}$$

and by adding and subtracting a term it can be put in the form:

$$p^2c^2 = \frac{m_o^2 c^2 \left[\frac{v^2}{c^2} - 1\right]}{1 - \frac{v^2}{c^2}} + \frac{m_o^2 c^4}{1 - \frac{v^2}{c^2}} = -m_o^2 c^4 + (mc^2)^2$$

which may be rearranged to give the expression for energy.This means, the relativistic energy of a particle can also be expressed in terms of its momentum in the expression:

$$E = mc^2 = \sqrt{p^2c^2 + {m_o}^2 c^4}$$

For a particle with zero momentum $p = 0$.

$$E = m_0 c^2$$

A light photon has $m_0 = 0$, but it does have momentum p,

$$E = pc$$

IV. The wave equation

Wave equation (Traveling wave)

$$\frac{\partial^2}{\partial x^2}\vec{E} = \frac{1}{v^2}\frac{\partial^2}{\partial t^2}\vec{E}, \quad \frac{\partial^2}{\partial x^2}\vec{H} = \frac{1}{v^2}\frac{\partial^2}{\partial t^2}\vec{H}, \quad \text{where } v = \frac{1}{\sqrt{\mu\varepsilon}}$$

The configuration or state of a quantum object is completely specified by a wavefunction denoted as $\psi(x)$.

Sinusoidal form

$$\vec{E}(\vec{r}.t) = \vec{E}_o cos(\vec{k} \cdot \vec{r} - \omega t + \phi)$$

Exponential form

$$\vec{E}(\vec{r}.t) = \vec{E}_o \cdot e^{-i(\vec{k}\cdot\vec{r} - \omega t + \phi)}$$

Whereas, the program of classical mechanics is to determine the position of the particle at any given time $x(t)$.Once we know that, we can figure out the velocity $\left(v = \frac{dx}{dt}\right)$, the momentum ($p = mv$),the kinetic energy $\left(KE = \frac{1}{2}mv^2\right)$, or any other dynamical variable of interest.

The value of (position x at any time t) for any microscopic object can be find by applying Newton's second law $F = ma = m\frac{\partial^2 x}{\partial t^2}$, the force can be expressed as the derivate of a potential energy function $F = -\frac{\partial V}{\partial t}$.From these two form of force, we can determine the position $x(t)$, with applying an appropriate initial condition (typically the position and velocity at time $t = 0$). Newton's law determines $x(t)$ for all future time.

While in the quantum mechanics approaches, this same problem is dealt differently. In this case, what we're looking for is the wave equation,$\Psi(r.t)$, [in one dimension like x for example a wave function or equation represents a function of x, for any given time t]; of the particle.

The Schrödinger equation plays a role logically analogous to Newton Second law. Given suitable initial conditions [typically,$\psi(r.0)$], the Schrödinger equation determines $\psi(x.t)$ for all future time, just as, in classical mechanics,

The Born's statistical interpretation of the wave function has been used to describe the state of particle, which says that $|\Psi(x.t)|^2$ gives the probability of finding the particle at point x, at time t - or more precisely;

$$|\Psi(x.t)|^2dx = \begin{pmatrix}\text{probability of finding the particle} \\ \text{between } x \text{ and } (x+dx).\text{at time } t\end{pmatrix}$$

The statistical interpretation introduces a kind of indeterminacy into QM and because of the statistical interpretation, probability plays a control role in QM. For example, when an electron manifests as a wave, it is described by

$$\psi(z) \propto exp(ikz) \qquad \text{and} \qquad \frac{\partial^2}{\partial z^2}\psi(z) = -k^2\psi(z)$$

And a generalization of this wave into three dimensions' yields

$$\nabla^2\psi(r) = -k^2\psi(r)$$

The statistical interpretation of the wave function $|\Psi(x.t)|^2$is the probability density for finding the particle at point x at time t.The value of the integral of the probability density must be equal 1, so that the particle's go to be somewhere

$$\int_{-\infty}^{+\infty} |\Psi(x.t)|^2dx = 1$$

This mathematical relation represents the normalization of the probability density for finding the particle over all region.

i. Uncertainty principle (Heisenberg principle)

- It is impossible to simultaneously describe the absolute accuracy position and momentum of a particle.
- It is impossible to simultaneously describe the absolute accuracy energy of particle and momentum of a particle.

$$\Delta p\Delta x \geq \hbar \qquad\qquad \exp(kx)$$

$$\Delta E\Delta t \geq \hbar \qquad\qquad \exp(\omega t)$$

- The Uncertainty principle is only significant for subatomic particles

ii. Operators in quantum mechanics

An operator is a rule or an instruction which transforms a function into another function. Or (An operator is a rule for building one function from another).

Example include the identity $\hat{1}$ such that $\hat{1}f(x) = f(x)$, the spatial derivative $\widehat{D} = \frac{\partial}{\partial x}$ such that $\widehat{D}f(x) = \frac{\partial f(x)}{\partial x}$, the position $\hat{x} = x$ such that $\hat{x}f(x) = xf(x)$. Notationally, operators will be distinguished by hats on top of symbols.

All operator's com with a small set of special functions of their own. For an operator $\hat{A}$, if

$$\hat{A}f(x.A) = A \cdot f(x.A)$$

for a given $A \in C$, then $f(x)$ is an eigenfunction of the operator $\hat{A}$ and A is the corresponding eigenvalue. Operators act on eigenfunctions in a way identical to multiplying the eigenfunction by a constant number.
In physics or specially in quantum mechanics, to every observable quantity is associated a corresponding operator.
For instance,

- The momentum operator $\hat{p} = -i\hbar\nabla.$

$$\hat{p}_x = -i\hbar\frac{\partial^2}{\partial x^2}, \quad \hat{p}_y = -i\hbar\frac{\partial^2}{\partial y^2}. \hat{p}_z = -i\hbar\frac{\partial^2}{\partial z^2}$$

- The position operator $\hat{x} = x$
- The Hamiltonian operator $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$
- The energy operator $\hat{E} = i\hbar\frac{\partial}{\partial t}$
- The kinetic energy operator $\hat{T} = -\frac{\hbar^2}{2m}\nabla$
- The angular momentum operator

$$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right). \quad \hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right). \hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right).$$

These operators are derived as the same, such as in the case of the classic mechanics for the particle and from the relation following

$$L = r \times p = \begin{vmatrix} i & j & k \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$

V. The Schrödinger's wave Equation

Schrödinger in 1924 provided a formulation called wave mechanics which incorporated

- The principle of quanta (Planck).
- Wave -particle duality (de Broglie).

Based on the wave-particle duality principle, we will describe the motion of electron in a crystal by wave

Classical physics

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

Wave mechanics

$$\Updownarrow$$

$$\boldsymbol{p} \longrightarrow -i\hbar\frac{\partial}{\partial x} \qquad \boldsymbol{E} \rightarrow i\hbar\frac{\partial}{\partial t}$$

Schrödinger's wave Equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x.t)}{\partial x^2}+V(x)\Psi(r.t)=i\hbar\frac{\partial\Psi(r.t)}{\partial t}$$

$\psi(r.t)$: wavefunction, $V(x)$: Potential function, m : mass of the particle.

i. The Schrödinger equation derivative

The wave function $\Psi(x.t)$ of a particle moving in x-direction in terms of p_x and E can be expressed as:

$$\Psi(r.t)=A\exp\left[-i\left(\frac{Et}{\hbar}-\frac{p_x x}{\hbar}\right)\right] \tag{1}$$

From this equation

$$\frac{\partial\Psi}{\partial t}=-\frac{iE}{\hbar}\Psi \tag{2}$$

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

$$\frac{\partial\Psi}{\partial x}=\frac{ip_x}{\hbar}\Psi \tag{4}$$

$$-i\hbar\frac{\partial\Psi}{\partial x}=p_x\Psi \tag{5}$$

Differentiating Eq. 1, again with respect to *x*, we have

$$-i\hbar\frac{\partial^2\Psi}{\partial x^2}=p_x\frac{\partial\Psi}{\partial x}=i\frac{{p_x}^2}{\hbar}\Psi \tag{6}$$

$$-\hbar^2\frac{\partial^2\Psi}{\partial x^2}={p_x}^2\Psi \tag{7}$$

For a non-relativistic free particle, the total energy E of the particle moving in x -direction is equal to its kinetic energy T.

$$E=T=\frac{{p_x}^2}{2m}$$

Multiplying both sides of above equation by Ψ, we have

$$E\Psi=\frac{{p_x}^2}{2m}\Psi \tag{8}$$

Making use of Eqns. (2) and (7) we can write Eqn. (8) as:

$$i\hbar\frac{\partial\Psi}{\partial t}=\frac{-\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} \tag{9}$$

This equation is known as time-dependent Schrödinger for a free particle. If the particle is moving in a force field described by potential energy function **V**, its total energy is

$$E=\frac{{p_x}^2}{2m}+V$$

and the Schrödinger equation, it will be now in the form of

$$i\hbar\frac{\partial\Psi}{\partial t}=\frac{-\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V\Psi \tag{10}$$

in three dimensions, it is represented by:

$$i\hbar\frac{\partial\Psi}{\partial t}=\frac{-\hbar^2}{2m}\nabla^2\Psi+V\Psi \tag{11}$$

is known as the time-dependent Schrödinger equation of a particle in three dimensions.

The Schrödinger equation is motivated by further energy balance that total energy is equal to the sum of potential energy and kinetic energy. Defining the potential energy to be V (r), the energy balance equation becomes

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\Psi(r.t) = E\Psi(r.t)$$

However, it predicts many experimental outcomes, as well as predicting the existence of electron orbitals inside an atom, and how electron would interact with other particles.

ii. Stationary state (Time-independent Schrödinger Equation)

When the potential energy V is independent of time, the wave function may be written as product of two wave functions, of which one is function of *x* and the other is function of *t* only.
Assume the position and time parameters in wavefunction is separable.

$$\Psi(r.t) = \psi(r)\phi(t) \qquad in\ 3D$$

or

$$\Psi(x.t) = \psi(x)\phi(t) \qquad in\ 1D$$

The Schrödinger equation Eq. (10) can be written with this new form of the wavefunction as

$$\frac{-\hbar^2}{2m}\cdot\phi(t)\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x)\phi(t) = i\hbar\psi(x)\frac{\partial\phi(t)}{\partial t}$$

Divided the equation above be $\psi(x)\phi(t)$ we get

$$\frac{-\hbar^2}{2m}\cdot\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) = i\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t}$$

The left side of equation is a function of position *x* only and the right side is a function of time *t* only, which implies each side of this equation must be equal to same constant.

$$\frac{-\hbar^2}{2m}\cdot\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) = i\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t} = \eta\ (constant)$$

iii. Physical meaning of η

$$i\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t} = \eta\ (constant)$$

$\Rightarrow\ \phi(t) = e^{-i(\eta/\hbar)t} = e^{-i\omega t}$ The position-independent wavefunction is always in a form of exponential term $e^{-i\omega t}$.

Where $\frac{\eta}{\hbar} = \omega$

$\because E = \hbar\omega \quad \Rightarrow \eta = E$ The separation constant is the total energy *E* of the particle.

Whereas, the wave equation can be written as $\Psi(x.t) = \psi(x)\phi(t) = \psi(x)\, e^{-i\omega t}$

Then we can find two solutions to the time-independent Schrödinger equation:

$$\frac{-\hbar^2}{2m}\cdot\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) = i\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t} = E$$

Or

$$\frac{-\hbar^2}{2m}\cdot\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) - E = 0$$

$$\frac{\partial^2\psi(x)}{\partial x^2} + k^2\psi(x) = 0$$

Case 1: $k = \frac{2m[E-V(x)]}{\hbar^2} > 0$ if $E > V(x) \Rightarrow \psi(x) = A\exp(\pm ikx)$

Case 2: $\gamma = \frac{2m[V(x)-E]}{\hbar^2} > 0$ if $V(x) > E \Rightarrow \psi(x) = A\exp(\pm i\gamma x)$

iv. Physical meaning of the wave equation

- Max Born postulated in 1926 that the wavefunction $|\Psi(x.t)|^2dx$ is the probability of finding the particle between x and dx at a given

$$|\Psi(x.t)|^2 = \Psi(x.t)\cdot\Psi(x.t)^*$$
$$= \psi(x)e^{-i(E/\hbar)t}\cdot\psi(x)^*e^{+i(E/\hbar)t}$$
$$= \psi(x)\cdot\psi(x)^*$$

Probability $\quad |\Psi(x.t)|^2 = \psi(x)\cdot\psi(x)^*$

- The probability density function is independent of time.
- Fortunately, the Schrödinger equation has the property that it automatically preserves the normalization of the wave function.

$$\frac{d}{dt}\int_{-\infty}^{+\infty}|\Psi(x.t)|^2dx = \int_{-\infty}^{+\infty}\frac{\partial}{\partial t}|\Psi(x.t)|^2dx$$

[Note that the integral is a function only of x, so we use a total derivative $(\frac{d}{dt})$ in the first term, but the integrand is a function of x as well as t, so it's partial derivative $(\frac{\partial}{\partial t})$ in the second one].

$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{\partial}{\partial t}(\Psi^*\Psi) = \Psi^*\frac{\partial\Psi}{\partial t} + \frac{\partial\Psi^*}{\partial t}\Psi$$

Now the Schrödinger equation says that

$$\frac{\partial\Psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} - \frac{i}{\hbar}V\Psi$$

And hence (taking the complex conjugate of equation above)

$$\frac{\partial\Psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + \frac{i}{\hbar}V\Psi^*$$

So

$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \frac{\partial^2\Psi^*}{\partial x^2}\Psi\right) = \frac{\partial\Psi}{\partial x}\left[\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\right]$$

The integral of equation above can be now evaluated explicitly by the equation:

$$\frac{d}{dt}\int_{-\infty}^{+\infty}|\Psi(x.t)|^2dx = \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \frac{\partial^2\Psi^*}{\partial x^2}\Psi\right)\Bigg|_{-\infty}^{+\infty}$$

But $\Psi(x.t)$ must go to zero as x goes to $(\mp)$ infinity – otherwise the wave function would not be normalizable. It follows that

$$\frac{d}{dt}\int_{-\infty}^{+\infty}|\Psi(x.t)|^2dx = 0$$

And hence that the integral on the left is constant (independent of time); if Ψ is normalize at $t = 0$, it stays normalize for all future time.

- The state of a particle has to be more richly endowed and described by a wave function or state function (x, t). The state function (also known as a state vector) is a vector in the infinite dimensional space.
- The state of a particle in quantum mechanics is described by a state function, which has infinitely many degrees of freedom.
- In the Schrödinger equation, the wave function (x, t) is a continuous function of the position variable x at any time instant t; hence, it is described by infinitely many numbers, and has infinite degrees of freedom.

v. Boundary condition for wavefunction

- The probability of finding the particle over the entire space must be equal to 1

$$\int_{-\infty}^{+\infty} |\Psi(x.t)|^2 dx = \int_{-\infty}^{+\infty} \psi(x) \cdot \psi(x)^* \, dx = 1$$

- $\psi(x)$ must be finite, single-valued and continuous.
- $\partial\psi(x)/\partial x$ must be finite, single-valued and continuous.
- If the probability were to become infinite at some point in space, then the probability of finding the particle at the position would be certain, that violate the uncertainty principle.
- The second derivative must finite which implies that the first derivative must be continuous.
- The first derivative is related to the particle momentum, which must be finite and single-valued.
- The finite first derivative implies that the function itself must be continuous.

vi. Probabilistic Interpretation of the wave function

The final, most accepted interpretation of this wave function (one that also agrees with experiments) is that its magnitude squared corresponds to the probabilistic density function. In other words, the probability of finding an electron in an interval $[x;\ x\ +\ \Delta x]$ is equal to

$$|\Psi(x.t)|^2\ \Delta x$$

For the 3D case, the probability of finding an electron in a small volume ΔV in the vicinity of the point r is given by

$$|\Psi(x.t)|^2\ \Delta V$$

Since the magnitude squared of the wavefunction represents a probability density function, it must satisfy the normalization condition of a probability density function, viz.,

$$\int |\Psi(x.t)|^2\ \mathrm{d}V = 1$$

The magnitude squared of this wave function is like some kind of "energy" that cannot be destroyed. Electrons cannot be destroyed and hence, charge conservation is upheld by the Schrödinger equation.

Motivated by the conservation of the "energy" of the wave function, we shall consider an "energy" conserving system where the classical Hamiltonian will be a constant of motion. In this case, there is no "energy" loss from the system. Therefore, the Schrödinger equation that governs the time evolution of the wave function is:

$$\hat{H}\Psi = i\hbar\frac{\partial\Psi}{\partial t} \quad (1)$$

where $\hat{H}$ is the Hamiltonian operator, one can solve (1) formally to obtained:

$$\Psi(t) = e^{-i\frac{\hat{H}}{\hbar}t}\Psi(t=0) \quad (2)$$

Since the above is a function of an operator, it has meaning only if this function acts on the eigenvectors of the operator $\hat{H}$. It can be shown easily that if $\bar{A}\cdot V_i = \lambda_i V_i$,

$$exp(\bar{A})\cdot V_i = exp(\lambda_i)\, V_i \quad (3)$$

If $\hat{H}$ is a Hermitian operator, then there exists Eigenfunctions, or special wave functions, Ψ_n, such that

$$\hat{H}\Psi_n = E_n\Psi_n \quad (4)$$

where E_n is purely real. In this case, the time evolution of ψ_n from (2) is

$$\Psi(t) = e^{-i\frac{E_n}{\hbar}t}\Psi_n(t=0) = e^{-i\omega_n t}\Psi_n(t=0) \quad (5)$$

In the above, $E_n = \hbar\omega_n$, or the energy E_n is related to frequency ω_n via the reduced Planck constant $\hbar$.

Scalar variables that are measurable in classical mechanics, such as p and x, are known as observables in quantum mechanics. They are elevated from scalar variables to operators in quantum mechanics, denoted by a "^" symbol here. In classical mechanics, for a one particle system, the Hamiltonian is given by

$$H = T + V = \frac{p^2}{2m} + V \quad (6)$$

The Hamiltonian contains the information from which the equations of motion for the particle can be derived. But in quantum mechanics, this is not sufficient, and H becomes an operator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V} \quad (7)$$

This operator works in tandem with a wavefunction to describe the state of the particle. The operator acts on a wave function $\Psi(t)$, where in the coordinate x representation, is $\Psi(x.t)$.

When $\Psi(x.t)$ is an Eigenfunction with energy E_n, it can be expressed as

$$\Psi(x.t) = \Psi_n(x)e^{-i\omega_n t} \quad (8)$$

where $E_n = \hbar\omega_n$. The Schrödinger equation for $\psi_n(x)$ then becomes

$$\hat{H}\Psi_n(x) = \left(\frac{\hat{p}^2}{2m} + \hat{V}\right)\Psi(x) = E_n\Psi(x) \quad (9)$$

For simplicity, we consider an electron moving in free space where it has only a constant kinetic energy but not influenced by any potential energy. In other words, there is no force acting on the electron. In this case, $\hat{V} = 0$, and this equation becomes

$$\frac{\hat{p}^2}{2m}\Psi(x) = E_n\Psi(x) \quad (10)$$

It has been observed by de Broglie that the momentum of a particle, such as an electron which behaves like a wave, has a momentum

$$p = \hbar k \quad (11)$$

where $k = 2\pi/\lambda$ is the wavenumber of the wave function; This motivates that the operator $\hat{p}$ can be expressed by

$$\hat{p} = -i\hbar\frac{d}{dx} \quad (12)$$

in the coordinate space representation. This is chosen so that if an electron is described by a state function $\psi(x) = c_1 e^{ikx}$, then $\hat{p}\psi(x) = \hbar k \psi(x)$. The above motivation for the form of the operator $\hat{p}$ is highly heuristic. Equation (10) for a free particle is then

$$\frac{i\hbar}{2m}\frac{d}{dx}\Psi_n(x) = E_n \Psi_n(x) \tag{13}$$

Since this is a constant coefficient ordinary differential equation, the solution is of the form

$$\psi_n(x) = e^{\pm ikx} \tag{14}$$

which when used in (13), yields

$$\frac{\hbar^2 k^2}{2m} = E_n \tag{15}$$

Namely, the kinetic energy T of the particle is given by

$$T = \frac{\hbar^2 k^2}{2m} \tag{16}$$

where $p = \hbar k$ is in agreement with de Broglie's finding.
In many problems, the operator $\hat{V}$ is a scalar operator in coordinate space representation which is a scalar function of position $V(x)$. This potential traps the particle within it acting as a potential well. In general, the Schrödinger equation for a particle becomes

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x.t) = i\hbar\frac{\partial}{\partial t}\Psi(x.t) \tag{17}$$

For a particular eigenstate with energy E_n as indicated by (8), it becomes

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi_n(x) = E_n \Psi_n(x) \tag{18}$$

The above is an eigenvalue problem with eigenvalue E_n and Eigenfunction $\Psi_n(x)$. These eigenstates are also known as stationary states, because they have a time dependence indicated by (8). Hence, their probability density functions $|\Psi(x.t)|^2$ are time independent.
These Eigenfunctions correspond to trapped modes in the potential well defined by $V(x)$ very much like trapped guided modes in a dielectric waveguide. These modes are usually countable and they can be indexed by the index n.
In the special case of a particle in free space, or the absence of the potential well, the particle or electron is not trapped and it is free to assume any energy or momentum indexed by the continuous variable k. In (15), the index for the energy should rightfully be k and the Eigenfunctions are uncountably infinite. Moreover, the above can be generalized to two and three dimensional cases.

iv. Application of Schrödinger wave Equation

We have now enough knowledge to study some simple solutions of time-independent Schrödinger equation such as:

1. **Electron in free space.**
2. **Electron in infinite potential well.**
3. **Step potential function (The potential step).**
4. **Potential barrier (The Finite Square Well Potential).**
5. **Potential barrier and well.**
6. **Harmonic oscillator.**

1. Electron in free space (Free particle: Continuous states).

- This simplest one-dimensional problem (Electron in free space means no force acting on the electron), it corresponding to $V(x) = 0$ for any value of x.
- We must have $E > V(x)$ to assure the motion of electron.

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + (V(x) - E)\psi(x) = 0 \qquad (1\text{-}1)$$

This is above time-independent Schrödinger's wave equation, and since $V(x) = 0$, this equation become

$$\frac{\partial^2\psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\psi(x) = 0 \quad \text{(free space)} \qquad (1\text{-}2)$$

Or

$$\left(\frac{\partial^2}{\partial x^2} + k^2\right)\psi(x) = 0 \qquad (1\text{-}3)$$

Where $k^2 = 2mE/\hbar^2$. k being the wave number; The most general solution to eq. above is a combination of two linearly independent wave planes $\psi_+ = e^{ikx}$ and $\psi_- = e^{-ikx}$

$$\psi_k(x) = A_+e^{ikx} + A_-e^{-ikx} \qquad (1\text{-}4)$$

Where A_+ and A_- are two arbitrary constants.

$$\because\ \phi(t) = e^{-i\omega t} \text{ and } \Psi(x.t) = \psi(x)\cdot\phi(t) \qquad (1\text{-}5)$$

Then

$$\underbrace{\Psi(x.t) = A_+e^{i(kx-\omega t)}}_{\text{Right- going wave}} + \underbrace{A_-e^{-i(kx+\omega t)}}_{\text{Left-going wave}} \qquad (1\text{-}6)$$

This formula above of the wavefunction represents the stationary state, which can also be written as

$$\Psi(x.t) = A_+e^{i(kx-\hbar k^2t/2m)} + A_-e^{-i(kx+\hbar k^2t/2m)} \qquad (1\text{-}7)$$

Since $\omega = E/\hbar = \hbar k^2/2m$, the first term $\Psi_+(x.t) = A_+e^{i(kx-\omega t)}$, represents a wave travelling to the right, while the second term $\Psi_-(x.t) = A_-e^{-i(kx+\omega t)}$,represents a wave travelling to the left. The intensities of these waves are given by $|A_+|^2$ and $|A_-|^2$, respectively.

We should note that the wave $\Psi_+(x.t)$ and $\Psi_-(x.t)$ are associated, respectively, with a free particle travelling to the right and to the left with well-defined momenta and energy; $p_\pm = \pm\hbar k$, $E_\pm = \hbar^2k^2/2m$.

We will comment on the physical implications of this in moment. Since there are no boundary conditions, there are no restrictions on k or on E, all vales yield solutions to the equation.

Remember the postulate of de Broglie's wave-particle principle:

$$\lambda = \frac{h}{p}$$

We also have

$$p = \sqrt{2mE} \quad \text{and} \quad E = p^2/2m$$

Which implies the consistency of wave-particle principle and wave mechanics in free space (wave mechanics is based on energy quanta and wave particle duality).

The free particle problem is simple to solve mathematically, yet it presents a number of physical subtleties. Let us discuss briefly three of these subtleties.

First, the probability density corresponding to either solutions

$$P_{\pm}(x.t) = |\Psi_{\pm}(x.t)|^2 = |A_{\pm}|^2 \qquad (1\text{-}8)$$

are constant, for they depend neither on x and t. This is due to the complete loss of information about the position and time for a state with definite values of momentum, $p_{\pm} = \pm\hbar k$, and energy, $E_{\pm} = \hbar^2k^2/2m$. This is consequence of Heisenberg's uncertainty principle: when the momentum and energy of a particle are known exactly, $\Delta p = 0$ and $\Delta E = 0$, there must be total uncertainty about its position and time: $\Delta x \to \infty$ and $\Delta t \to \infty$.

Second, an apparent discrepancy between the speed of the wave and the speed of the particle**;** it is supposed to represent**.** The speed of the plane waves $\Psi_{\pm}(x.t)$ is given by

$$\upsilon_{wave} = \frac{\omega}{k} = \frac{E}{\hbar k} = \frac{\hbar^2k^2/2m}{\hbar k} = \frac{\hbar k}{2m} \qquad (1\text{-}9)$$

On the other hand, the classical speed of the particle is given by

$$\upsilon_{classical} = \frac{p}{m} = \frac{\hbar k}{m} = 2\upsilon_{wave} \qquad (1\text{-}10)$$

This means that the particle travels twice as fast as the wave that represents it.

Third, the wavefunction is not normalizable:

$$\int_{-\infty}^{+\infty} \Psi_{\pm}^{*}(x.t)\Psi_{\pm}(x.t)\,dx = |A_{\pm}|^2 \int_{-\infty}^{+\infty} dx \to \infty \qquad (1\text{-}11)$$

The solution $\Psi_{\pm}(x.t)$ are thus unphysical; physical wavefunctions must be square integrable. The problem can be traced to this; a free particle cannot have sharply defined momenta and energy.

In view of these three subtleties above, the solution of the Schrödinger equation related to this case, that are physically acceptable cannot be planes waves. The answer is provided wave packet

$$\Psi(x.t) = \frac{1}{\sqrt{2}}\int_{-\infty}^{+\infty} \emptyset(k)e^{i(kx-\omega t)}dk. \qquad (1\text{-}12)$$

Where $\emptyset(k)$, the amplitude of the wave packet, is given by the Fourier transform of $\psi(x.0)$ as

$$\emptyset(k) = \frac{1}{\sqrt{2}}\int_{-\infty}^{+\infty} \psi(x.0)e^{ikx}dx. \qquad (1\text{-}13)$$

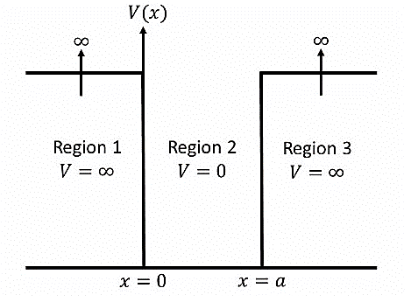
The wave packet solution cures and avoids all the subtleties raised above. First, the momentum, the position and the energy of the particle are no longer known exactly; only probabilistic outcomes are possible. Second, the wave packet (1-12) and the particle travel with the same speed $v_g = p/m$, called the *group* speed or the speed of the whole packet.

Third, the wave packet (1-12) is normalizable. To summarize, a free particle cannot be represented by a single (monochromatic) plane wave; it has to be represented by a wave packet. The physical solutions of the Schrödinger equation are thus given by wave packets, not by stationary solutions.

2. Electron in infinite potential well (bound particle)

a. The Asymmetric square well.

Consider a particle of mass m confined to move inside an infinitely deep asymmetric potential well.



$$V(x)=\begin{cases}+\infty & x<0.\\ 0 & 0\le x\le a.\\ +\infty & x>a.\end{cases} \qquad (2.1)$$

Classically, the particle remains confined inside the well, moving at constant momentum $p=\pm\sqrt{2mE}$ back and forth as a result of repeated reflection from the walls of the wsell.

Quantum mechanically, we expect this particle to have only bound state solutions and a discrete nondegenerate energy spectrum. Since $V(x)$ is infinite outside the region $0\le x\le a.$ the wavefunction of the particle must be zero outside the boundary.

Region 1 & 3	Region 2
$V(x)=\infty$ and $V(x)>E$	$V(x)=o$ and $E>V(x)$
⇒ Decaying wave	⇒ Travelling wave
$\frac{\partial^2\psi(x)}{\partial x^2}+\frac{2m}{\hbar^2}[V(x)-E]\psi(x)=0$	$\frac{\partial^2\psi(x)}{\partial x^2}+\frac{2mE}{\hbar^2}\psi(x)=0$

Hence we can look for solutions only inside the well, in the same way that we have learned in “Fundamental physics"

$$\frac{\partial^2\psi(x)}{\partial x^2}+k^2\psi(x)=0. \quad \text{with} \quad k^2=\frac{2mE}{\hbar^2} \qquad (2\text{-}2)$$

So that, the solution will be

$$\psi(x)=Ae^{ikx}+Be^{-ikx}\Rightarrow \psi(x)=Acos(kx)+Bsin(kx) \qquad (2\text{-}3)$$

Boundary conditions

$\psi(x)$ must continuous (at boundaries and the wavefunction vanishes at the walls).

$$\psi(0)=\psi(a)=0$$
$$\psi(x=0^+)=\psi(x=0^-)=0 \qquad (2\text{-}4)$$

And

$$\psi(x=a^+)=\psi(x=a^-)=0 \qquad (2\text{-}5)$$

Since $\quad Acos(k0)=Acos(ka)=0$

Then $\quad A=0$

Because $\quad cos(k0)\neq o$ and $cos(ka)\neq 0$

But $\quad Bsin(ka)=0$

Then $\quad sin(ka)=0$

Because $\quad B\neq 0$

And $\quad k_na=n\pi \qquad (n=1.2.3.\cdots)$

This condition above determines the energy

$$E_n=\frac{\hbar^2}{2m}k_n^2=\frac{\hbar^2\pi^2}{2ma^2}n^2 \quad (n=1.2.3.\cdots) \qquad (2\text{-}6)$$

The energy is *quantized*; only certain values are permitted. This is expected since the *states* of a particle which is confined to a limited region of space are bounded and the energy spectrum is discrete. This is in sharp contrast to classical physics where the energy of the particle, given by $E = p^2/2m$, takes any value; the classical energy evolves *continuously*.

As it can be inferred from (2-6), we should note that the energy between adjacent levels is not constant:

$$E_{n+1} - E_n = 2n + 1 \qquad (2\text{-}7)$$

Which leads

$$\frac{E_{n+1} - E_n}{E_n} = \frac{(n+1)^2 - n^2}{n^2} = \frac{2n+1}{n^2} \qquad (2\text{-}8)$$

In the classical limit $n \to \infty$,

$$\lim_{n\to\infty} \frac{E_{n+1} - E_n}{E_n} = \lim_{n\to\infty} \frac{2n+1}{n^2} = 0 \qquad (2\text{-}9)$$

The levels become so close together as to be practically indistinguishable.

Since $A = 0$ and $k_n = n\pi/a$, then the wavefunction yields $\psi_n(x) = B sin(n\pi x/a)$, and we can choose the constant B so that $\psi_n(x)$ is normalized (total probability equal one):

$$1 = \int_0^a |\psi_n(x)|^2\, dx = |B|^2 \int_0^a sin^2(n\pi x/a)\, dx \qquad (2\text{-}10)$$

$$\int_0^a \big(B sin\,(kx)\big)^2\, dx = 1 \qquad (2\text{-}11)$$

$$\int sin^2(kx)\, dx = \frac{x}{2} - \frac{sin2kx}{4k} \qquad (2\text{-}12)$$

$$\int_0^a \big(B sin\,(kx)\big)^2\, dx = 1 = B^2 \left(\frac{x}{2} - \cancelto{0}{\frac{sin2kx}{4k}}\right)\Big|_0^a \qquad (2\text{-}13)$$

$$B = \sqrt{\frac{2}{a}}$$

Hence

$$\psi_n(x) = \sqrt{\frac{2}{a}}\, sin\left(\frac{n\pi x}{a}\right) \quad (n = 1.2.3.\cdots) \qquad (2\text{-}14)$$

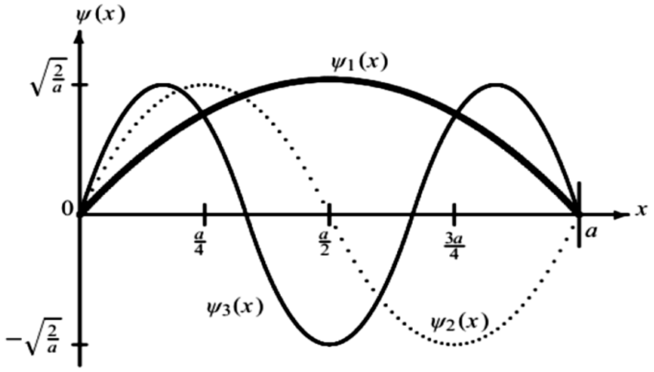
The solution of the time-independent Schrödinger equation has thus given us the energy (2-6) and the wave function (2-14). There is then an infinite sequence of discrete energy levels corresponding to the positive integer values of the *quantum number* n. It is clear that $n = 0$, yields an uninteresting result: $\psi_0(x) = 0$ and $E_o = 0$;later, we will examine in more detail the physical implications of this. So, the lowest energy, or *ground state* energy, corresponds to $n = 1$; it is $E_1 = \hbar^2\pi^2/(2ma^2)$. As will be explained later, this is called the *zero-point energy*, for there exists no state with zero energy. The states corresponding to $n = 2.3.4.\cdots$ are called *excited states*; their energies are given by $E_n = n^2 E_1$. As shown in Figure above, we can see that each function $\psi_n(x)$ has$(n-1)$ nodes, and the functions $\psi_{2n+1}(x)$ are *even* and the functions $\psi_{2n}(x)$ are *odd* with respect to the center of the well;

Note that none of the energy levels is degenerate (there is only one eignfunction for each energy level) and that the wavefunctions corresponding to different energy levels are orthogonal:

$$\int_0^a \psi_m^*(x)\psi_n(x)dx = \delta_{mn} \qquad (2\text{-}15)$$

Since we are dealing with stationary states and since $E_n = n^2 E_1$, the most general solutions of the time-dependent Schrödinger equation are given by

$$\Psi(x.t) = \sum_{n=1}^{\infty} \psi_n(x)e^{-iE_nt/\hbar} = \sqrt{\frac{2}{a}}\sum_{n=1}^{\infty} sin\left(\frac{n\pi x}{a}\right)e^{-in^2E_1t/\hbar} \qquad (2\text{-}16)$$



Quantization of energy levels

$$\because k = \sqrt{\frac{2mE}{\hbar^2}}$$

Discrete Wave vector

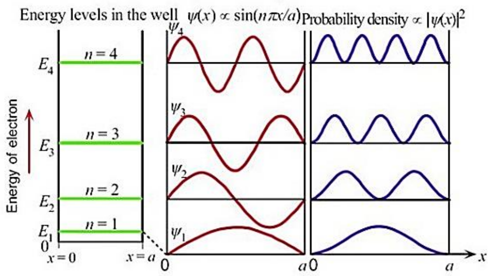
$$k = \frac{n\pi}{a}$$

discrete energy

$$E = E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$$

Infinite well

$$E_n \propto n^2$$



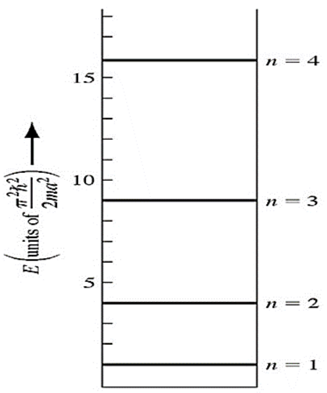
Example: infinite potential well

Infinite potential well width of $5\dot{A}$

$$E = E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2} = \frac{n^2(1.054 \times 10^{-34})^2\pi^2}{2(9.11 \times 10^{-34})(5 \times 10^{-10})^2} = n^2(2.41 \times 10^{-19})J$$

$$= \frac{n^2(2.41 \times 10^{-19})}{1.6 \times 10^{-19}} = n^2(1.51)eV$$

$E_1 = 1.51\ eV$
$E_2 = 6.04\ eV = 4E_1$
$E_3 = 13.59\ eV = 9E_1$
For potential, well, $E_n \propto n^2$



b. The symmetric potential well

In this case, the potential well that previously described, is translated to the left by a distance of $a/2$ to become symmetric

$$V(x) = \begin{cases} +\infty & x < 0. \\ 0 & 0 \leq x \leq a. \\ +\infty & x > a. \end{cases}$$

First, we would expect the energy spectrum (ii-6) to remain unaffected by this translation, since the Hamiltonian is invariant under spatial translations; as it contains only a kinetic part, it commutes with the particle's momentum, $[\hat{H}.\hat{P}] = 0$. The energy spectrum is discrete and nondegenerate.

Second, earlier in this chapter we saw that for symmetric potentials, $V(-x) = V(x)$, the wave function of bound states must be either even or odd. The wave function corresponding to the potential that described in Eq. above can be written as follows:

$$\psi_n(x) = \sqrt{\frac{2}{a}}\, sin\left[\frac{n\pi}{a}\left(x + \frac{a}{2}\right)\right] = \begin{cases} \sqrt{\frac{2}{a}}\, cos\left(\frac{n\pi}{a}x\right) & (n = 1.3.5.\cdots). \\ \sqrt{\frac{2}{a}}\, sin\left(\frac{n\pi}{a}x\right) & (n = 2.4.6.\cdots). \end{cases}$$

That is, the wave functions corresponding to odd quantum numbers are symmetric $n = 1.3.5.\cdots$, are symmetric $(-x) = \psi(x)$, and those corresponding to even numbers $n = 2.4.6.\cdots$are antisymmetric, $\psi(-x) = \psi(x)$.

3. Step potential function (The potential step)

Another sample problem consists of particle that is free everywhere, but beyond a particle point, say $x = 0$, the potential increases sharply (i.e., it becomes repulsive or attractive). A potential of this type is called a potential step, as shown in Figure below.

$$V(x) = \begin{cases} 0. & x < 0. \\ V_o. & x \geq 0 \geq. \end{cases} \tag{3-1}$$

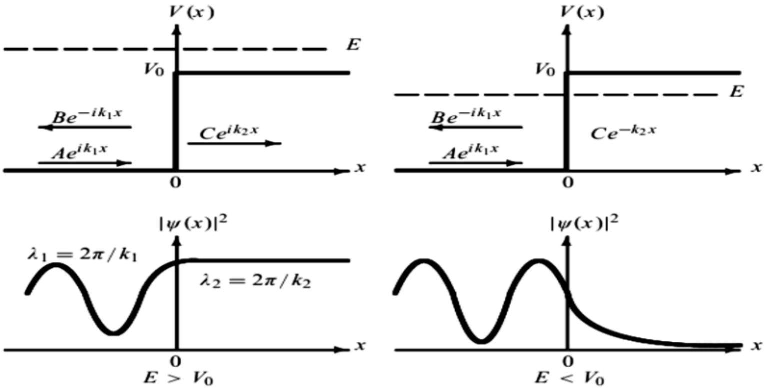


Figure: Potential step and propagation directions of the incident, reflected, and transmitted waves, plus their probability densities $|\psi\,(x)|^2$ when $E > V_O$ and $E < V_O$.

In this problem, we try to analyze the dynamics of a flux of particles (all having the same mass m and moving with the same velocity) moving from left to the right. We are going to consider two cases, depending on whether the energy of the particles is larger or smaller than V_0.

a) Case $E > V_o$

The particles are free for $x < 0$ and feel a repulsive potential V_0 that starts at $x = 0$ and stays flat (constant) for $x > 0$. Let us analyze the dynamics of this flux of particles classically and then quantum mechanically.

Classically, the particles approach the potential step or barrier from the left with a constant momentum $\sqrt{2mE}$. As the particles enter the region $x \geq 0$, where the potential now is $V = V_o$, they slow down to a momentum $\sqrt{2m(E-V_O)}$; they will then conserve this momentum as they travel to the right. Since the particles have sufficient energy to penetrate into the region $x \geq 0$, there will be *total transmission*: all the particles will emerge to the right with a smaller kinetic energy $E - V_O$. This is then a simple *scattering* problem in one dimension.

Quantum mechanically, the dynamics of the particle is regulated by the Schrödinger equation which is given in these two regions by

$$\left(\frac{d^2}{dx^2} + k_1^2\right)\psi_1(x) = 0 \qquad (x < 0) \tag{3-2}$$

$$\left(\frac{d^2}{dx^2} + k_2^2\right)\psi_2(x) = 0 \qquad (x \geq 0) \tag{3-3}$$

Where $k_1^2 = 2mE/\hbar^2$ and $k_2^2 = 2m(E-V_O)/\hbar^2$.The most general solutions to these two equations are plane waves:

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \qquad (x < 0) \tag{3-4}$$

$$\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x} \qquad (x \geq 0) \tag{3-5}$$

Where Ae^{ik_1x} and Ce^{ik_2x} represent waves moving in the positive *x*-direction, but Be^{-ik_1x} and De^{-ik_2x} correspond to waves moving in the negative *x*-direction. We are interested in the case where the particles are initially incident on the potential step from the left: they can be reflected or transmitted at $x = 0$. Since no wave is reflected from the region $x > 0$ to the left, the constant D must vanish. Since we are dealing with stationary states, the complete wave function is thus given by:

$$\Psi(x.t) = \begin{cases} \psi_1(x)e^{-i\omega t} = Ae^{i(k_1x-\omega t)} + Be^{-i(k_1x-\omega t)} & x < 0 \\ \psi_2(x)e^{-i\omega t} = Ce^{i(k_2x-\omega t)} & x \geq 0 \end{cases} \tag{3-6}$$

where $\mathrm{Ae}^{i(k_1x-\omega t)}$, $\mathrm{Be}^{-i(k_1x-\omega t)}$, and $\mathrm{Ce}^{i(k_2x-\omega t)}$ represent the incident, the reflected, and the transmitted waves, respectively; they travel to the right, the left, and theright (Figure above). Note that the probability density $|\psi(x)|^2$ shown in the lower left plot of Figure above is a straight line for $x > 0$, since $|\psi(x)|^2 = \left|\mathrm{Ce}^{i(k_2x-\omega t)}\right|^2 = |\mathrm{C}|^2$.

Let us now evaluate the reflection and transmission coefficients, R and T, as defined by

$$R = \left|\frac{\text{reflected current density}}{\text{incident current density}}\right| = \left|\frac{J_{reflected}}{J_{incident}}\right| \quad T = \left|\frac{J_{transmited}}{J_{incident}}\right|; \tag{3-7}$$

R represents the ratio of the reflected to the incident beams and T the ratio of the transmitted to the incident beams. To calculate R and T, we need to find *Jincident*, *Jreflected*, and *Jtransmitted* .

Since the incident wave is $\psi_i(x) = Ae^{ik_1x}$, the incident current density (or incident flux) is given by

$$RJ_{incident} = \frac{i\hbar}{2m}\left(\psi_i(x)\frac{d\psi_i^*(x)}{dx} - \psi_i^*(x)\frac{d\psi_i(x)}{dx} = \frac{\hbar k_1}{m}|A|^2\right) \tag{3-8}$$

Similarly, since the reflected and transmitted waves are $\psi_r(x) = Be^{-ik_1x}$, and $\psi_t(x) = Ce^{ik_2x}$,we can verify that the reflected and transmitted fluxes are

$$J_{reflected} = \frac{\hbar k_1}{m}|B|^2. \quad J_{transmitted} = \frac{\hbar k_2}{m}|C|^2 \tag{3-9}$$

So that, we can expressed the *reflection* and *transmission coefficients* by the equation

$$R = \frac{|B|^2}{|A|^2}. \qquad T = \frac{|C|^2}{|A|^2}\ ; \tag{3-10}$$

Thus, the calculation of R and T is reduced to determining the constants B and C. For this, we need to use the boundary conditions of the wave function at $x = 0$. Since both the wave function and its first derivative are continuous at $x = 0$,

$$\psi_1(0) = \psi_2(0). \quad \frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx} \tag{3-11}$$

equations (3-4) and (3-5) yield

$$A + B = C. \quad k_1(A - B) = k_2C \tag{3-12}$$

Hence

$$B = \frac{k_1 - k_2}{k_1 + k_2}A. \quad C = \frac{2k_1}{k_1 + k_2}A \tag{3-13}$$

As for the constant *A*, it can be determined from the normalization condition of the wave function, but we don't need it here, since *R* and *T* are expressed in terms of ratios. A combination of (iii-10) with (iii-3) leads to

$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} = \frac{(1-\kappa)^2}{(1+k_2)^2}. \quad T = \frac{4k_1k_2}{(k_1 + k_2)^2} \tag{3-14}$$

Where $\kappa = k_2/k_1 = \sqrt{1 - V_o/E}$. The sum of R and T is equal to 1, as it should be.
In contrast to classical mechanics, which states that none of the particles get reflected, equation (iii-14) shows that the quantum mechanical reflection coefficient R is not zero: there are particles that get reflected in spite of their energies being higher than the step V_o. This effect must be attributed to the *wavelike behavior* of the particles.
From (iii-14) we see that as E gets smaller and smaller, T also gets smaller and smaller so that when $E = V_o$ the transmission coefficient T becomes zero and $R = 1$. On the other hand, when $E > V_o$ 0, we have $\kappa = \sqrt{1 - V_o/E} \cong 1$; hence $R = 0$ and $T = 1$. This is expected since, when the incident particles have very high energies, the potential step is so weak that it produces no noticeable effect on their motion.

Remark: physical meaning of the boundary conditions
Throughout this chapter, we will encounter at numerous times the use of the boundary condition of the wave function and its first derivative as in Eq. (iii-11). What is the underlying physics behind these continuity conditions? We can make two observations:

- Since the probability density $|\psi(x)|^2$ of finding the particle in any small region varies continuously from one point to another, the wave function $\psi(x)$ must, therefore, be a continuous function of *x*; thus, as shown in (11), we must have $\psi_1(0) = \psi_2(0)$
- Since the linear momentum of the particle, $\hat{P}\psi(x) = -\hbar\, d\psi(x)/dx$, must be a continuous function of x as the particle moves from left to right, the first derivative of the wave function, $d\psi(x)/dx$, must also be a continuous function of x, notably at $x=0$. Hence, as shown in (iii-11), we must have $d\psi_1(0)/dx = d\psi_2(0)/dx$.

b) Case $E < V_o$
Classically, the particles arriving at the potential step from the left (with momenta $p= 2mE$) will come to a stop $x=0$ and then all will bounce back to the left with the magnitudes of their momenta unchanged. None of the particles will make it into the

right side of the barrier $x=0$; there is total reflection of the particles. So the motion of the particles is reversed by the potential barrier.

Quantum mechanically, the picture will be somewhat different. In this case, the Schrödinger equation and the wave function in the region $x < 0$ are given by (3-1) and (3-3), respectively.

But for $x > 0$ the Schrödinger equation is given by

$$\left(\frac{d^2}{dx^2} + {k_2'}^2\right)\psi_2(x)=0 \qquad (x \geq 0) \tag{3-15}$$

Where ${k'}_2^2 = 2m(V_o - E)/\hbar^2$. This equation's solution is

$$\psi_2(x) = Ce^{-k_2'x} + De^{k_2'x} \qquad (x \geq 0) \tag{3-16}$$

Since the wave function must be finite everywhere, and since the term $e^{k_2'x}$ diverges when $\rightarrow \infty$, the constant D has to be zero. Thus, the complete wave function is

$$\Psi(x.t) = \begin{cases} Ae^{i(k_1x-\omega t)} + Be^{-i(k_1x-\omega t)} & x < 0 \\ Ce^{-k_2'x}e^{-i\omega t} & x \geq 0 \end{cases} \tag{3-17}$$

Let us now evaluate, as we did in the previous case, the reflected and the transmitted coefficients. First we should note that the transmitted coefficient, which corresponds to the transmitted wave function $\psi_t(x) = Ce^{-k_2'x}$, is zero since $\psi_t(x)$ is a *purely real* function ($\psi_t^*(x) = \psi_t(x)$) and therefore

$$J_{transmitted} = \frac{\hbar}{2im}\left(\psi_t(x)\frac{d\psi_t(x)}{dx} - \psi_t(x)\frac{d\psi_t(x)}{dx}\right) \tag{3-18}$$

Hence, the reflected coefficient R must be equal to 1. We can obtain this result by applying the continuity conditions at $x=0$ for (3-4) and (3-16):

$$B = \frac{k_1 - ik_2'}{k_1 + ik_2'}A. \quad C = \frac{2k_1}{k_1 + ik_2'}A \tag{3-19}$$

Thus, the reflected coefficient is given by

$$R = \frac{|B|^2}{|A|^2} = \frac{k_1^2 + {k'}_2^2}{k_1^2 + {k'}_2^2} = 1 \tag{3-20}$$

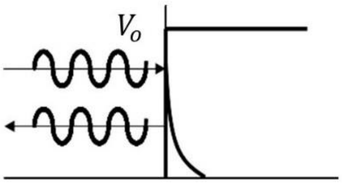
We therefore have total reflection, as in the classical case. There is, however, a difference with the classical case: while none of the particles can be found classically in the region $x=0$, quantum mechanically there is a *nonzero probability* that the wave function penetrates this *classically forbidden* region. To see this, note that the relative probability density

$$P(x) = |\psi_t(x)|^2 = |C|^2 = \frac{4k_1^2|A|^2}{k_1^2 + {k'}_2^2}\, e^{-2k_2'x} \tag{3-21}$$

is appreciable near $x=0$ and falls exponentially to small values as x becomes large; the behavior of the probability density is shown in Figure above.

Example: Penetration depth

$$\psi_t(x) = Be^{-k_2x}. \qquad k_2 = \sqrt{\frac{2m(V_o - E)}{\hbar^2}} > 0$$



The penetration depth defined as $k_2d = 1$

$$d = \frac{1}{k_2} = \sqrt{\frac{\hbar^2}{2m(V_o - E)}} = \sqrt{\frac{\hbar^2}{2m(2E_o - E)}}$$

$$= \frac{1.054 \times 10^{-34}}{\sqrt{2(9.11 \times 10^{-31})(4.56 \times 10^{-31})}} = 11.6 \times 10^{-10} m$$

$$d = 11.6\,\dot{A}$$

4. Potential barrier (The Finite Square Well Potential)

Consider a particle of mass m moving in the following symmetric potential

$$V(x) = \begin{cases} V_{o.} & x < -a/2. \\ 0. & -a/2 \le x \le a/2. \\ V_{o.} & x > a/2. \end{cases} \qquad (4\text{-}1)$$

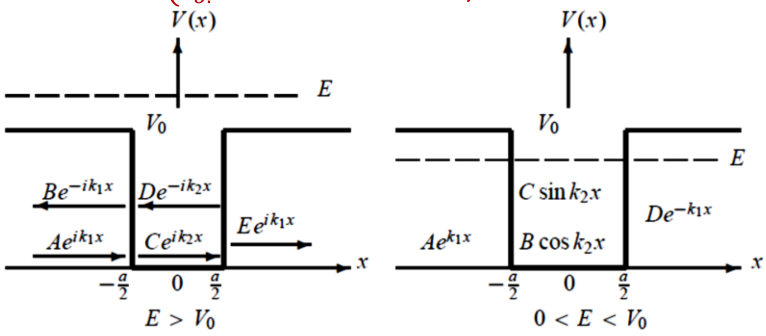


Figure: Finite square well potential and propagation directions of the incident, reflected and transmitted waves when $E > V_o$ and $0 < E < V_o$.

The two physically interesting cases are $E > V_o$ and $E < V_o$. We expect the solutions to yield a *continuous* doubly-degenerate energy spectrum for $E > V_o$ and a *discrete* nondegenerate spectrum for $0 < E < V_o$.

a. The Scattering Solutions ($E > V_o$)

Classically, if the particle is initially incident from left with constant momentum $\sqrt{2m(E - V_o)}$, it will speed up to $\sqrt{2mE}$ between $-a/2 \le x \le a/2$ and then slow down to its initial momentum in the region $x > a$. All the particles that come from the left will be transmitted, none will be reflected back; therefore $T = 1$ and $R = 0$. Quantum mechanically, and as we did for the step and barrier potentials, we can verify that we get a *finite* reflection coefficient. The solution is straightforward to obtain; just follow the procedure outlined in the previous two sections. The wave function has an oscillating pattern in all three regions (see Figure above).

b. The Bound State Solutions ($0 < E < V_o$)

Classically, when $E < V_o$ the particle is completely confined to the region $-a/2 \le x \le a/2$; it will bounce back and forth between $x = -a/2$ and $x = a/2$ with constant momentum $p = \sqrt{2mE}$.

Quantum mechanically, the solutions are particularly interesting for they are expected to yield a *discrete* energy spectrum and wave functions that decay in the two regions $x < -a/2$ and $x > a/2$, but oscillate in $-a/2 \le x \le a/2$. In these three regions, the Schrödinger equation can be written as

$$\left(\frac{d^2}{dx^2} - k_1^2\right)\psi_1(x) = 0 \qquad (x < -a/2) \tag{4-2}$$
$$\left(\frac{d^2}{dx^2} + k_2^2\right)\psi_2(x) = 0 \qquad (-a/2 \le x \le -a/2) \tag{4-3}$$
$$\left(\frac{d^2}{dx^2} - k_1^2\right)\psi_3(x) = 0 \qquad (x > a/2) \tag{4-4}$$

Where $k_1^2 = 2m(E - V_o)$ and $k_2^2 = 2mE/\hbar^2$. Eliminating the physically unacceptable solutions which grow exponentially for large values of $|x|$, we can write the solution to this Schrödinger equation in the regions $x < -a/2$and $x > a/2$as follows:

$$\psi_1(x) = Ae^{k_1x} \qquad (x < -a/2). \tag{4-5}$$
$$\psi_3(x) = De^{-k_1x} \qquad (x < -a/2). \tag{4-6}$$

Since the bound state eigenfunctions of symmetric one dimensional Hamiltonians are either even or odd under space inversion, the solutions of (v-2) to (v-4) are then either **antisymmetric (odd)**

$$\psi_a(x) = \begin{cases} Ae^{k_1x}. & x < -a/2. \\ Csin(k_2x). & -a/2 \le x \le a/2. \\ De^{-k_1x}. & x > a/2. \end{cases} \tag{4-7}$$

Or **symmetric (even)**

$$\psi_s(x) = \begin{cases} Ae^{k_1x}. & x < -a/2. \\ Bcos(k_2x). & -a/2 \le x \le a/2. \\ De^{-k_1x}. & x > a/2. \end{cases} \tag{4-8}$$

To determine the eigenvalues, we need to use the continuity conditions at $x = \pm a/2$. The continuity of the logarithmic derivative,$(1/\psi_a(x))\, d\psi_a(x)/dx$ at $x = \pm a/2$ yields

$$k_2 cot\left(\frac{k_2a}{2}\right) = -k_1. \tag{4-9}$$

Similarly, the continuity of $(1/\psi_s(x))\, d\psi_s(x)/dx$ at $x = \pm a/2$ gives

$$k_2 tan\left(\frac{k_2a}{2}\right) = -k_1. \tag{4-10}$$

The transcendental equations (4-9) and (4-10) cannot be solved directly; we can solve them either graphically or numerically. To solve these equations graphically, we need only to rewrite them in the following suggestive forms:

$$-\alpha_n cot\alpha_n = \sqrt{R^2 - \alpha_n^2}. \quad \text{(for odd states).} \tag{4-11}$$

$$\alpha_n tan\alpha_n = \sqrt{R^2 - \alpha_n^2}. \quad \text{(for even states).} \tag{4-12}$$

where $\alpha_n^2 = (k_2a/2)^2 = ma^2E_n/(2\hbar^2)$ and $R^2 = ma^2V_o/(2\hbar^2)$; these equations are obtained by inserting $k_1 = \sqrt{2m(V_o - E)/\hbar^2}$and $k_2 = \sqrt{2mE/\hbar^2}$ into (4-9) and (4-10). The left-hand sides of (4-11) and (4-12) consist of trigonometric functions; the right-hand sides consist of a circle of radius R. The solutions are given by the points where the circle $\sqrt{R^2 - \alpha_n^2}$ intersects the functions $-\alpha_n cot\alpha_n$and $\alpha_n tan\alpha_n$ (see Figure below). The solutions form a *discrete* set. As illustrated in Figure below, the intersection of the small circle with the curve $\alpha_n tan\alpha_n$ yields only one bound state, $n = 0$, whereas the intersection of the larger circle with $\alpha_n tan\alpha_n$ yields two bound states, $n = 0.2$, and its intersection with $-\alpha_n cot\alpha_n$yields two other bound states, $n = 1.3$.

The number of solutions depends on the size of R, which in turn depends on the depth V_o and the width a of the well, since $R = \sqrt{ma^2V_o/(2\hbar^2)}$. The deeper and broader the well, the larger the value of R, and hence the greater the number of bound states. Note that there is always at least one bound state (i.e., one intersection) no matter how small V_o is. When

$$0 < R < \frac{\pi}{2}. \quad \text{or} \quad 0 < V_o < \left(\frac{\pi}{2}\right)^2 \frac{2\hbar^2}{ma^2}. \tag{4-13}$$

there is only one bound state corresponding to $n = 0$ (see Figure below); this state—the ground state—is even. Then, and when

$$\frac{\pi}{2} < R < \pi. \quad \text{or} \quad \left(\frac{\pi}{2}\right)^2 \frac{2\hbar^2}{ma^2} < V_o < \pi^2 \frac{2\hbar^2}{ma^2}. \tag{4-14}$$

there are two bound states: an even state (the ground state) corresponding to $n = 0$ and the first odd state corresponding to $n = 1$. Now, if

$$\pi < R < \frac{3\pi}{2}. \quad \text{or} \quad \pi^2 \frac{2\hbar^2}{ma^2} < V_o < \left(\frac{3\pi}{2}\right)^2 \frac{2\hbar^2}{ma^2}. \tag{4-15}$$

there exist three bound states: the ground state (even state), $n = 0$, the first excited state (odd state), corresponding to $n = 1$, and the second excited state (even state), which corresponds to $n = 2$. In general, the well width at which n states are allowed is given by

$$tan\alpha_n \to \infty \quad \Rightarrow \alpha_n = \frac{2n+1}{2}\pi. \quad (\mathrm{n} = 0.1.2.3.\cdots). \tag{4-16}$$

$$cot\alpha_n \to \infty \quad \Rightarrow \alpha_n = n\pi. \qquad (\mathrm{n} = 1.2.3.\cdots). \tag{4-17}$$

Combining these two cases, we obtain

$$\alpha_n = \frac{n\pi}{2} \quad (\mathrm{n} = 1.2.3.\cdots). \tag{4-18}$$

Since $\alpha_n^2 = ma^2E_n/(2\hbar^2)$ we see that we recover the energy expression for the infinite well:

$$\alpha_n = \frac{n\pi}{2} \to E_n = \frac{\pi^2\hbar^2}{2ma^2}n^2 \tag{4-19}$$

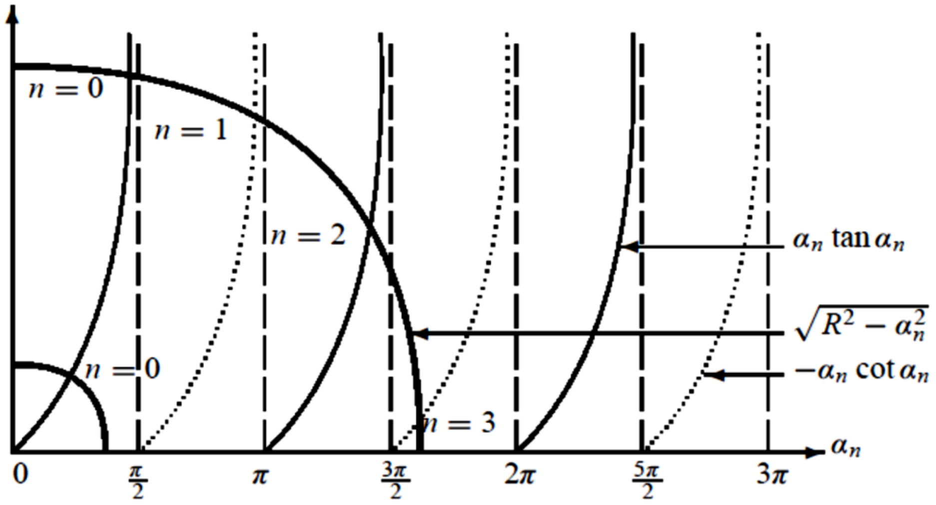


Figure: Graphical solutions for the finite square well potential: they are given by the intersections of $\sqrt{R^2 - \alpha_n^2}$ with $\alpha_n tan\alpha_n$ and $-\alpha_n cot\alpha_n$. Where $\alpha_n^2 = ma^2 E_n/(2\hbar^2)$ and $R^2 = ma^2 V_o/(2\hbar^2)$.

Example

Find the number of bound states and the corresponding energies for the finite square well potential when: (a) $R = 1$ (i.e., $\sqrt{ma^2 V_o/(2\hbar^2)} = 1$), and (b) $R = 2$.

Solution

(a) From Figure above, when $= \sqrt{ma^2 V_o/(2\hbar^2)} = 1$, there is only one bound state since $\alpha_n < R$. This bound state corresponds to $n = 0$. The corresponding energy is given by the intersection of $\alpha_0 tan\alpha_o$ with $\sqrt{1 - \alpha_0^2}$

$$\alpha_0 tan\alpha_o = \sqrt{1 - \alpha_0^2} \Rightarrow \alpha_0^2(1 + tan^2\alpha_o) = 1 \Rightarrow cos^2\alpha_o = \alpha_0^2$$

The solution of $cos^2\alpha_o = \alpha_0^2$ is given numerically by $\alpha_o = 0.73909$. Thus, the corresponding energy is determined by the relation $\sqrt{ma^2 E_o/(2\hbar^2)} = 0.73909$, which yields $E_o \cong 1.1\, \hbar^2/(ma^2)$.

(b)When $R = 2$ there are two bound states resulting from the intersections of $\sqrt{4 - \alpha_0^2}$ with $\alpha_o tan\alpha_o$ and $-\alpha_1 cot\alpha_1$;they correspond to $n = 0$ and $n = 1$, respectively. The numerical solutions of the corresponding equations

$$\alpha_0 tan\alpha_o = \sqrt{4 - \alpha_0^2} \Rightarrow 4cos^2\alpha_o = \alpha_0^2$$

$$-\alpha_1 cot\alpha_1 = \sqrt{4 - \alpha_1^2} \Rightarrow 4sin^2\alpha_1 = \alpha_1^2$$

Yield $\alpha_o = 1.03$ and $\alpha_1 = 1.9$, respectively. The corresponding energies are

$$\alpha_o = \sqrt{\frac{ma^2 E_o}{2\hbar^2}} = 1.03 \quad \Rightarrow E_o = \frac{2.12\hbar^2}{ma^2}$$

$$\alpha_1 = \sqrt{\frac{ma^2E_1}{2\hbar^2}} = 1.9 \quad \Rightarrow E_1 = \frac{7.22\hbar^2}{ma^2}$$

5. The potential barrier and well

Consider a beam of particles of mass *m* that are sent from the left on a potential barrier

$$V(x) = \begin{cases} 0. & x < 0. \\ V_{o.} & 0 \leq x \leq a. \\ 0. & x > a \end{cases} \qquad (5\text{-}1)$$

This potential, which is repulsive, supports no bound states (Figure below). We are dealing here, as in the case of the potential step, with a one-dimensional *scattering* problem.

Again, let us consider the following two cases which correspond to the particle energies being respectively larger and smaller than the potential barrier.

a. The case $E > V_o$

Classically, the particles that approach the barrier from the left at constant momentum, $p_1 = \sqrt{2mE}$, as they enter the region $0 \leq x \leq a$ will slow down to a momentum $p_1 = \sqrt{2m(E - V_o)}$They will maintain the momentum p_2 until they reach the point $x = 0$. Then, as soon as they pass beyond the point $x = a$, they will accelerate to a momentum $p_2 = \sqrt{2mE}$ and maintain this value in the entire region $x > a$. Since the particles have enough energy to cross the barrier, none of the particles will be reflected back; all the particles will emerge on the right side of $x = a$: *total transmission*.

It is easy to infer the quantum mechanical study from the treatment of the potential step presented in the previous section. We need only to mention that the wave function will display an oscillatory pattern in all three regions; its amplitude reduces every time the particle enters a new region (see Figure below):

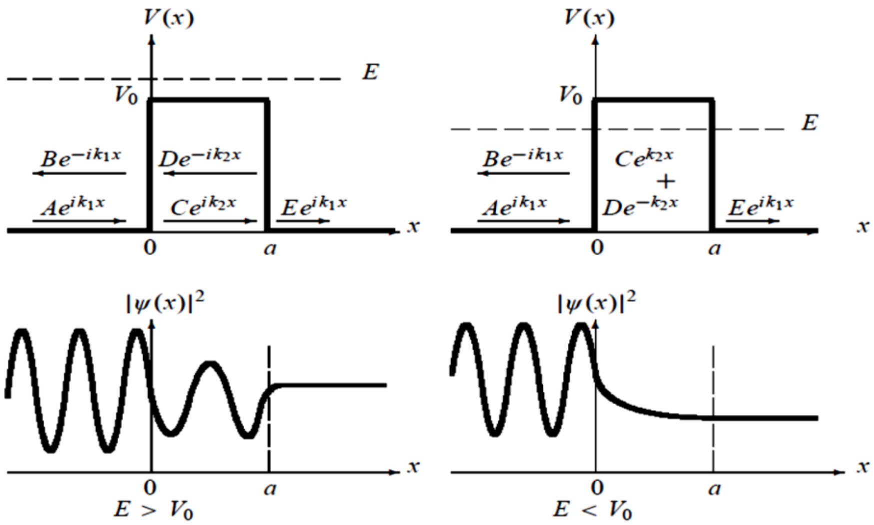


Figure: Potential barrier and propagation directions of the incident, reflected, and transmitted waves, plus their probability densities $|\psi(x)|^2$ when $E > V_o$ and $E < V_o$.

$$\psi(x) = \begin{cases} \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}. & x \le 0. \\ \psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}. & 0 < x < a. \\ \psi_3(x) = Ee^{ik_1x}. & x \ge a \end{cases} \tag{5-2}$$

where $k_1 = \sqrt{2mE/\hbar^2}$ and $k_2 = \sqrt{2m(E - V_o)/\hbar^2}$. The constants B, C, D, and E can be obtained in terms of A from the boundary conditions: $\psi(x)$ and $d\psi(x)/dx$must be continuous at $x = 0$ and $x = a$, respectively

$$\psi_1(0) = \psi_2(0). \qquad \frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx}. \tag{5-3}$$

$$\psi_2(a) = \psi_3(a). \qquad \frac{d\psi_2(a)}{dx} = \frac{d\psi_3(a)}{dx}. \tag{5-4}$$

These equations yield

$$A + B = C + D. \qquad ik_1(A - B) = ik_2(C - D). \tag{5-5}$$

$$Ce^{ik_2a} + De^{-ik_2a} = Ee^{ik_1a}. \; ik_2\left(Ce^{ik_2a} + De^{-ik_2a}\right) = ik_1Ee^{ik_1a}. \tag{5-6}$$

Solving for E, we obtain

$$\begin{aligned} E &= 4k_1k_2\, Ae^{-ik_1a}\left[(k_1 + k_2)^2e^{-ik_2a} - (k_1 - k_2)^2e^{ik_2a}\right]^{-1} \\ &= 4k_1k_2\, Ae^{-ik_1a}[4k_1k_2cos(k_2a) - 2i(k_1^2 + k_2^2)^2sin(k_2a)]^{-1} \end{aligned} \tag{5-7}$$

The transmission coefficient is thus given by

$$\begin{aligned} T &= \frac{k_1|E|^2}{k_1|A|^2} = \left[1 + \frac{1}{4}\left(\frac{k_1^2 - k_2^2}{k_1k_2}\right)^2 sin^2(k_2a)\right]^{-1} \\ &= \left[1 + \frac{V_o^2}{4E(E - V_o)}sin^2\left(a\sqrt{2mV_o/\hbar^2}\,\sqrt{E/V_o} - 1\right)\right]^{-1} \end{aligned} \tag{5-8}$$

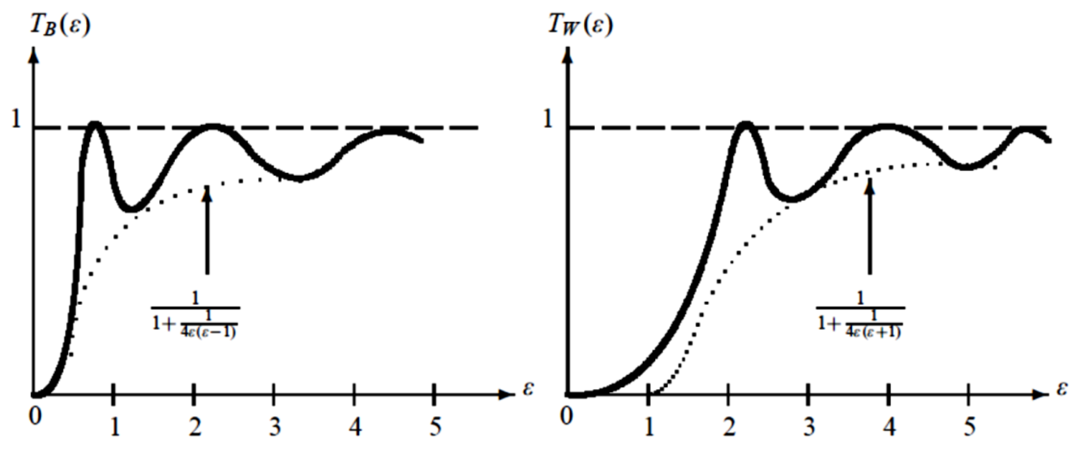


Figure: Transmission coefficients for a potential barrier, $T_B(\varepsilon) = \frac{4\varepsilon(\varepsilon-1)}{4\varepsilon(\varepsilon-1)+sin^2(\lambda\sqrt{\varepsilon-1})}$, and for a potential well, $T_W(\varepsilon) = \frac{4\varepsilon(\varepsilon+1)}{4\varepsilon(\varepsilon+1)+sin^2(\lambda\sqrt{\varepsilon+1})}$.

because

$$\left(\frac{k_1^2 - k_2^2}{k_1 k_2}\right)^2 = \frac{V_o^2}{E(E - V_o)}. \qquad (5\text{-}9)$$

Using the notation $\lambda = a\sqrt{2mV_o/\hbar^2}$ and $\varepsilon = E/V_o$

$$T = \left[1 + \frac{1}{4\varepsilon(\varepsilon - 1)} sin^2\left(\lambda\sqrt{\varepsilon - 1}\right)\right]^{-1}. \qquad (5\text{-}10)$$

Similarly, we can show that

$$R = \frac{sin^2\left(\lambda\sqrt{\varepsilon - 1}\right)}{4\varepsilon(\varepsilon - 1) + sin^2\left(\lambda\sqrt{\varepsilon - 1}\right)} = \left[1 + \frac{4\varepsilon(\varepsilon - 1)}{sin^2\left(\lambda\sqrt{\varepsilon - 1}\right)}\right]^{-1}. \qquad (5\text{-}11)$$

Special cases

- If $E > V_o$, and hence $\varepsilon \gg 1$, the transmission coefficient T becomes asymptotically equal to unity, $T \cong 1$, and $R \cong 0$. So, at very high energies and weak potential barrier, the particles would not feel the effect of the barrier; we have total transmission.
- We also have total transmission when $sin\left(\lambda\sqrt{\varepsilon - 1}\right) = 0$ or $\lambda\sqrt{\varepsilon - 1} = n\pi$. As shown in Figure above, the total transmission, $T(\varepsilon_n) \cong 1$, occurs whenever $\varepsilon_n = E/V_o = n^2\pi^2\hbar^2/(2ma^2V_o) + 1$ or whenever the incident energy of the particle is $E_n = n^2\pi^2\hbar^2/2ma^2$ with $n = 1.2.3.\cdots$ The maxima of the transmission coefficient coincide with the energy eigenvalues of the infinite square well potential; these are known as resonances. This resonance phenomenon, which does not occur in classical physics, results from a constructive interference between the incident and the reflected waves. This phenomenon is observed experimentally in a number of cases such as when scattering low-energy $(E \sim 0.1\ eV)$ electrons off noble atoms (known as the *Ramsauer–Townsend effect*, a consequence of symmetry of noble atoms) and neutrons off nuclei.
- In the limit $\varepsilon \to 1$ we have $sin\left(\lambda\sqrt{\varepsilon - 1}\right) \sim \lambda\sqrt{\varepsilon - 1}$, hence (5-10) and (5-11) become

$$T = \left(1 + \frac{ma^2V_o}{2\hbar^2}\right)^{-1}. \ R = \left(1 + \frac{2\hbar^2}{ma^2V_o}\right)^{-1}. \qquad (5\text{-}12)$$

The potential well($\mathbf{V_o < 0}$)

The transmission coefficient (v-10) was derived for the case where $V_o > 0$, i.e., for a *barrier potential*. Following the same procedure that led to (v-10), we can show that the transmission coefficient for a finite *potential well*, $V_o < 0$, is given by

$$T_W = \left[1 + \frac{1}{4\varepsilon(\varepsilon - 1)} sin^2\left(\lambda\sqrt{\varepsilon - 1}\right)\right]^{-1}. \qquad (5\text{-}13)$$

where $\varepsilon = E/|V_o|$ and $\lambda = a\sqrt{2m|V_o|/\hbar^2}$. Notice that there is total transmission whenever $sin\left(\lambda\sqrt{\varepsilon - 1}\right) = 0\ or\ \lambda\sqrt{\varepsilon - 1} = n\pi$. As shown in Figure above, the total transmission, $T_W = 1$, occurs whenever $\varepsilon_n = E/|V_o| = n^2\pi^2\hbar^2/(2mV_o) - 1$ or whenever the incident energy of the particle is $E_n = n^2\pi^2\hbar^2/(2m) - |V_o|$with $n = 1.2.3.\cdots$.

b. The case $E < V_o$ Tunneling

Classically, we would expect total reflection: every particle that arrives at the barrier ($x = 0$) will be reflected back; no particle can penetrate the barrier, where it would have a negative kinetic energy.

We are now going to show that the quantum mechanical predictions differ sharply from their classical counterparts, for the wave function is not zero beyond the barrier. The solutions of the Schrödinger equation in the three regions yield expressions that are similar to (v-2) except that $\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}$should be replaced with $\psi_2(x) = Ce^{k_2x} + De^{-k_2x}$:

$$\psi(x) = \begin{cases} \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}. & x \le 0. \\ \psi_2(x) = Ce^{k_2x} + De^{-k_2x}. & 0 < x < a. \\ \psi_3(x) = Ee^{ik_1x}. & x \ge a \end{cases} \tag{5-14}$$

where $k_1^2 = 2mE/\hbar^2$ and $k_2^2 = 2m(E - V_o)/\hbar^2$. The behavior of the probability density corresponding to this wave function is expected, as displayed in Figure above, to be oscillatory in the regions $x < 0$ and $x > a$, and exponentially decaying for $o \le x \le a$.

To find the reflection and transmission coefficients

$$R = \frac{|B|^2}{|A|^2}. \quad T = \frac{|E|^2}{|A|^2} \tag{5-15}$$

We need only to calculate B and E in terms of A. The continuity conditions of the wave function and its derivative at $x = 0$ and $x = a$ yield

$$A + B = C + D. \tag{5-16}$$

$$ik_1(A - B) = k_2(C - D). \tag{5-17}$$

$$Ce^{k_2a} + De^{-k_2a} = Ee^{ik_1a}. \tag{5-18}$$

$$k_2(Ce^{k_2a} - De^{-k_2a}) = ik_1Ee^{ik_1a}. \tag{5-19}$$

The last two equations lead to the following expressions for C and D:

$$C = \frac{E}{2}\left(1 + i\frac{k_1}{k_2}\right)e^{(ik_1 - k_2)a}. \quad D = \frac{E}{2}\left(1 - i\frac{k_1}{k_2}\right)e^{(ik_1 + k_2)a} \tag{5-20}$$

Inserting these two expressions into the two equations (5-16) and (5-17) and dividing by A, we can show that these two equations reduce, respectively, to

$$1 + \frac{B}{A} = \frac{E}{A}e^{ik_1a}\left[cosh(k_2a) - i\frac{k_1}{k_2}sinh(k_2a)\right]. \tag{5-21}$$

$$1 - \frac{B}{A} = \frac{E}{A}e^{ik_1a}\left[cosh(k_2a) + i\frac{k_1}{k_2}sinh(k_2a)\right]. \tag{5-22}$$

Solving these two equations for B/A and E/A , we obtain

$$\frac{B}{A} = -i\frac{k_1^2 + k_2^2}{k_1 k_2} sinh(k_2 a)\left[2cosh(k_2 a) + i\frac{k_2^2 - k_1^2}{k_1 k_2} sinh(k_2 a)\right]^{-1}. \qquad (5\text{-}23)$$

$$\frac{E}{A} = 2e^{-ik_1 a}\left[2cosh(k_2 a) + i\frac{k_2^2 - k_1^2}{k_1 k_2} sinh(k_2 a)\right]^{-1}. \qquad (5\text{-}24)$$

Thus, the coefficients R and T become

$$R = \frac{|B|^2}{|A|^2} = \left(\frac{k_1^2 + k_2^2}{k_1 k_2}\right)^2 sinh^2(k_2 a)\left[4cosh^2(k_2 a) + \left(\frac{k_2^2 + k_1^2}{k_1 k_2}\right)^2 sinh^2(k_2 a)\right]^{-1}. \qquad (5\text{-}25)$$

$$T = \frac{|E|^2}{|A|^2} = 4\left[4cosh^2(k_2 a) + \left(\frac{k_2^2 - k_1^2}{k_1 k_2}\right)^2 sinh^2(k_2 a)\right]^{-1}. \qquad (5\text{-}26)$$

We can rewrite R in terms of T as

$$R = \frac{1}{4}T\left(\frac{k_2^2 - k_1^2}{k_1 k_2}\right) sinh^2(k_2 a) \;. \qquad (5\text{-}27)$$

Since $cosh^2(k_2 a) = 1 + sinh^2(k_2 a)$we can reduce (5-26) to

$$T= \left[1 + \frac{1}{4}\left(\frac{k_2^2 - k_1^2}{k_1 k_2}\right)^2 sinh^2(k_2 a)\right]^{-1}. \qquad (5\text{-}28)$$

Note that T is *finite*. This means that the probability for the transmission of the particles into the region $x \geq a$ is *not zero* (in classical physics, however, the particle can in no way make it into the $x \geq 0$ region). This is a purely quantum mechanical effect which is due to the *wave aspect* of microscopic objects; it is known as the *tunneling effect*: *quantum mechanical objects can tunnel through classically impenetrable barriers*. This *barrier penetration* effect has important applications in various branches of modern physics ranging from particle and nuclear physics to semiconductor devices. For instance, radioactive decays and charge transport in electronic devices are typical examples of the tunneling effect.

Now since

$$\left(\frac{k_2^2 - k_1^2}{k_1 k_2}\right)^2 = \left(\frac{V_o}{\sqrt{E(V_o - E)}}\right)^2 = \frac{V_o^2}{E(V_o - E)}. \qquad (5\text{-}29)$$

We can rewrite (v-27) and (v-28) as follows:

$$R = \frac{1}{4}\frac{V_o{}^2 T}{E(V_o - E)} sinh^2\left(\frac{a}{\hbar}\sqrt{2m(V_o - E)}\right). \qquad (5\text{-}30)$$

$$T= \left[1 + \frac{1}{4}\frac{V_o^2}{E(V_o - E)} sinh^2\left(\frac{a}{\hbar}\sqrt{2m(V_o - E)}\right)\right]^{-1}. \qquad (5\text{-}31)$$

Or

$$R = \frac{T}{4\varepsilon(1-\varepsilon)} sinh^2\left(\lambda\sqrt{1-\varepsilon}\right). \qquad (5\text{-}32)$$

$$T= \left[1 + \frac{1}{4\varepsilon(1-\varepsilon)} sinh^2\left(\lambda\sqrt{1-\varepsilon}\right)\right]^{-1}. \qquad (5\text{-}33)$$

Where $\lambda = a\sqrt{2mV_o/\hbar^2}$ and $\varepsilon = E/V_o$.

Special cases

- If $E \ll V_o$. Hence $\varepsilon \ll 1$ or $\lambda\sqrt{1-\varepsilon} \gg 1$. we may approximate $sinh\left(\lambda\sqrt{1-\varepsilon}\right) \cong \frac{1}{2}exp\left(\lambda\sqrt{1-\varepsilon}\right)$. We can thus show that the transmission coefficient (v-33) becomes

$$T \cong \left\{\frac{1}{4\varepsilon(1-\varepsilon)}\left[e^{\left(\lambda\sqrt{1-\varepsilon}\right)}\right]^2\right\}^{-1} = 16\varepsilon(1-\varepsilon)e^{-2\lambda\sqrt{1-\varepsilon}}$$
$$= 16\left(1-\frac{E}{V_o}\right)e^{-(2a/\hbar)\sqrt{2m(V_o-E)}} \qquad (5\text{-}34)$$

This shows that the transmission coefficient is not zero, as it would be classically, but has a finite value. So, quantum mechanically, there is a finite tunneling beyond the barrier $x > a$.

- When $E \cong V_o$, hence $\varepsilon \cong 1$, we can verify that (5-32) and (5-33) lead to the relations (5-12).
- Taking the classical limit $\hbar \to 0$, the coefficients (5-32) and (5-33) reduce to the classical result: $R \to 1$ and $T \to 0$.

c. The Tunneling Effect

In general, the tunneling effect consists of the propagation of a particle through a region where the particle's energy is smaller than the potential energy $E < V(x)$. Classically this region, defined by $x_1 < x < x_2$ (Figure below-a), is forbidden to the particle where its kinetic energy would be negative; the points $x = x_1$ and $x = x_2$ are known as the *classical turning points*.
Quantum mechanically, however, since particles display wave features, the quantum waves can tunnel through the barrier.

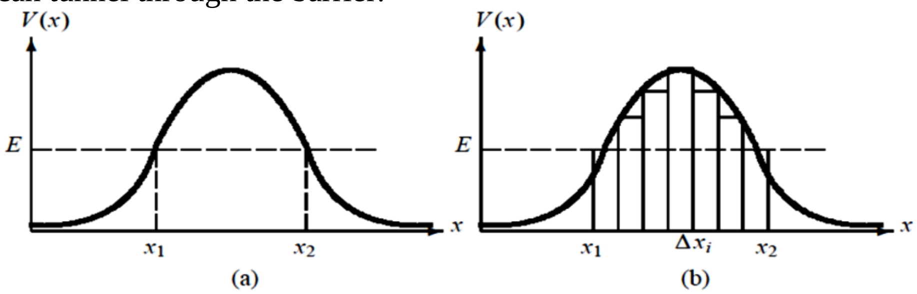


Figure: (a)Tunneling though a potential barrier. (b) Approximation of a smoothly varying potential $V(x)$ by square barriers.

As shown in the square barrier example, the particle has a finite probability of tunneling through the barrier. In this case, we managed to find an analytical expression (5-33) for the tunneling probability only because we dealt with a simple square potential. Analytic expressions cannot be obtained for potentials with arbitrary spatial dependence. In such cases one needs approximations. The Wentzel–Kramers Brillouin (WKB) method provides one of the most useful approximation methods. We will show that the transmission coefficient for a barrier potential $V(x)$ is given by:

$$T \sim exp\left\{-\frac{2}{\hbar}\int_{x_1}^{x_2} dx\sqrt{2m[V(x)-E]}\right\}. \qquad (5\text{-}35)$$

The transmission probability for the general potential of Figure above, where we divided the region $x_1 < x < x_2$ into a very large number of small interval , is given by

$$T \sim \lim_{N\to\infty} \prod_{i=1}^{N} exp\left[-\frac{2\Delta x_i}{\hbar}\sqrt{2m(V(x_i)-E)}\right]$$
$$= exp\left[-\frac{2}{\hbar}\lim_{\Delta x_i\to 0}\sum_i \Delta x_i\sqrt{2m(V(x_i)-E)}\right] \qquad (5\text{-}36)$$
$$\to exp\left[-\frac{2}{\hbar}\int_{x_1}^{x_2} dx\sqrt{2m[\mathrm{V(x)}-E]}\right]$$

The approximation leading to this relation is valid, only if the potential $\mathrm{V(x)}$ is a smooth, slowly varying function of x.

6. Harmonic oscillator.

The harmonic oscillator is one of those few problems that are important to all branches of physics. It provides a useful model for a variety of vibrational phenomena that are encountered ,for instance, in classical mechanics, electrodynamics, statistical mechanics, solid state, atomic ,nuclear, and particle physics. In quantum mechanics, it serves as an invaluable tool to illustrate the basic concepts and the formalism.
The paradigm for a classical harmonic oscillator is a mass m attached to a spring of force constant k. The motion is governed by Hooke's law.

$$F = -kx = m\frac{d^2x}{dt^2} \qquad (6\text{-}1)$$

(as always, we ignore friction), and the solution is

$$x(t) = Asin(\omega t) + Bcos(\omega t) \qquad (6\text{-}2)$$

Where $\omega \equiv \sqrt{\frac{k}{m}}$ is the (angular) frequency of oscillation. The potential energy is

$$V(x) = \frac{1}{2}kx^2 \qquad (6\text{-}3)$$

Its graph is a parabola.
Of course, there's no such thing as a perfect simple harmonic oscillator-if you stretch it too far the spring is going to break, and typically **Hook's law** fails long before that point is reached. But practically any potential is *approximately* parabolic, in the neighborhood of a local minimum (Figure below). Formally, if we expand $V(x)$ in a **Taylor series** about the minimum:

$$V(x) = V(x_o) + V'(x_o)(x-x_o) + \frac{1}{2}V''(x_o)(x-x_o)^2 + \cdots \qquad (6\text{-}4)$$

Subtract $V(x_o)$ [you can add a constant to $V(x_o)$ with impunity, since that doesn't change the force], recognize that $V' = 0$ (since x_o is a minimum), and drop the higher –order terms [which are negligible as long as $(x-x_o)$ stays small], the potential becomes

$$V(x) \cong \frac{1}{2}V''(x_o)(x-x_o)^2 \qquad (6\text{-}5)$$

Which described simple harmonic oscillation (about the point x_o), with an effective spring constant $k = V''(x_o)$. That's why the simple harmonic oscillator is so important:

virtually any oscillatory motion is approximately simple harmonic, as long as the amplitude is small.

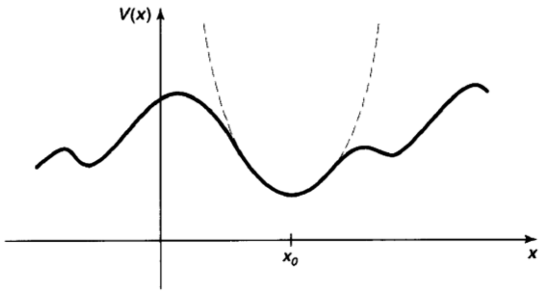


Figure: Parabolic approximation (dashed curve) to an arbitrary potential, in the neighborhood of a local minimum.

The quantum mechanics problem is to solve the Schrödinger equation for the potential

$$V(x) = \frac{1}{2}m\omega^2 x^2 \qquad (6\text{-}6)$$

(it is customary to eliminate the spring constant in favor of the classical frequency, using Equation (6-6). As we have seen, it suffices to solve the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi = E\omega \qquad (6\text{-}7)$$

In the literature you will find two entirely different approaches to this problem. The first called the *analytic method*, which is a straightforward "brute force" solution to differential equation, using the method of power series expansion; it has the virtue that the same strategy can be applied to many others potentials. The second method is a diabolically clever algebraic technique, using so-called the ladder or algebraic method, does not deal with solving the Schrödinger equation, but deals instead with operator algebra involving operators known as the *creation* and *annihilation* or ladder operators.

a. Algebraic method

To begin with, let's rewrite Equation (6-7) in a more suggestive form

$$\frac{1}{2m}\left[\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 + (m\omega\, x\,)^2\right]\psi = E\psi \qquad (6\text{-}8)$$

The idea is to factor the term in square brackets. If these were numbers, it would be

$$u^2 + v^2 = (u - iv)(u + iv)$$

Here, however, it's not quite so simple, because u and v are operators, and operators do not, in general, commute (uv is not the same as vu). Still, this does invite us to take a look at the expressions

$$a_{\pm} \equiv \frac{1}{\sqrt{2m}}\left(\frac{\hbar}{i}\frac{d}{dx} \pm im\omega\, x\,\right) \qquad (6\text{-}9)$$

What is their product, $a_- a_+$? Warring: operators can be slippery to work with in the abstract, and you are bound to mike mistake unless you give them a "test fuction", $f(x)$, to act on. At the end you can throw away the test function, and you'll be left with an equation involving the operators alone. In the present case, we have

$$(a_-a_+)f(x) = \frac{1}{2m}\left(\frac{\hbar}{i}\frac{d}{dx} - im\omega\, x\right)\left(\frac{\hbar}{i}\frac{d}{dx} + im\omega\, x\right)f(x)$$
$$= \frac{1}{2m}\left(\frac{\hbar}{i}\frac{d}{dx} - im\omega\, x\right)\left(\frac{\hbar}{i}\frac{df}{dx} + im\omega\, xf\right)$$
$$= \frac{1}{2m}\left[-\hbar^2\frac{d^2f}{dx^2} + \hbar m\omega\,\frac{d}{dx}(xf) - m\omega\, x\frac{df}{dx} + (m\omega\, x)^2 f\right] \qquad (6\text{-}10)$$
$$= \frac{1}{2m}\left[\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 + (m\omega\, x)^2 + \hbar m\omega\right] f(x)$$

[I used $d(xf)/dx = x(df/dx) + f$ in the last step]. Discarding the test function, we conclude that

$$a_-a_+ = \frac{1}{2m}\left[\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 + (m\omega\, x)^2\right] + \frac{1}{2}\hbar\omega \qquad (6\text{-}11)$$

Evidently, Equation (vi-8) does not factor perfectly – there's an extra term $(1/2)\hbar\omega.$ However, if we pull this over to the other side, the Schrödinger equation becomes

$$\left(a_-a_+ - \frac{1}{2}\hbar\omega\right)\psi = E \qquad (6\text{-}12)$$

Notice that the ordering of the factors a_+ and a_- is important here, the same argument with a_+ on the left yields

$$a_+a_- = \frac{1}{2m}\left[\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 - (m\omega\, x)^2\right] - \frac{1}{2}\hbar\omega \qquad (6\text{-}13)$$

Thus

$$a_-a_+ - a_+a_- = \hbar\omega \qquad (6\text{-}14)$$

And the Schrödinger equation can also be written

$$\left(a_+a_- + \frac{1}{2}\hbar\omega\right)\psi = E\psi \qquad (6\text{-}15)$$

Now, here comes the crucial step: I claim that if 1/; satisfies the Schrödinger equation, with energy E, then a+1l/ satisfies the Schrödinger equation with energy (E +hw). Proof:

$$\left(a_+a_- + \frac{1}{2}\hbar\omega\right)(a_+\psi) = \left(a_+a_-a_+ + \frac{1}{2}\hbar\omega\, a_+\right)\psi$$
$$= a_+\left(a_-a_+ + \frac{1}{2}\hbar\omega\right)\psi = a_+\left[\left(a_-a_+ - \frac{1}{2}\hbar\omega\right)\psi + \hbar\omega\psi\right]$$
$$= a_+(E\psi + \hbar\omega\psi) = (E + \hbar\omega)(a_+\psi).\, QED$$

Notice that whereas the ordering of a_+ and a_- does matter, the ordering of $a_\pm$ and any constants (such as $\hbar$, ω, and E) does not.] By the same token, $a_-\psi$ is a solution with energy$(E - \hbar\omega)$:

$$\left(a_-a_+ - \frac{1}{2}\hbar\omega\right)(a_-\psi) = a_-\left(a_+a_- - \frac{1}{2}\hbar\omega\right)\psi$$
$$= a_-\left[\left(a_+a_- + \frac{1}{2}\hbar\omega\right)\psi - \hbar\omega\psi\right] = a_-(E\psi - \hbar\omega\psi)$$
$$= (E - \hbar\omega)(a_-\psi).\, QED$$

Here, then, is a wonderful machine for grinding out new solutions, with higher and lower energies—if we can just find one solution, to get started! We call $a_\pm$ ladder operators, because they allow us to climb up and down in energy; a_+ is called *the raising operator*, and a_- *the lowering operator*. The "ladder" of states is illustrated in Figure below.

But wait! What if I apply the lowering operator repeatedly? Eventually I'm going to reach a state with energy less than zero, which (according to the general theorem) does not exist! At some point the machine must fail. How can that happen? We know that $a_-\psi$ is a new solution to the Schrödinger equation, but there is no guarantee that it will be normalizable—it might be zero, or its square integral might be infinite. Conclusion: There must occur a "lowest rung" (let's call it ψ_o) such that

$$a_-\psi = 0 \tag{6-16}$$

That is to say

$$\frac{1}{\sqrt{2m}}\left(\frac{\hbar}{i}\frac{d\psi_o}{dx} - im\omega\, x\, \psi_o\right) = 0$$

Or

$$\frac{d\psi_o}{dx} = -\frac{m\omega}{\hbar} x\, \psi_o$$

This differential equation for ψ_o is easy to solve:

$$\int \frac{d\psi_o}{\psi_o} = -\frac{m\omega}{\hbar}\int x dx \quad \Rightarrow \quad ln\psi_o = -\frac{m\omega}{2\hbar}x^2 + constant,$$

So

$$\psi_o(x) = A_o e^{-\frac{m\omega}{2\hbar}x^2}. \tag{6-17}$$

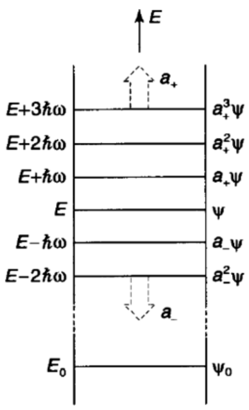


Figure: the ladder of stationary states for the simple harmonic oscillator.

To determine the energy of this state, we plug it into the Schrödinger equation {in the form of Equation (6-15}, $\left(a_+a_- + \frac{1}{2}\hbar\omega\right)\psi_o = E_o\psi_o$, and exploit the fact that $a_-\psi = 0$. Evidently

$$E_o = \frac{1}{2}\hbar\omega \tag{6-18}$$

With our foot now securely planted on the bottom rung" (the ground state of the quantum oscillator), we simply apply the raising Operator to generate the excited states":

$$\psi_n(x) = A_n(a_+)^n e^{-\frac{m\omega}{2\hbar}x^2}, \qquad with\ E_n = \left(n + \frac{1}{2}\right)\hbar\omega \tag{6-19}$$

(This method does not immediately determine the normalization factor A_n; For example,

$$\psi_1(x) = A_1 a_+ e^{-\frac{m\omega}{2\hbar}x^2} = A_1\frac{1}{\sqrt{2m}}\left(\frac{\hbar}{i}\frac{d}{dx} - im\omega\, x\right)e^{-\frac{m\omega}{2\hbar}x^2}$$

$$= \frac{A_1}{\sqrt{2m}}\left(\frac{\hbar}{i}\left(-\frac{m\omega}{\hbar}x\right)e^{-\frac{m\omega}{2\hbar}x^2} + im\omega\, xe^{-\frac{m\omega}{2\hbar}x^2}\right)$$

Which simplify to

$$\psi_1(x) = \left(iA_1\omega\sqrt{2m}\right)xe^{-\frac{m\omega}{2\hbar}x^2} \qquad (6\text{-}20)$$

I wouldn't want to calculate ψ_{50} in this way, but never mind: We have found all the allowed energies, and in principle we have determined the stationary states—the rest is just computation.

a. Analytical Method

We return now to the Schrödinger equation for the harmonic oscillator (Equation 6-7):

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\omega$$

Things look a little cleaner if we introduce the dimensionless variable

$$\xi \equiv \sqrt{\frac{m\omega}{\hbar}}\, x \qquad (6\text{-}21)$$

In term of ξ, the Schrödinger reads

$$\frac{d^2\psi}{dx^2} = (\xi^2 - K)\psi \qquad (6\text{-}22)$$

Where K is the energy, in units of $(1/2)\hbar\omega$:

$$K \equiv \frac{2E}{\hbar\omega} \qquad (6\text{-}23)$$

Our problem is to solve Equation 6-22, and in the process obtain the "allowed" values of K (and hence of E).

To begin with, note that at very large ξ (which is to say, at very large x), ξ^2completely dominates over the constant K, so in this regime

$$\frac{d^2\psi}{d\xi^2} \approx \xi^2\psi \qquad (6\text{-}24)$$

which has the approximate solution (check it!)

$$\psi(\xi) \approx Ae^{-\xi^2/2} + Be^{+\xi^2/2} \qquad (6\text{-}25)$$

The B term is clearly not normalizable (it blows up as $|x| \to \infty$); the physically acceptable solutions, then, have the asymptotic for

$$\psi(\xi) \approx (\,)e^{-\xi^2/2}, \quad \text{at large } \xi \qquad (6\text{-}26)$$

This suggests that we "peel off ' the exponential part,

$$\psi(\xi) = h(\,\xi\,)e^{-\xi^2/2}, \qquad (6\text{-}27)$$

in hopes that what remains [$h(\,\xi\,)$] has a simpler functional form than $\psi(\xi)$ itself.

Differentiating Equation 6-26, we have

$$\frac{d\psi}{d\xi} = \left(\frac{dh}{d\xi} - \xi h\right)e^{-\xi^2/2}$$

And

$$\frac{d^2\psi}{d\xi^2} = \left(\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (\xi^2 - 1)\right)e^{-\xi^2/2}$$

So the Schrödinger equation (Equation 6-21) becomes

$$\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (K-1)h = 0, \qquad (6\text{-}28)$$

I propose to look for a solution to Equation 6-28 in the form of a power series in ξ:

$$h(\xi) = a_o + a_1\xi + a_2\xi^2 + \cdots = \sum_{j=0}^{\infty} a_j\xi^j, \qquad (6\text{-}29)$$

Differentiating the series term by term,

$$\frac{dh}{d\xi} = a_1 + 2a_2\xi + 3a_3\xi^2 \ldots = \sum_{j=0}^{\infty} ja_j\xi^{j-1}, \qquad (6\text{-}30)$$

And

$$\frac{d^2h}{d\xi^2} = 2a_2 + 2\cdot 3a_3\xi + 3\cdot 4a_4\xi^2 + \cdots = \sum_{j=0}^{\infty}(j+1)(j+2)a_{j+2}\xi^j, \qquad (6\text{-}31)$$

Putting these into Equation vi-27, we find

$$\sum_{j=0}^{\infty}[(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j]\xi^j = 0\ , \qquad (6\text{-}32)$$

It follows (from the uniqueness of power series expansions") that the coefficient of *each power* of ξ must vanish

$$(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j = 0$$

And hence that

$$a_{j+2} = \frac{(2j+1-K)}{(j+1)(j+2)}a_j, \qquad (6\text{-}33)$$

This **recursion formula** is entirely equivalent to the Schrödinger equation itself.

Given a_o it enables us (in principle) to generate $a_2, a_4, a_6, \ldots$ and given a_1 it generates $a_3, a_5, a_7, \ldots$. Let us write

$$h(\xi) = h_{even}(\xi) + h_{odd}(\xi) \qquad (6\text{-}34)$$

Where

$$h_{even}(\xi) = a_o + a_2\xi^2 + a_4\xi^4 + \cdots$$

is an even function of ξ (since it involves only even powers), built on a_o, and

$$h_{odd}(\xi) = a_1\xi + a_3\xi^3 + a_5\xi^5 + \cdots$$

is an odd function, built on a_1. Thus Equation vi-31 determines $h(\xi)$ in terms arbitrary constants (a_o and a_1)—which is just what we would expect, for a second order differential equation.

However, not all the solutions so obtained are normalizable. For at very large j, the recursion formula becomes (approximately)

$$a_{j+2} \approx \frac{2}{j}a_j,$$

With the (approximate) solution

$$a_j \approx \frac{C}{(j/2)!},$$

For some constant C, and this yields (at large ξ, where the higher powers dominate)

$$h(\xi) \approx C\sum\frac{1}{(j/2)!}\xi^j \approx C\sum\frac{1}{k!}\xi^{2k} \approx Ce^{\xi^2}$$

Now, if h goes like $exp(\xi^2)$, then ψ (remember ψ?——that's what we're trying to calculate) goes like $\exp(\xi^2/2)$, (Equation vi-27), which is precisely the asymptotic behavior we don 't want." There is only one way to wiggle out of this: For normalizable solutions the power series must terminate. There must occur some "highest" j (call it n) such that the recursion formula spits out $a_{n+2} = 0$ (this will truncate either the series h_{even} or the series h_{odd}; the other one must be zero from the start). For physically acceptable solutions, then, we must have

$$K = 2n + 1,$$

for some positive integer n , which is to say (referring to Equation 6-23) that the energy must be of the form

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad for\; n = 0,1,2, ... \tag{6-35}$$

Thus we recover, by a completely different method, the fundamental quantization condition we found algebraically in Equation 6-19.

For the allowed values of K, the recursion formula reads

$$a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)} a_j \tag{6-36}$$

If $n = 0$, there is only one term in the series (we must pick a_1 to kill h_{odd}, and $j = 0$ in Equation. 6-36 yields $a_1 = 0$):

$$h_0(\xi) = a_0,$$

And hence

$$\psi_0(\xi) = a_0 e^{-\xi^2/2}$$

(which reproduces Equation 6-17). For $n = 0$ we pick $a_0 = 0$, and Equation 6-36 with $j = 0$ yields $a_3 = 0$, so

$$h_1(\xi) = a_1\xi,$$

And hence

$$\psi_1(\xi) = a_1\xi e^{-\xi^2/2}$$

(confirming Equation 6-20). For $n = 2$, $j = 0$yields $a_2 = -2a_0$, andj $j = 2$ gives $a_4 = 0$, so

$$h_2(\xi) = a_o(1 - 2\xi^2),$$

And

$$\psi_2(\xi) = a_o(1 - 2\xi^2)e^{-\xi^2/2}$$

and so on.

In general, $h_n(\xi)$ will be a polynomial of degree n in ξ, involving even powers only, if n is an even integer, and odd powers only, if n is an odd integer. Apart from the overall factor (a_o or a_1) they are the so-called Hermite polynomials, $H_n(\xi)$.

The Hermite polynomials is:

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n}{dx^n} e^{\xi^{-2}}$$

The first few of them are listed in Table below. By tradition, the arbitrary multiplicative factor is chosen so that the coefficient of the highest power of 'ξ is 2^n". With this convention, the normalized stationary states for the harmonic oscillator are

$$\psi_n(\xi) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2} \tag{6-37}$$

They are identical (of course) to the ones we obtained algebraically in Equation 6-19.

In Figure below a I have plotted $\psi_n(x)$ for the first few n's.

The quantum oscillator is strikingly different from its classical counterpart—not only are the energies quantized, but the position distributions have some bizarre features. For instance, the probability of finding the particle outside the classically allowed range (that is, with x greater than the classical amplitude for the energy in question) is not zero, and in all odd states the probability of

Table: The first few Hermite polynomials, $H_n(\xi)$.

$H_o = 1,$	For $n = 0,$
$H_1 = 2x,$	For $n = 1,$
$H_2 = 4x^2 - 2,$	For $n = 2,$
$H_3 = 8x^3 - 12x,$	For $n = 3,$
$H_4 = 16x^4 - 48x^2 + 12,$	For $n = 4,$
$H_5 = 32x^5 - 160x^3 + 120x,$	For $n = 5,$

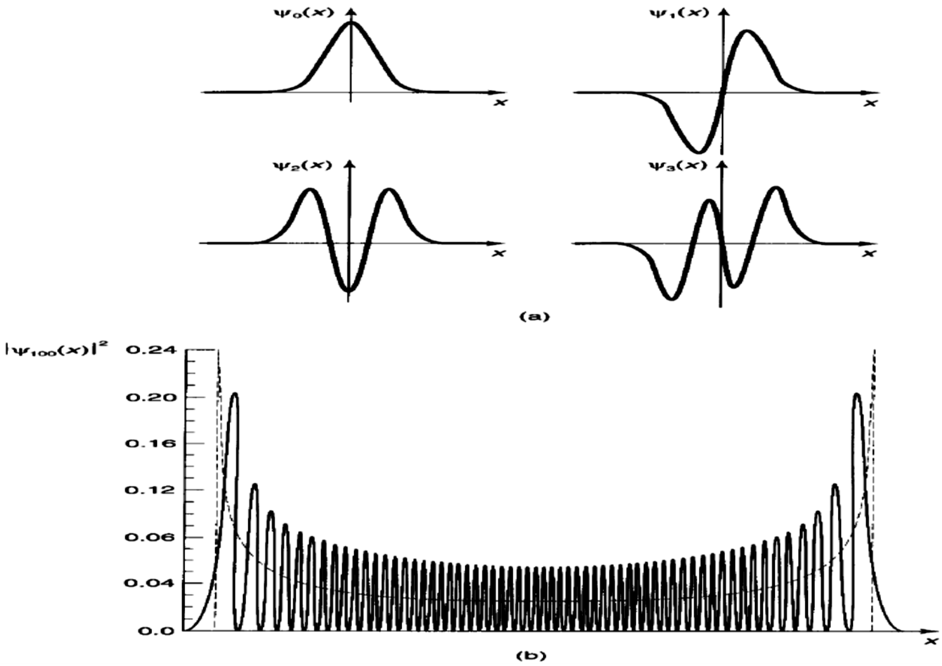


Figure: (a) The first four stationary states of the harmonic oscillator.

(b) Graph of $|\psi_1(x)|^2$, with the classical distribution (dashed curve) superimposed.

finding the particle at the center of the potential well is zero. Only at relatively large n do we begin to see some resemblance to the classical case. In Figure above-b I have superimposed the classical position distribution on the quantum one (for $= 100$); if you smoothed out the bumps in the latter, the two would fit pretty well (however, in the classical case we are talking about the distribution of positions over *time* for *one* oscillator, whereas in the quantum case we are talking about the distribution over an ensemble of identically-prepared systems).

Solved Problem in Quantum Mechanics in One Dimension

Problem1:-Wave Function for a Free Particle

A free electron has wave function

$$\Psi(x,t) = sin(kx - \omega t) \qquad (1)$$

1. Determine the electron's de Broglie wavelength, momentum, kinetic energy and speed when $k = 50nm^{-1}$.
2. Determine the electron's de Broglie wavelength, momentum, total energy, kinetic energy and speed when $k = 50\ pm^{-1}$.

Solution:-

1. The equations relating the speed v, momentum p, de Broglie wavelength λ, wave number k, kinetic energy E, angular frequency ω and group velocity v_g for a nonrelativistic particle of mass m are:

$$p = mv = \frac{h}{\lambda} = \hbar k \qquad (2)$$

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \hbar\omega \qquad (3)$$

$$v_g = \frac{d\omega}{dk} = v \qquad (4)$$

When $k = 50\ nm^{-1}$,

$$\lambda = 126\text{ pm}, \qquad p = 9.87\text{KeV/c} \qquad (5)$$

And, for an electron $(m = 511\ keV/c^2)$,

$$E = 95.2\text{eV}, \qquad v = 1.93 \times 10^{-2}c \qquad (6)$$

2. The equations relating the speed v, momentum p, de Broglie wavelength λ, wave number k, total energy E, kinetic energy K, angular frequency ω and group velocity v_g for a relativistic particle of mass m are:

$$p = \gamma mv = \frac{h}{\lambda} = \hbar k \qquad (7)$$

$$E = \gamma mc^2 = mc^2 + K = \sqrt{p^2c^2 + m^2c^4} = \hbar\omega \qquad (8)$$

$$v_g = \frac{d\omega}{dk} = v = \frac{pc^2}{E} \qquad (9)$$

$$\gamma = \frac{1}{\sqrt{1-\beta^2}} \qquad (10)$$

$$\beta = v/c \qquad (11)$$

When $k = 50\ pm^{-1}$,

$$\lambda = 126\text{ fm}, \qquad p = 9.87\text{MeV/c} \qquad (12)$$

And, for an electron $(m = 511\ keV/c^2)$,

$$E = 9.88\ \text{MeV}, \qquad K = 9.37\text{MeV} \qquad v = 0.9987\ c \qquad (13)$$

Problem2:- Potential Energy of a Particle

In a region of space, a particle with mass m and with zero energy has a time-independent wave function

$$\psi(x) = Axe^{-x^2/L^2} \tag{14}$$

Where A and L are constants.

Determine the potential energy U(x) of the particle.

Solution:-

The time-independent Schrödinger equation for the wavefunction (x) of a particle of mass m in a potential $U(x)$ is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\,\psi(x) = E\psi(x) \tag{15}$$

When a particle with zero energy has wavefunction (x) given by Eq. (14), it follows on substitution into Eq. (15) that

$$U(x) = \frac{2\hbar^2}{mL^4}\left(x^2 - \frac{3L^2}{2}\right) \tag{16}$$

$U(x)$ is a parabola centred at $x = 0$ with $U(x) = \frac{-3\hbar^2}{mL^2}$.

Problem3:- Photon Energy From a Transition in an Infinite Square Well Potential.

A proton is confined in an infinite square well of width $10\ fm$. (The nuclear potential that binds protons and neutrons in the nucleus of an atom is often approximated by an infinite square well potential.)

1. Calculate the energy and wavelength of the photon emitted when the proton undergoes a transition from the first excited state ($n = 2$) to the ground state ($n = 1$).
2. In what region of the electromagnetic spectrum does this wavelength belong?

Solution:-

1. The energy E_n of a particle of mass m in the nth energy state of an infinite square well potential with width L gives as:

$$E_n = \frac{n^2h^2}{8mL^2} \tag{17}$$

The energy E and wavelength λ of a photon emitted as the particle makes a transition from the $n = 2$ state to the $n = 1$ state are

$$E = E_2 - E_1 = \frac{3h^2}{8mL^2} \tag{18}$$

$$\lambda = \frac{hc}{E} \tag{19}$$

For a proton ($m = 938\ MeV/c^2$), $E = 6.15MeV$ and $\lambda = 202\ f$m. The wavelength is in the gamma ray region of the spectrum.

Problem4:- Wave Functions for a Particle in an Infinite Square Well Potential

A particle with mass m is in an infinite square well potential with walls at $x = -L/2$ and $x = L/2$.
Write the wave functions for the states $n = 1, n = 2$ and $n = 3$.

Solution:-

The normalized wave functions for a particle in an infinite square well potential with walls at $x = 0$ and $x = L$ gives as $\psi_n(x) = \sqrt{\frac{2}{L}} sin\left(\frac{n\pi x}{L}\right)$.To obtain the wavefunctions $\psi_n(x)$ for a particle in an infinite square potential with walls at $x = -L/2$ and $x = L/2$ we replace x in aforementioned Eq. by $x + L = 2$:

$$\psi_n(x) = \sqrt{\frac{2}{L}} sin\left(\frac{n\pi(x + L/2)}{L}\right) \tag{20}$$

Which satisfies $\psi_n(-L/2) = \psi_n(L/2) = 0$ as required. Thus,

$$\psi_1(x) = \sqrt{\frac{2}{L}} cos\left(\frac{\pi x}{L}\right) \tag{21}$$

$$\psi_2(x) = -\sqrt{\frac{2}{L}} sin\left(\frac{2\pi x}{L}\right) \tag{22}$$

$$\psi_2(x) = -\sqrt{\frac{2}{L}} cos\left(\frac{3\pi x}{L}\right) \tag{23}$$

Problem5:- Position Probability for a Particle in an Infinite Square Well Potential

A particle is in the nth energy state $\psi_n(x)$ of an infinite square well potential with width L.

1. Determine the probability $P_n(1/a)$ that the particle is confined to the first $1/a$ of the width of the well.
2. Comment on the *n*-dependence of $P_n(1/a)$.

Solution:-

The wave function $\psi_n(x)$ for a particle in the nth energy state in an infinite square box with walls at $x = 0$ and $x = L$ is

$$\psi_n(x) = \sqrt{\frac{2}{L}} sin\left(\frac{n\pi x}{L}\right) \tag{24}$$

The probability $P_n(1/a)$ that the electron is between $x = 0$ and $x = L$ in the state $\psi_n(x)$is

$$P_n\left(\frac{1}{a}\right) = \int_0^{L/2} |\psi_n(x)|^2 \, dx = \frac{2}{L}\int_0^{L/2} sin^2\left(\frac{n\pi x}{L}\right) dx \\ = \frac{1}{a} - \frac{sin(2n\pi/a)}{2n\pi} \tag{25}$$

$P_n(1/a)$ is the probability that the particle in the state $\psi_n(x)$ is confined to the first $1/a$ of the width of the well. The sinusoidal n-dependent term decreases as n increases and vanishes in the limit of large n:

$$P_n\left(\frac{1}{a}\right) \to \frac{1}{a} \quad as \quad n \to \infty \tag{26}$$

$P_n(1/a) = 1/a$ is the classical result. The above analysis is consistent with the correspondence principle, which may be stated symbolically as

$$\text{quantum physics} \;\; \to \;\; \text{classical physics as } n \to \infty \tag{27}$$

Where n is a typical quantum number of the system.

<u>Problem</u>6:- Energy Levels for a Particle in a Finite Square Well Potential

A particle with energy E is bound in a finite square well potential with height U and width $2L$ situated at $-L \leq x \leq +L$.
The potential is symmetric about the midpoint of the well. The stationary state wave functions are either symmetric or antisymmetric about this point.

1. Show that for $E < U$, the conditions for smooth joining of the interior and exterior wave functions leads to the following equation for the allowed energies of the symmetric wave functions:

$$k\tan kL = \alpha \tag{28}$$

Where

$$\alpha = \sqrt{\frac{2m(E-U)}{\hbar^2}} \tag{29}$$

And

$$k = \sqrt{\frac{2mE}{\hbar^2}} \tag{30}$$

k is the wave number of oscillation in the interior of the well.

2. Show that Eq. (28) can be rewritten as

$$k\sec kL = \frac{\sqrt{2mU}}{\hbar} \tag{31}$$

3. Apply this result to an electron trapped at a defect site in a crystal, modeling the defect as a finite square well potential with height $5\ eV$ and width $200\ pm$.

<u>Solution</u>:-

The wavefunction $\psi(x)$ for a particle with energy E in a potential $U(x)$ satisfies the time-independent Schrödinger equation.
Inside the well ($-L \leq x \leq +L$), the particle is free. The wavefunction symmetric about $x = 0$ is

$$\psi(x) = A\cos kx \quad where\ k = \sqrt{\frac{2mE}{\hbar^2}} \tag{32}$$

Outside the well ($-\infty < x < -L$ and $L < x < \infty$), the potential has constant value $U > E$. The wavefunction symmetric about $x = 0$ is

$$\psi(x) = Be^{-\alpha|x|} \quad where\ \alpha = \sqrt{\frac{2m(U-E)}{\hbar^2}} \tag{33}$$

$\psi\,(x)$ and its derivative are continuous at $x = L$:

$$AcoskL = Be^{-\alpha L} \tag{34}$$

$$AksinkL = B\alpha e^{-\alpha L} \tag{35}$$

From which

$$ktankL = \alpha \tag{36}$$

Or, alternatively,

$$\theta sec\theta = \pm a \tag{37}$$

Where

$$\theta = kL \tag{38}$$

And

$$\alpha = \sqrt{\frac{2mUL^2}{\hbar^2}} \tag{39}$$

Eq. (36) are equations for the allowed values of k. The equation with the positive sign yields values of θ in the first quadrant. The equation with the negative sign yields values of θ in the third quadrant.
Solving Eq. (37) numerically for an electron in a well with $U = 5\,eV$ and $L = 100\,pm$ yields the ground state energy $E = 2.43\,eV$.

Problem7:-Wave Function

An electron is trapped in an infinitely deep potential well of width L = 10^6 fm.
Calculate the wavelength of photon emitted from the transition $E_4 \longrightarrow E_3$.

Solution:-

$$E_n = \frac{n^2h^2}{8mL^2} = \frac{\pi^2n^2\hbar^2c^2}{8mc^2L^2} = \frac{\pi^2 \times (197.3\text{ MeV fm})^2n^2}{2 \times 0.511(\text{MeV}) \times (10^2\text{ fm})^2} = 0.038\,n^2\text{ eV} \tag{40}$$

$$E_1 = 0.038\text{ eV},\; E_2 = 0.152\text{ eV},\; E_3 = 0.342\text{ eV},\;\; E_4 = 0.608\text{ eV}, \tag{41}$$

$$\Delta E_{43} = E_4 - E_3 = 0.608 - 0.342 = 0.266\text{eV} \tag{42}$$

$$\lambda = \frac{1.241}{0.266} = 4.665\text{ nm}$$

Problem8:-Wave Function

If $\psi(x) = \frac{N}{x^2+a^2}$, calculate the normalization constant N.

Solution:-

Normalization condition is

$$\int_{-\infty}^{+\infty} |\psi|^2 dx = 1 \tag{43}$$

$$N^2 \int_{-\infty}^{+\infty} (x^2 + a^2)^{-2} dx = 1 \tag{44}$$

Put $x = a\tan\theta;\, dx = sec2\theta\; d\theta$

$$\left(\frac{2N^2}{a^3}\right)\int_0^{\pi/2} cos^2\theta d\theta = N^2\pi/2a^3 = 1 \tag{45}$$

Therefore,

$$N = \left(\frac{2a^3}{\pi}\right)^{1/2}$$

<u>Problem9</u>:-Wave Function

Find the flux of particles represented by the wave function

$$\psi(x) = A\,e^{ikx} + Be^{-ikx}$$

<u>Solution</u>:-

The flux is

$$J_x = \left(\frac{\hbar}{2im}\right)\left[\psi^*\frac{d\psi}{dx} - \psi\frac{d\psi^*}{dx}\right] \tag{46}$$

$$J_x = \left(\frac{\hbar}{2im}\right)\left[\left(A\,e^{-ikx} + Be^{ikx}\right)ik\left(A\,e^{ikx} - Be^{-ikx}\right) + \left(A\,e^{ikx} + Be^{-ikx}\right)ik\left(A\,e^{-ikx} + Be^{ikx}\right)\right] \tag{47}$$

$$J_x = \left(\frac{\hbar k}{2m}\right)\left[A^2 - B^2 - ABe^{-2ikx} + ABe^{2ikx} + A^2 - B^2 + ABe^{-2ikx} - ABe^{2ikx}\right] = \left(\frac{\hbar k}{m}\right)\left[A^2 - B^2\right] \tag{48}$$

<u>Problem10</u>:-Wave Function

(a) Find the normalized wave functions for a particle of mass m and energy E trapped in a square well of width $2a$ and depth $V_o > E$.

(b) Sketch the first two wave functions in all the three regions. In what respect do they differ from those for the infinite well depth.

<u>Solution</u>:-

(a)

$$\begin{aligned} \psi_1 &= Ae^{\beta x} && (-\infty < x < -a) \\ \psi_2 &= D cos\alpha x && (-a < x < +a) \\ \psi_1 &= Ae^{-\beta x} && (a < x < \infty) \end{aligned} \tag{49}$$

Normalization implies that

$$\int_{-\infty}^{-a} |\psi_1|^2 dx + \int_{-a}^{a} |\psi_2|^2 dx + \int_{a}^{\infty} |\psi_3|^2 dx = 1 \tag{50}$$

$$\int_{-\infty}^{-a} A^2 e^{2\beta x} dx + \int_{-a}^{a} D^2 cos^2\alpha x dx + \int_{a}^{\infty} A^2 e^{-2\beta x} dx = 1 \tag{51}$$

$$A^2\,e^{-2\beta a}/2\beta + D^2[a + sin\,(2\alpha a)/2\alpha] + A^2\,e^{-2\beta a}/2\beta = 1 \tag{52}$$

Or

$$A^2\,e^{-2\beta a}/\beta + D^2[a + sin\,(2\alpha a)/2\alpha] = 1 \tag{53}$$

Boundary condition at $x = a$ gives

$$D cos\alpha a = ae^{-\beta a} \tag{54}$$

Combining (53) and (54) gives

$$D = \left(a + \frac{1}{\beta}\right)^{-1}$$
$$A = e^{\beta a} cos\alpha a \left(a + \frac{1}{\beta}\right)^{-1} \quad (55)$$

(b)The difference between the wave functions in the infinite and finite potential wells is that in the former the wave function within the well terminates at the potential well, while in the latter it penetrates the well.

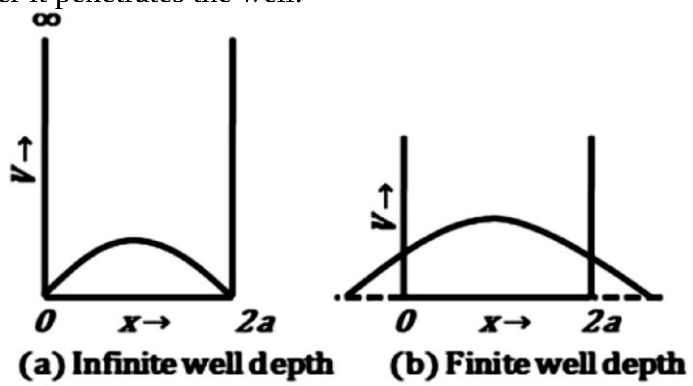


Figure: Wave functions in potential wells of infinite and finite depths.

<u>Problem11</u>:-Wave Function

The state of a free particle is described by the following wave function (Fig. below)

$$\psi(x) = \begin{cases} 0 & x < -3a \\ c & -3a < x < a \\ 0 & x > a \end{cases}$$

(a) Determine c using the normalization condition.

(b) Find the probability of finding the particle in the interval [0, a].

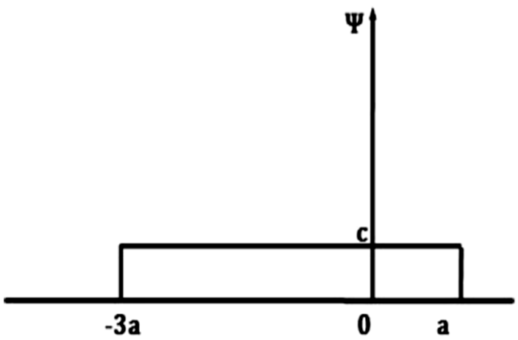


Fig.: Uniform distribution of ψ.

<u>Solution</u>:-

(a)The normalization condition requires

$$\int_{-\infty}^{\infty} |\psi|^2 dx = \int_{-3a}^{a} |c|^2 dx = 1 = 4a\,|c|^2 \quad (56)$$

Therefore, $c = 1/2\sqrt{a}$

(b)The probability is

$$\int_0^a |\psi|^2 dx = \int_0^a c^2 dx = 1/4 \qquad (57)$$

<u>Problem11</u>:-Potential Wells and Barriers

(a) The one-dimensional time-independent Schrödinger equation is

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

Give the meanings of the symbols in this equation.

(b) A particle of mass m is contained in a one-dimensional box of width a.The potential energy $U(x)$ is infinite at the walls of the box ($x = 0$ and $x = a$) and zero in between ($0 < x < a$).
Solve the Schrodinger equation for this particle and hence show that the normalized solutions have the form $\psi_n(x) = \left(\frac{a}{2}\right)^2 sin\left(\frac{n\pi x}{a}\right)$, with energy $E_n = h^2n^2/8ma^2$, where n is an integer ($n > 0$).

(c) For the case $n = 3$, find the probability that the particle will be located in the region $a/3 < x < 2a/3$.

(d) Sketch the wave-functions and the corresponding probability density distributions for the cases n = 1, 2 and 3.

<u>Solution</u>:-

(a) The term $\frac{-\hbar^2 d^2}{2mdx^2}$ is the kinetic energy operator, $U(x)$ is the potential energy operator, $\psi(x)$ is the eigen function and E is the eigen value.

(b)Put $U(x) = 0$ in the region $0 < x < a$ in the Schrödinger equation to obtain

$$\left(\frac{-\hbar^2}{2m}\right)\frac{d^2\psi(x)}{dx^2} = E\psi(x) \qquad (58)$$

Or

$$\frac{d^2\psi(x)}{dx^2} + \left(\frac{2mE}{\hbar^2}\right)\psi(x) = 0 \qquad (59)$$

Writing

$$\alpha^2 = \frac{2mE}{\hbar^2} \qquad (60)$$

Eq. (58) become

$$\frac{d^2\psi(x)}{dx^2} + \alpha^2\psi(x) = 0 \qquad (61)$$

Which has the solution

$$\psi(x) = Asin\alpha x + Bcos\alpha x \qquad (62)$$

Where A and B are constants of integration. Take the origin at the left corner, Fig. below.

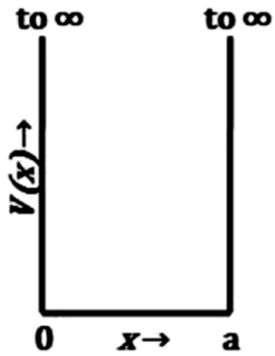


Fig.: Square potential well of infinite depth.

Boundary condition

$$\psi(0) = 0, \quad \psi(a) = 0,$$

The first one gives $B = 0$. We are left with

$$\psi(x) = Asin\alpha x \tag{63}$$

The second one gives

$$\alpha a = n\pi, \qquad n = 1,2,3, \dots \tag{64}$$

$n = 0$ is excluded as it would give a trivial solution.
Using the value of α in Eq. (62).

$$\psi(x) = Asin\left(\frac{n\pi x}{a}\right) \tag{65}$$

This is an unnormalized solution. The constant A is determined from normalization condition.

$$\int_0^a \psi_n^*(x)\psi(x)dx = 1$$

$$A^2\int_0^a sin^2\left(\frac{n\pi x}{a}\right)dx = 1$$

$$\left(\frac{A^2}{2}\right)\left(x - cos\left(\frac{n\pi x}{a}\right)\right)\Big|_0^a = Aa^2 = 1$$

Therefore,

$$A = \left(\frac{2}{a}\right)^{\frac{1}{2}} \tag{66}$$

The normalized wave function is

$$\psi(x) = \left(\frac{2}{a}\right)^{\frac{1}{2}} sin\left(\frac{n\pi x}{a}\right) \tag{67}$$

Using the value of α from (63) in (59), the energy is

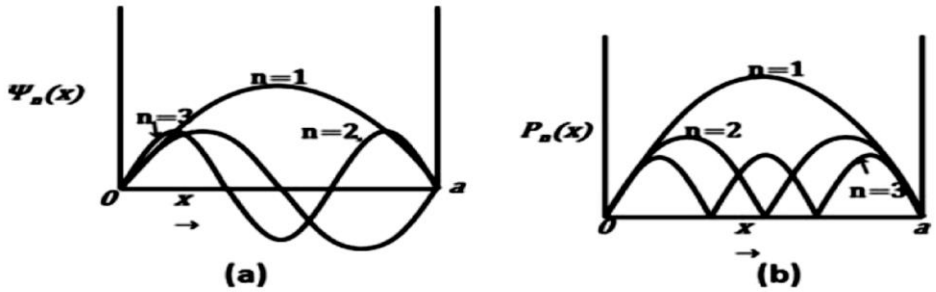
$$E_n = \frac{n^2\hbar^2}{8ma^2} \tag{68}$$

(c) Probability

$$p = \int_0^a |\psi_3(x)|^2 dx = \int_{\frac{a}{3}}^{\frac{2a}{3}} \left(\frac{2}{a}\right) sin^2\left(\frac{3\pi x}{a}\right)dx = \frac{1}{3} \tag{69}$$

(d) $\psi(n)$ and probability density $P(x)$ distributions for $n = 1,2$ and 3 are sketched in

Fig below.



Problem12:-Potential Wells and Barriers

A particle of mass m_e trapped in an infinite depth well of width L = 1nm.
Consider the transition from the excited state n = 2 to the ground state n = 1.
Calculate the wavelength of light emitted. In which region of electromagnetic spectrum does it fall?

Solution:-

Referring to the previous question, the energy of the nth level is

$$E_n = \frac{n^2\hbar^2}{8mL^2} \tag{70}$$

And

$$E_{n+1} = \frac{(n+1)^2\hbar^2}{8mL^2} \tag{71}$$

Therefore,

$$E_{n+1} - E_n = \frac{(2n+1)\hbar^2}{8mL^2} \tag{72}$$

The ground state corresponds to n = 1 and the first excited state to $n = 2, m = 8\, m_e$ and $L = 1nm = 10^6\, fm$. Putting $n = 1$ in (70)

$$hv = E_2 - E_1 = \frac{3\hbar^2}{8mL^2} = \frac{3\pi^2\hbar^2c^2}{16m_ec^2L^2}$$

$$= 3\pi^2(197.3)^2MeV^2.fm^2/(16\times 0.511\ MeV)(10^6)^2fm^2 = 0.14\times 10^{-6}MeV$$
$$= 0.14\ eV$$

$$\lambda(nm) = \frac{1.241}{E(eV)} = \frac{1.241}{0.14} = 8864 \text{ nm}$$

This corresponds to the microwave region of the electro-magnetic spectrum

Problem 13: Explain what was learned about quantization of radiation or mechanical system from the following experiments:

(a) Photoelectric effect.
(b) Black body radiation spectrum.

Solution:-

(a) Photoelectric effect:

This refers to the emission of electrons observed when one irradiates a metal under vacuum with ultraviolet light. It was found that the magnitude of the electric current thus produced is proportional to the intensity of the striking radiation provided that the frequency of the light is greater than a minimum value characteristic of the metal, while the speed of the electrons does not depend on the light intensity, but on its frequency. These results could not be explained by classical physics.

Einstein in 1905 explained these results by assuming light, in its interaction with matter, consisted of corpuscles of energy $h\nu$, called photons. When a photon encounters an electron of the metal it is entirely absorbed, and the electon, after receiving the energy $h\nu$, spends an amount of work W equal to its binding energy in the metal, and leaves with a kinetic energy

$$\frac{1}{2}mv^2 = h\nu - W$$

This quantitative theory of photoelectricity has been completely verified by experiment, thus establishing the corpuscular nature of light.

(b) Black body radiation spectrum.

A black body is one which absorbs all the radiation falling on it. The spectral distribution of the radiation emitted by a black body can be derived from the general laws of interaction between matter and radiation. The expressions deduced from the classical theory are known as Wien law and Rayleigh law. The former is in good agreement with experiment in the short wavelength end of the spectrum only, while the latter is in good agreement with the long wavelength results but leads to divergency in total energy.

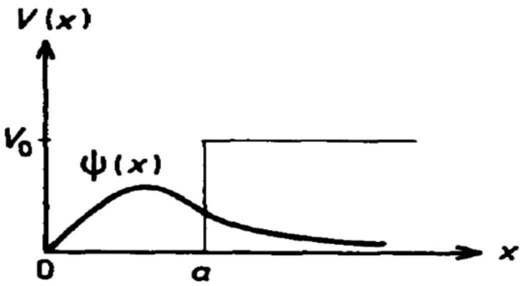
Planck in 1900 succeeded in removing the difficulties encountered by classical physics in black body radiation by postulating that energy exchanges between matter and radiation do not take place in a continuous manner but by discrete and indivisible quantities, or quanta, of energy. He showed that by assuming that the quantum of energy was proportional to the frequency, $E = h\nu$, he was able to obtain an expression for the spectrum which is in complete agreement with experiment:

$$E_\nu = \frac{8\pi h\nu^3}{c^3}\frac{L}{e^{\frac{h\nu}{kT}} - 1}$$

where h is a universal constant, now known as Planck constant. Planck hypothesis has been confirmed by a whole array of elementary processes and it directly reveals the existence of discontinuities of physical processes on the microscopic scale, namely quantum phenomena.

Problem 14: Consider the one-dimensional problem of a particle of mass m in a potential (See Figure below)

$$V = \begin{cases} \infty & x < 0, \\ 0 & 0 \leq x \leq a, \\ V_0 & x > a, \end{cases}$$



(a) Show that the bound state energies ($E < V_0$) are given by the equation

$$\tan\sqrt{\frac{2mEa}{\hbar}} = -\sqrt{\frac{E}{V_0 - E}}$$

(b)Without solving any further, sketch the ground state wave function.

Solution:-

(a) The Schrödinger equations for the two regions are

$$\psi'' + \frac{2mE\psi}{\hbar^2} = 0, \qquad 0 \le x \le a,$$

$$\psi'' - \frac{2m(V_0 - E)\psi}{\hbar^2} = 0, \qquad x > a,$$

with respective boundary conditions $\psi = 0$ for $x = 0$ and $\psi \to 0$ for $x \to +\infty$. The solutions for $E < V_0$ are then

$$\psi = sin(2mEx/\hbar), \qquad 0 \le x \le a,$$

$$\psi = Ae^{-\sqrt{2m(V_0-E)x/\hbar}}, \qquad x > a,$$

where A is a constant. The requirement that ψ and ψ' are continuous at $x = a$ gives

$$tan\sqrt{\frac{2mEa}{\hbar}} = -\sqrt{\frac{E}{V_0 - E}}$$

(b) The ground-state wave function is as shown in Fig. above.

Problem 15: The dynamics of a particle moving one-dimensionally in a potential $V(x)$ is governed by the Hamiltonian $H_0 = p^2/2m + V(x)$, where $p = -i\hbar d/dx$ is the momentum operator. Let $E_n^0, n = 1,2,3, \ldots$, be the eigenvalues H_0 . Now consider a new Hamiltonian $H = H_0 + \lambda p/m$, where λ is a given parameter. Given A, m and E_n^0,), find the eigenvalues of H.

Solution:-

The new Hamiltonian is

$$H = H_0 + \lambda p/m = p^2/2m + \lambda p/m + V(x),$$
$$= (p + \lambda)^2/2m + V(x) - \lambda^2/2m,$$

Or

$$H' = \frac{p'^2}{2m} + V(x),$$

Where $H' = H + \frac{\lambda^2}{2m}, p' = p + \lambda,$

The eigenfunctions and eigenvalues of H' are respectively E_n^0 and ψ_n^0.

AS the wave number is $k' = \frac{p'}{\hbar} = \frac{1}{\hbar}(p + \lambda)$,the new eigenfunction are

$$\psi = \psi^0 e^{-\lambda x/\hbar}$$

and the corresponding eigenvalues are

$$E_n = E_n^0 - \lambda^2/2m.$$

Problem 16: Use the uncertainty principle to obtain the ground state energy of a linear Oscillator.

Solution:-

$$\Delta x \Delta p \sim \hbar/2$$

$$p = \frac{\hbar}{2x}$$

$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

$$E = \frac{\hbar^2}{8mx^2} + \frac{1}{2}m\omega^2 x^2$$

The ground state energy is obtained by setting $\frac{\partial E}{\partial x} = 0$

$$\frac{\partial E}{\partial x} = -\frac{\hbar^2}{4mx^3} + m\omega^2 x = 0$$

Whence $x^2 = \frac{\hbar}{2m\omega}$

$$\therefore E = 1/4\hbar\omega + 1/4\hbar\omega = \frac{1}{2}\hbar\omega$$

Problem 17: Consider a particle of mass *m* trapped in a potential well of finite depth V_o.

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

Discuss the solutions and eigen values for the class I and II solutions graphically.

Solution:-

Consider a finite potential well. Take the origin at the centre of the well.

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

$$\frac{d^2\psi}{dx^2} + \left(\frac{2m}{\hbar^2}\right)[E - V(r)]\psi = 0$$

Region 1 $(E < V_o)$

$$\frac{d^2\psi}{dx^2} - \left(\frac{2m}{\hbar^2}\right)[V_o - E]\psi = 0 \qquad (1)$$

$$\frac{d^2\psi}{dx^2} - \beta^2\psi = 0 \qquad (2)$$

Where $\beta^2 = \left(\frac{2m}{\hbar^2}\right)(V_o - E)$ (3)

$$\psi_1 = Ae^{\beta x} + Be^{-\beta x} \qquad (4)$$

where A and B are constants of integration.

Since x is negative in region 1, and ψ_1 has to remain finite we must set $B = 0$, otherwise the wave function grows exponentially. The physically accepted solution is

$$\psi_1 = Ae^{\beta x} \qquad (5)$$

Region 2; $(V = 0)$

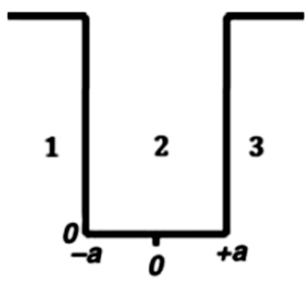


Fig: Square potential well of finite depth.

$$\frac{d^2\psi}{dx^2} + \left(\frac{2mE}{\hbar^2}\right)\psi = 0$$

$$\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0 \qquad (6)$$

With $\alpha^2 = \frac{2mE}{\hbar^2}$ (7)

$$\psi_2 = Csin\alpha x + Dcos\alpha x \qquad (8)$$

odd even

In this region either odd function must belong to a given value E or even function, but not both,

Region 3; ($E < V_o$)

Solution will be identical to (Eq. 4)

$$\psi_3 = Ae^{\beta x} + Be^{-\beta x}$$

But physically accepted solution will be

$$\psi_3 = Be^{-\beta x} \tag{9}$$

Because we must put $A = 0$ in this region where x takes positive values if the wave function has to remain finite.

Class I ($C = 0$)

$$\psi_2 = Dcos\alpha x \tag{10}$$

Boundary conditions

$$\psi_2(a) = \psi_3(a) \tag{11}$$

$$d\psi_2/dx|_{x=a} = d\psi_3/dx|_{x=a} \tag{11a}$$

These lead to

$$Dcos\alpha x = Be^{-\beta x} \tag{12}$$

$$-D\alpha cos\alpha x = -B\beta e^{-\beta a} \tag{13}$$

Dividing (13) by (12)

$$\alpha tan\alpha a = \beta \tag{14}$$

Class II ($D = 0$)

$$\psi_2 = Csin\,\alpha x \tag{15}$$

Boundary conditions:

$$\psi_2(-a) = \psi_1(a) \tag{16}$$

$$d\psi_2/dx|_{x=-a} = d\psi_1/dx|_{x=-a} \tag{17}$$

These lead to

$$Csin(-\alpha a) = -Csin(\alpha a) = Ae^{\beta a} \tag{18}$$

$$C\alpha cos(\alpha x) = A\beta e^{\beta a} \tag{19}$$

Dividing (19) by (18)

$$\alpha cot(\alpha a) = -\beta \tag{20}$$

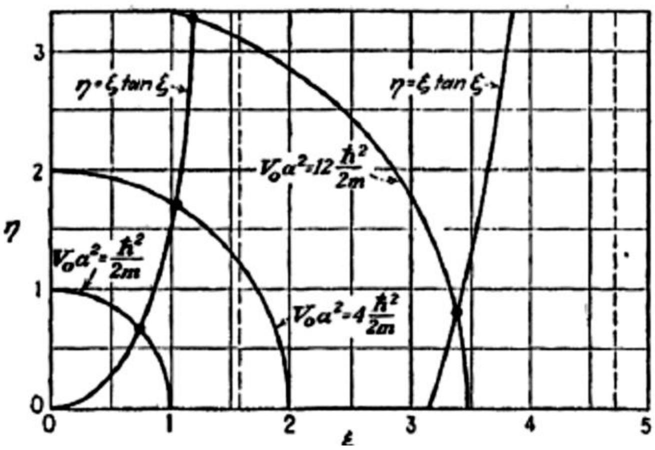


Fig.: $\eta - \xi$ curves for class I solutions. For explanation see the text.

Note that from (15) and (2), $\alpha^2 = -\beta^2$, which is absurd because this implies that $\alpha^2 + \beta^2 = 0$ that is $2mV_o/\hbar^2 = 0$, but $V_o = 0$. This simply means that class I and class II solutions cannot coexist

Energy levels:
Class I: set $\xi = \alpha a$; $\eta = \beta a$
where α and β are positive.
Equation (15) then becomes

$$\xi tan\xi = \eta \qquad (21)$$

with $\xi^2 + \eta^2 = a^2(\alpha^2 + \beta^2) = 2mV_o a^2/\hbar^2 = constant \qquad (22)$

The energy levels are determined from the intersection of the curve $\xi tan\xi$ plotted against η with the circle of known radius $\left(\frac{2mV_o a^2}{\hbar^2}\right)^{1/2}$, in the first quadrant since ξ and η are restricted to positive values.
The circles, Eq. (22), are drawn for $V_o a^2 = \hbar^2/2m,\ 4\hbar^2/2m,$ and $9\hbar^2/2m.$ for curves 1, 2 and 3 respectively Fig 3.9. For the first two values there is only one solution while for the third one there are two solutions.
For class II, energy levels are obtained from intersection of the same circles with the curves of $-\xi cot\xi$ in the first quadrant, Fig above.
Curve (1) gives no solution while the other two yield one solution each.
Thus the three values of $V_o a^2$ in the increasing order give, one, two and three energy levels, respectively. Note that for a given particle mass the energy levels depend on the combination $V_o a^2$. With the increasing depth and/or width of the potential well, greater number of energy levels can be accommodated.
For $\xi = 0$ to $\pi/2$, that is $V_o a^2$ between 0 and $\pi^2\hbar^2/8m$ there is just one level of class I

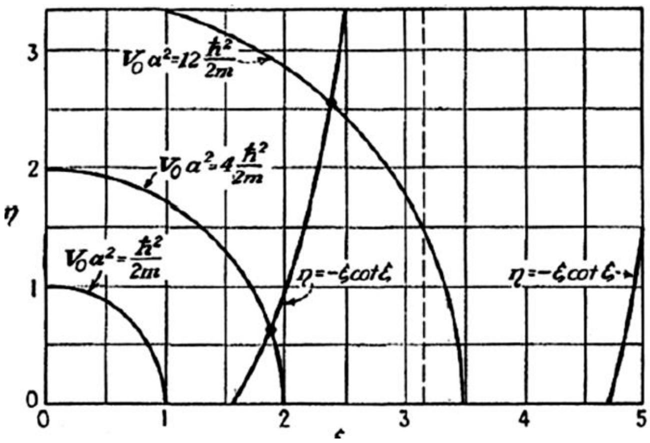


Fig.: η − ξ curves for class II solutions. For explanation see the text.

For $V_o a^2$ between $2\pi^2\hbar^2/8m$ and $4\pi^2\hbar^2/8m$ *m* there is one energy level of each class or two altogether. As $V_o a^2$ increases, energy levels appear successively first of one class and next of the other.

Problem 18: Consider a stream of particles with energy E travelling in one dimension from $x = -\infty$ to ∞. The particles have an average spacing of distance L. The particle stream encounters a potential barrier at *x* = 0. The potential can be written as

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

Suppose the particle energy is smaller than the potential barrier, i.e., $< V_b$.

(a) For each of the three regions, write down Schrodinger's equation and calculate the wave-function ψ and its derivative $d\psi/dx$.

Use the constants to represent the amplitude of the reflected and transmitted particle streams respectively and take

$$k_1^2 = \frac{2mE}{\hbar^2} \text{ and } k_2^2 = \frac{2m(V_b - E)}{\hbar^2}$$

(b) At the boundaries to the potential barrier, ψ and $d\psi/dx$ must be continuous.Equate the solutions that you have at $x = 0$ and x =a and manipulate these equations to derive the following expression for the transmission amplitude.

$$\tau = \frac{4ik_1k_2e^{-ik_1a}}{[(ik_1 - k_2)^2e^{-k_2a}] - [(ik_1 - k_2)^2e^{k_2a}]}$$

Solution:- Schrodinger's equation in one dimension

(a) $\frac{d^2\psi}{dx^2} + \left(\frac{2m}{\hbar^2}\right)(E - V)\psi = 0$

Region 1: $(x < 0)\ V = 0;\ \frac{d^2\psi}{dx^2} + k_1^2\psi = 0$

where $k_1^2 = \frac{2mE}{\hbar^2}$

Solution: $\psi_1 = \exp(ik_1x) + A\exp(-ik_1x)$

Region 2: $(0 < x < a)\ V = V_b;\ \frac{d^2\psi}{dx^2} - k_2^2\psi = 0$

where $k_2^2 = \frac{2m}{\hbar^2}(V_b - E)$

Solution: $\psi_2 = \mathrm{B}\exp(k_2x) + C\exp(-k_2x)$

Region 3: $(x > 0)\ V = 0;$

Solution: $\psi_3 = \mathrm{D}\exp(ik_1x)$

(b) Boundary conditions:

$$\psi_1(0) = \psi_2(0) \to 1 + A = B + C \qquad (1)$$

$$\frac{d\psi_1}{dx}\Big|_{x=0} = \frac{d\psi_2}{dx}\Big|_{x=0} \to ik_1(1 - A) = k_2(B - C) \qquad (2)$$

$$\psi_2(a) = \psi_3(a) \to \mathrm{B}\exp(k_2a) + C\exp(-k_2a) = \mathrm{D}\exp(ik_1a) \qquad (3)$$

$$\frac{d\psi_2}{dx}\Big|_{x=a} = \frac{d\psi_3}{dx}\Big|_{x=a} \to k_2(\mathrm{B}\exp(k_2a) - C\exp(-k_2a)) = ik_1\mathrm{D}\exp(ik_1a) \qquad (4)$$

Eliminate A between (1) and (2) to get

$$\mathrm{B}(k_2 - ik_1) - C(k_2 + ik_1) = 2ik_1 \qquad (5)$$

Eliminate D between (3) and (4) to get

$$k_2(\mathrm{B}\exp(k_2a) - C\exp(-k_2a)) = ik_1(\mathrm{B}\exp(k_2a) - C\exp(-k_2a)) \qquad (6)$$

Solve (5) and (6) to get

$$B = \frac{2ik_1(k_2+ik_1)}{[(k_2+ik_1)^2 - e^{2k_2a}(k_2-ik_1)^2]} \qquad (7)$$

$$C = \frac{2ik_1(k_2-ik_1)e^{2k_2a}}{[(k_2+ik_1)^2 - e^{2k_2a}(k_2-ik_1)^2]} \qquad (8)$$

Using the values of B and C in (3),

$$\tau = D = \frac{4ik_1k_2e^{-ik_1a}}{[(ik_1-k_2)^2e^{-k_2a}] - [(ik_1-k_2)^2e^{k_2a}]} \qquad (9)$$

Problem 19: In Problem above,

(a) Show that the fraction of transmitted particles is given by $F_{trans} = \tau^* \tau$ which when calculated evaluates to

$$F_{trans} = \left[1 + \frac{V_b^2 sinh^2(k_2 a)}{4E(V_b - E)}\right]^{-1}$$

(b) How would F_{trans} vary if $E > V_b$

Solution: - (a)

$$F_{trans} = \tau^* \tau = |D|^2 = 16\frac{k_1^2 k_2^2}{(k_1^2 + k_2^2)^2(e^{2k_2 a} + e^{-2k_2 a}) - 2(k_2^4 - 6k_2^2 k_1^2 + k_1^4)}$$

$$F_{trans} = T = 16\frac{4k_1^2 k_2^2}{(k_1^2+k_2^2)^2 sinh^2(k_2 a) + 4k_1^2 k_2^2} \qquad (10)$$

The expression simplifies to

Use $k_1^2 = 2mE/\hbar^2$ and $k_2^2 = 2m(V_b - E)/\hbar^2$

The reflection coefficient R is obtained by substituting (7) and (8) in (1) to find the value of A. After similar algebraic manipulations we find

$$R = |A|^2 = \frac{(k_1^2+k_2^2)^2 sinh^2(k_2 a)}{(k_1^2+k_2^2)^2 sinh^2(k_2 a) + 4k_1^2 k_2^2} \qquad (11)$$

Note that $R + T = 1$

When $E > V_b, k_2$ becomes imaginary and

$$\sinh(k_2 a) = i \sinh(k_2 a) \qquad (12)$$

Using (11) in (9) and noting $k_1^2 + k_2^2 = \frac{2mV_b}{\hbar^2}$

$$k_2^2 = \frac{2mV_b}{\hbar^2}$$

And $k_1^2 k_2^2 = \left(\frac{2m}{\hbar^2}\right)^2 E(V_b - E)$

We find

$$T = \frac{1}{1 + \frac{V_b^2 sinh^2(k_2 a)}{4E(E - V_b)}} \qquad (13)$$

And

$$R = \frac{1}{1 + \frac{4E(E - V_b)}{V_0^2 sinh^2(k_2 a)}} \qquad (14)$$

A typical graph for T versus $\frac{E}{V_b}$ is shown in Fig. above.

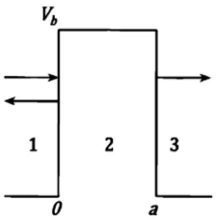


Fig. Transmission through a rectangular Potential barrier.

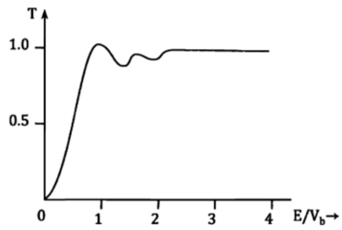


Fig. Transmission as a function of $\frac{E}{V_b}$

Problem 20: A particle of mass m is moving in a region where there is a potential step at $x = 0$: $V(x) = 0$ for $x < 0$ and $V(x) = U_o$ (a positive constant) $x \geq 0$

(a) Determine $\psi(x)$ separately for the regions $x \ll 0$ and $x \gg 0$ for the cases:

(i) $U_o < E$

(ii) $U_o > E$

(b) Write down and justify briefly the boundary conditions that $\psi(x)$ must satisfy at the boundary between the two adjacent regions. Use these conditions to sketch the form of $\psi(x)$ in the region around $= 0$ for the cases (i) and (ii).

Solution:- (a) Case (i) $U_o < E$ region $x \ll 0$

Putting $V(x) = 0$, Schrödinger's equation is reduced to

$$\frac{d^2\psi}{dx^2} + \left(\frac{2mE}{\hbar^2}\right)\psi = 0 \quad (1)$$

which has the solution

$$\psi_1 = Aexp(ik_1x) + Bexp(-ik_1x) \quad (2)$$

Where $k_1^2 = \frac{2mE}{\hbar^2}$ (3)

ψ_1 represents the incident wave moving from left to right (first term in (2)) plus the reflected wave (second term in (2)) moving from right to left

Region $x \gg 0$: $\frac{d^2\psi}{dx^2} + \left[\frac{2m(E-U_o)}{\hbar^2}\right]\psi = 0$ (4)

which has the physical solution

$$\psi_2 = Cexp(ik_2x) \quad (5)$$

Where $k_2^2 = \frac{2m(E-U_o)}{\hbar^2}$ (6)

It represents the transmitted wave to the right with reduced amplitude.

Note that the second term is absent in (5) as there is no reflected wave in the region $x > 0$

Case (ii), $U_o > E$

Region $x < 0$

$$\psi_3 = Aexp(ik_1x) + Bexp(-ik_1x) \quad (7)$$

Region $x > 0$

$$\frac{d^2\psi}{dx^2} - \frac{2m\psi(E-U_o)}{\hbar^2} = 0$$

$$\frac{d^2\psi}{dx^2} - \alpha^2\psi = 0$$

$$\psi_4 = Cexp(-\alpha^2x) + Dexp(\alpha^2x)$$

ψ must be finite everywhere including at $x = -\infty$. We therefore set $D = 0$. The physically accepted solution is then

$$\psi_4 = Cexp(-\alpha^2x) \quad (8)$$

(b) The continuity condition on the function and its derivative at $x = 0$ leads to Eqs. (9) and (10).

$$\psi_3(0) = \psi_4(0)$$

$$A + B = C \quad (9)$$

$$\frac{d\psi_3}{dx}\Big|_{x=0} = \frac{d\psi_4}{dx}\Big|_{x=0}$$

$$ik_1(A - B) = -C\alpha \quad (10)$$

Dividing (10) by (9) gives

$$\frac{ik_1(A-B)}{A+B} = -\alpha \quad (11)$$

Diagrams for ψ at around $x = 0$

(c)

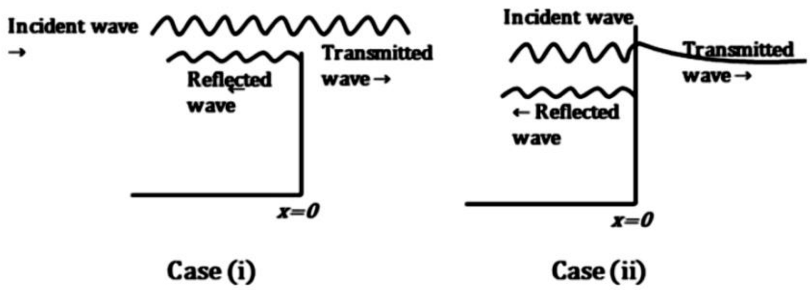
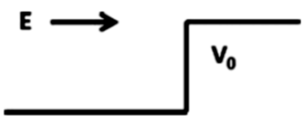


Fig. The sketch of the wave form $\psi(x)$ in case (i) & case (ii).

Problem 21: A steady stream of particles with energy $E(> V_o)$ is incident on a potential step of height V_o as shown in Fig. below.
The wave functions in the two regions are given by
$\psi_1(x) = A_o exp(ik_1x) + Aexp(-ik_1x)$
$\psi_2(x) = Bexp(ik_2x)$
Write down expressions for the quantities k_1 and k_2 in terms of E and V_o. Show that
$A = \left[\frac{k_1-k_2}{k_1+k_2}\right] A_o$ and $B = \left[\frac{2k_1}{k_1+k_2}\right] A_o$
and determine the reflection and transmission coefficients in terms of k_1 and k_2.
If $E = 4V_o/3$ show that the reflection and transmission coefficients are $1/9$ and $8/9$ respectively.
Comment on why $A^2 + B^2$ is not equal to 1.

Fig. Potential step



Solution:-

$k_1 = \left(\frac{2mE}{\hbar^2}\right)^{1/2}; \; k_2 = \left(\frac{2m(E-V_o)}{\hbar^2}\right)^{1/2}$ (1)

Boundary conditions at $x = 0$

$\psi_1(0) = \psi_2(0)$

$\frac{d\psi_1}{dx}\Big|_{x=0} = \frac{d\psi_2}{dx}\Big|_{x=0}$ (2)

These lead to

$A_o + A = B$ (3)

$ik_1(A_o - A) = ik_2B$

Or

$k_1(A_o - A) = k_2B$ (4)

Solving (3) and (4)

A=$\left[\frac{k_1-k_2}{k_1+k_2}\right] A_o$ (5)

B=$\frac{2k_1}{k_1+k_2} A_o$ (6)

Reflection coefficient,

$R = \frac{|A|^2}{|A_o|^2} = \frac{(k_1-k_2)^2}{(k_1+k_2)^2}$ (7)

Transmission coefficient,

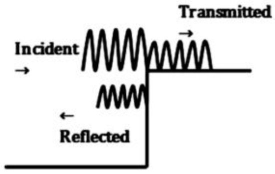
$T = \left(\frac{k_2}{k_1}\right)\frac{|B|^2}{|A_o|^2} = \frac{4k_1k_2}{(k_1+k_2)^2}$ (8)

Substituting the expressions for k_1 and k_2 from (1) and putting $E = 4V_o/3$
We find that $R = 1/9$ and $T = 8/9$.

From (7) and (8) it is easily verified that

$R + T = 1$

Fig. Graphs for probability density.



This is a direct result of the fact that the current density is constant for a steady state. Thus $|A_o|^2 v_1 = |A|^2 v_1 + |B|^2 v_2$

Where $v_1 = \frac{k_1 \hbar}{m}$ and $v_2 = \frac{k_2 \hbar}{m}$

$A^2 + B^2 \neq 1$ because the sum of the intensities of the reflected intensity and transmitted intensities does not add up to unity. What is true is relation (9) which is relevant to current densities

Problem 22:

(a)What boundary conditions do wave-functions obey?

A particle confined to a one-dimensional potential well has a wave-function given by

$$\psi(x) = 0 \quad \text{for} \quad x < -L/2$$
$$\psi(x) = A\cos\left(\frac{3\pi x}{L}\right) \quad \text{for} \quad -L/2 \leq x \leq L/2$$
$$\psi(x) = 0 \quad \text{for} \quad x > L/2$$

(b) Sketch the wave-function $\psi(x)$.

(c) Calculate the normalization constant A.

(d) Calculate the probability of finding the particle in the interval $-L/4 \leq x \leq L/4$

(e) By calculating $\frac{d^2\psi}{dx^2}$ and writing the Schrodinger equation as

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

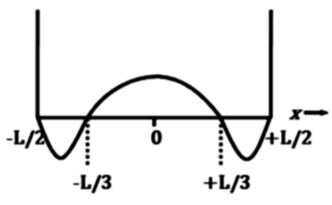
Show that the energy E corresponding to this wave-function is $\frac{9\pi^2\hbar^2}{2mL^2}$.

Solution:-

(a) The wave function must be finite, single-valued and continuous. At the boundary this is ensured by requiring the magnitude and the first derivative be equal.

(b)

Fig. Sketch of $\psi \sim cos\left(\frac{3\pi x}{L}\right)$



(c) $\int_{-\frac{L}{2}}^{\frac{L}{2}} |\psi|^2 dx = A^2 \int_{-\frac{L}{2}}^{\frac{L}{2}} cos^2 \frac{3\pi x}{L} dx = 1$

Or

$$A^2 \int_{-\frac{L}{2}}^{\frac{L}{2}} (1 + \cos 6\pi x/L) dx = A^2 L = 1$$

Therefore $A = 1/\sqrt{L}$

(d) $P\left(-\frac{L}{4}<x<\frac{L}{4}\right)=A^2\int_{-\frac{L}{4}}^{\frac{L}{4}}cos^2\left(\frac{3\pi x}{L}\right)dx=\left(\frac{1}{L}\right)\int_{-\frac{L}{4}}^{\frac{L}{4}}\frac{1}{2}\left(1+cos\left(\frac{6\pi x}{L}\right)\right)dx=$
$\frac{1}{4}+\frac{1}{6\pi}=0.303$

(e) $\frac{d^2\psi}{dx^2}=\frac{d^2}{dx^2}\,A\cos\left(\frac{3\pi x}{L}\right)=-9\pi^2\left(\frac{A}{L}\right)\cos\left(\frac{3\pi x}{L}\right)=-\left(\frac{9\pi^2}{L}\right)\psi$

Therefore, $\left(-\frac{\hbar^2}{2m}\right)\left(\frac{d^2\psi}{dx^2}\right)=-\left(\frac{9\pi^2\hbar^2}{2mL}\right)\psi-E\psi$

Or

$$E=\frac{9\pi^2\hbar^2}{2mL}$$

Problem 23:

(a) Sketch the one-dimensional "top hat" potential
(1) $V=0$ for $x<0$;
(2) $V=W$ constant, for $0\le x\le L$;
(3) $V=0$ for $x<L$;

(b) Consider particles, of mass m and energy $E<W$ incident on this potential barrier from the left ($x<0$). Including possible reflections from the barrier boundaries, write down general expressions for the wavefunctions in these regions and the form the time-independent Schrodinger equation takes in each region. What ratio of wavefunction amplitudes is needed to determine the transmission coefficient?

(c) Write down the boundary conditions for ψ and $d\psi/dx$ at $x=0$ and $x=L$.

(d) A full algebraic solution for these boundary conditions is time consuming. In the approximation for a tall or wide barrier, the transmission coefficient T is given by $T=16\left(\frac{E}{W}\right)\left(1-\frac{E}{W}\right)e^{-2\alpha L}$, where $\alpha^2=2m\left(\frac{W-E}{\hbar^2}\right)^2$
Determine T T for electrons of energy $E=2eV$, striking a potential of value $W=5eV$ and width $L=0.3nm$.

(e) Describe four examples where quantum mechanical tunneling is observed.

Solution:-

(a)

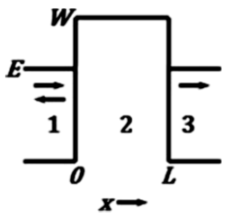


Fig. Penetration of a rectangular barrier.

(b) Region 1, $x<0$

$\frac{d^2\psi}{dx^2}+k^2\psi=0$

With $k^2=\frac{2mE}{\hbar^2}$

$\psi_1=Ae^{ik_1x}+Be^{-ik_1x}$

Incident reflected at $x=0$

Region 2, $0<x<L$

$\frac{d^2\psi}{dx^2}-\alpha^2\psi=0$

With $\alpha^2 = \frac{2m(W-E)}{\hbar^2}$
$\psi_2 = Ce^{-\alpha x} + De^{\alpha x}$
Region 3, $x > L$
$\frac{d^2\psi}{dx^2} + k^2\psi = 0$
With $k^2 = \frac{2mE}{\hbar^2}$
$\psi_3 = Fe^{ik_1x}$
The second term is absent as there is no reflected wave coming from right to left

The transmission coefficient $T = \frac{|F|^2}{|A|^2}$

(c) Boundary conditions
$\psi_1(0) = \psi_2(0)$
$\frac{d\psi_1}{dx}\Big|_{x=0} = \frac{d\psi_2}{dx}\Big|_{x=0}$
$\psi_2(L) = \psi_3(L)$
$\frac{d\psi_1}{dx}\Big|_{x=L} = \frac{d\psi_2}{dx}\Big|_{x=L}$

(d) $T = 16\left(\frac{E}{W}\right)\left(1-\frac{E}{W}\right)e^{-2\alpha L}$
$\alpha^2 = 2m\left(\frac{W-E}{\hbar^2}\right) \to \alpha = \frac{\sqrt{2mc^2(W-E)}}{\hbar c} = \frac{\sqrt{2\times0.511\times(5-2)\times10^{-6}}}{197.3\times10^{-15}} = 8.8748 \times 10^9\ m^{-1}$

Therefore $2\alpha L = 2 \times 8.8748 \times 10^9 \times 0.3 \times 10^{-9} = 5.3249$
$T = 16\left(\frac{2}{5}\right)\left(1-\frac{2}{5}\right)e^{-5.3249} = 0.0187$

(e) Examples of quantum mechanical tunneling
(i) $\alpha - decay$ Observed $\alpha - energy$ may be $\sim$ 5MeV although the Coulomb barrier height is 20 or 30MeV
(ii) *Tunnel diode.*
(iii) *Josephson effect* :In superconductivity electron emission in pairs through insulator is possible via tunneling mechanism
(iv) *Inversion spectral line* in ammonia molecule. This arises due to tunneling through the potential barrier between two equilibrium positions of the nitrogen atom along the axis of the pyramid molecule which is perpendicular to the plane of the hydrogen atoms. The oscillation between the two equilibrium positions causes an intense spectral line in the microwave region.

Problem 24: Show that the wavefunction $\psi_o(x) = A\,exp(-x^2/2a^2)$ is a solution to the time- independent Schrodinger equation for a simple harmonic oscillator (SHO) potential.

$$\left(-\frac{\hbar^2}{2m}\right)\frac{d^2\psi}{dx^2} + \left(\frac{1}{2}\right)m\omega_o x^2\psi = E\,\psi$$

with energy $E_o = \left(\frac{1}{2}\right)\hbar\omega_o$, and determine a in terms of m and ω_o.
The corresponding dimensionless form of this equation is

$$-\frac{d^2\psi}{dR^2}+R^2\psi=\varepsilon E$$
where $R = x/a$ and $\varepsilon = E/E_o$.
Show that putting $\psi(R)=AH(R)exp(-R^2/2)$ into this equation leads to Hermite's equation
$$-\frac{d^2H}{dR^2}-2R\left(\frac{dH}{dR}\right)+(\varepsilon-1)H=0$$
$H(R)$ is a polynomial of order n of the form $a_nR_n+a_n-2\,R_n-2+a_n-4\,R_n-4+\ldots$
Deduce that ε is a simple function of n and that the energy levels are equally spaced.

Solution:-
By substituting $\psi(R) = AH(R)\,exp\,(-R^2/2)$ in the dimensionless form of the equation and simplifying we easily get the Hermite's equation.
The problem is solved by the series method
$H = \Sigma H_n(R) = \Sigma_{n=0,2,4} a_n\,R_n$
$$\frac{dH}{dR}=a_nnR^{n-1}$$
$$\frac{d^2H}{dR^2}=\sum n(n-1)\,a_nR^{n-2}$$
$\Sigma n(n-1)a_nR^{n-2} - 2\Sigma a_nnR^n + (\varepsilon-1)\Sigma a_nR^n = 0$
Equating equal power of R_n
$$a_{n+2}=\frac{[2n-(\varepsilon-1)]a_n}{(n+1)(n+2)}$$
If the series is to terminate for some value of n then
$2n-(\varepsilon-1)=0$ because $a_n=0$. This gives $\varepsilon=2n+1$
Thus ε is a simple function of n
$E = \varepsilon E_o = (2n+1)1/2\hbar\omega, n = 0,2,4,\ldots$
$= 1/2\hbar\omega, 3\hbar\omega/2, 5\hbar\omega/2,\ldots$
Thus energy levels are equally spaced.

Problem 25: Show that for a simple harmonic oscillator in the ground state the probability for finding the particle in the classical forbidden region is approximately 16%.

Solution:-
$$u_o=\left[\frac{\alpha}{\sqrt{\pi}}\right]e^{-\zeta^2/2}H_o(\zeta);\zeta=\alpha x$$
$$P=1-\int_{-a}^{a}|u_o|^2\,dx=1-2\int_0^a\left(\alpha/\sqrt{\pi}\right)^2e^{-\zeta^2/2}\,dx=1-\frac{2}{\sqrt{\pi}}\int_0^{\alpha a}e^{-\zeta^2/2}d\zeta$$
$$E_o=1/2\,ka^2=\frac{\hbar\omega}{2}(n=0)$$
Therefore $a^2=\frac{\hbar\omega}{k}=\left(\frac{\hbar}{k}\right)\left(\frac{k}{m}\right)^{1/2}=\frac{\hbar}{\sqrt{km}}=\frac{1}{\alpha^2}$
Therefore $\alpha^2a^2=1$ or $\alpha a=1$
$$P=1-\frac{2}{\sqrt{\pi}}\int_0^1e^{-\zeta^2/2}d\zeta=1-\frac{2}{\sqrt{\pi}}\int_0^1\left[1-\zeta^2+\frac{\zeta^4}{2!}-\frac{\zeta^6}{3!}+\frac{\zeta^8}{4!}-\cdots\right]d\zeta$$

$$= 1 - \frac{2}{\sqrt{\pi}}\left[1 - \frac{1}{3} + \frac{1}{10} - \frac{1}{42} + \frac{1}{418} - \cdots\right] \approx 0.16$$

Therefore, $p \approx 16\%$.

Fig. Probability of the particle found outside the classical limits is shown shaded.

Problem 26: Show that when $n \to \infty$ the quantum mechanical simple harmonic oscillator gives the same probability distribution as the classical one.

Solution:-

The probability distribution for the quantum mechanical simple harmonic oscillator (S.H.O) is

$$P(x) = |\psi|^2 = \frac{\alpha exp(-\zeta^2)H_n^2(\zeta)}{\sqrt{\pi}\, 2^n n!} \quad (1)$$

$\zeta = \alpha x;\ \alpha^4 = mk/\hbar^2$

Stirling approximation gives

$$n! \to (2n\pi)^{1/2} n^n e^{-n} \quad (2)$$

Furthermore the asymptotic expression for Hermite function is

$$H_n(\zeta)(\text{for } n \to \infty) \to 2^{n+1}\frac{(n/2e)^{\frac{n}{2}}}{\sqrt{2cos\beta}} exp(n\beta^2) cos\left[(2n + {}^1\!/_2)\beta - \frac{n\pi}{2}\right] \quad (3)$$

Where $sin\beta = \zeta/\sqrt{2n}$ (4)

Using (2) and (3) in (1)

$$P(x) \to 2\alpha exp(-\zeta^2) exp(2n\beta^2)\frac{cos^2\left[(2n + {}^1\!/_2)\beta - \frac{n\pi}{2}\right]}{\pi\sqrt{2n}\, cos\beta}$$

But $\langle cos^2\left[(2n + {}^1\!/_2)\beta - \frac{n\pi}{2}\right]\rangle = \frac{1}{2}$

Therefore $P(x) = \frac{\alpha exp(-\zeta^2) exp(2n\beta^2)}{\pi\sqrt{2n}\, cos\beta}$. (5)

Classically, $E = \frac{ka^2}{2} = \left(n + \frac{1}{2}\right)\hbar\omega$ (quantum mechanically) $\approx n\hbar\omega (n \to \infty)$

Therefore $a^2 = \frac{2n\hbar\omega}{k} = \left(\frac{2n\hbar}{k}\right)\left(\frac{k}{m}\right)^{1/2} = \frac{2n\hbar}{\sqrt{km}} = \frac{2n}{\alpha^2}$

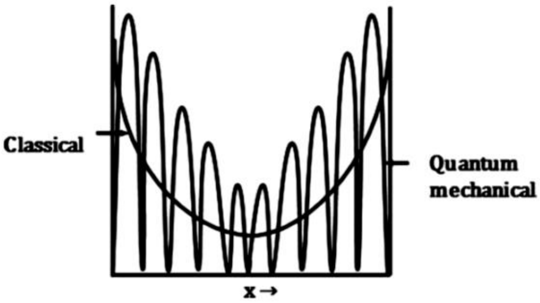


Fig: Probability distribution of quantum mechanical oscillator and classical oscillator.

$$\omega = \sqrt{\frac{k}{m}}$$

Or

$$a = \frac{\sqrt{2n}}{\alpha} \quad (6)$$

$$sin\beta = \frac{\zeta}{\sqrt{2n}} = \frac{\alpha x}{\sqrt{2n}} = \frac{x}{a}$$

Therefore

$$cos\beta = \frac{(a^2-x^2)^{\frac{1}{2}}}{a} \qquad (7)$$

Using (6) and (7) in (5)

$$P(x) = \frac{exp(-\zeta^2)exp(2n\beta^2)}{\pi(a^2-x^2)^{\frac{1}{2}}} \qquad (8)$$

Now when $n \to \infty, sin\,\beta \;\to\; \beta$ and

$\beta \;\to \zeta/\sqrt{2n},$ and $exp(-\zeta^2)exp(2n\beta^2) \to 1$

Therefore $P(x) = \frac{1}{\pi(a^2-x^2)^{\frac{1}{2}}}$ (classical).

Problem 27: Derive the probability distribution for a classical simple harmonic oscillator.

Solution:-

One can expect the probability of finding the particle of mass m at distance x from the equilibrium position to be inversely proportional to the velocity

$$P(x) = \frac{A}{v} \qquad (1)$$

where A =normalization constant. The equation for S.H.O. is

$$\frac{d^2x}{dt^2} + \omega^2 x = 0$$

which has the solution

$$x = a\,sin\,\omega t;\ (at\ t = 0, x = 0)$$

where a is the amplitude.

$$v = \frac{dx}{dt} = \omega\sqrt{a^2-x^2} \qquad (2)$$

Using (2) in (1)

$$P(x) = \frac{A}{\omega\sqrt{a^2-x^2}} \qquad (3)$$

We can find the normalization constant A.

$$\int P(x)dx = \int_{-a}^{a} \frac{Adx}{\omega\sqrt{a^2-x^2}} = \frac{\pi A}{\omega}=1$$

Therefore,

$$A = \frac{\omega}{\pi} \qquad (4)$$

Using (4) in (3), the normalized distribution is

$$P(x) = \frac{1}{\pi\sqrt{a^2-x^2}} \qquad (5)$$

Problem 28: The wave function (unnormalized) for a particle moving in a one dimensional potential well $V(x)$ is given by $\psi(x) = exp(-ax^2/2)$. If the potential is to have minimum value at $x = 0$, determine (a) the eigen value (b) the potential $V(x)$.

Solution:-

Schrodinger's equation in one dimension is

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

Given

$\psi = exp\left(-\frac{1}{2}ax^2\right)$ (2)

Differentiating twice,
We get

$\frac{d^2\psi}{dx^2} = exp\left(-\frac{1}{2}ax^2\right)(a^2x^2 - a)$ (3)

Inserting (2) and (3) in (1), we get

$V(x) = E + \left(\frac{\hbar^2}{2m}\right)(a^2x^2 - a)$ (4)

Minimum value of $V(x)$is determined from

$$\frac{dV}{dx} = \frac{\hbar^2 a^2 x}{m} = 0$$

Minimum of $V(x)$ occurs at $x = 0$

From (4) we find $0 = E - \frac{\hbar^2 a}{m}$

(a) Or the eigen value $E = \frac{\hbar^2 a}{m}$

(b) $V(x) = \frac{\hbar^2 a}{m} + \left(\frac{\hbar^2}{2m}\right)(a^2x^2 - a) = \frac{\hbar^2 a^2 x^2}{2m}$

Problem 29:

(a) Show that the wave-function $\psi_o x) = A\exp(-x^2/2a^2)$ with energy $E = \frac{\hbar\omega}{2}$(where A and a are constants) is a solution for all values of x to the one-dimensional time-independent Schrodinger equation (TISE) for the simple harmonic oscillator (SHO) potential $V(x) = \frac{m\omega^2 x^2}{2}$.

(b) Sketch the function $\psi_1(x) = Bx\,exp(-x^2/2a^2)$ (where B = constant), and show that it too is a solution of the TISE for all values of x.

(c) Show that the corresponding energy $E = (3/2)\hbar\omega$.

Solution:-

(a) $\psi_o(x) = Aexp(-x^2/2a^2)$

Differentiate twice and multiply by $-\hbar^2/2m$

$$\left(-\frac{\hbar^2}{2m}\right)\frac{d^2\psi_o}{dx^2} = \left(\frac{A\hbar^2}{2ma^2}\right)\left(1 - \frac{x^2}{a^2}\right) exp\left(\frac{-x^2}{2a^2}\right)$$

$$= \left(\frac{A\hbar^2}{2ma^4}\right)\psi_o - \left(\frac{\hbar^2 x^2}{2ma^2}\right)\psi_o$$

Or $-\left(\frac{\hbar^2}{2m}\right)\frac{d^2\psi_o}{dx^2} + \left(\frac{\hbar^2 x^2}{2ma^2}\right)\psi_o = \left(\frac{\hbar^2}{2ma^2}\right)\psi_o$

Compare the equation with the Schrodinger equation

$$E = \frac{\hbar^2}{2ma^2} = \frac{\hbar\omega}{2}$$

$\omega = \frac{\hbar}{ma^2}$

Or $a = \left(\frac{\hbar}{m\omega}\right)^{\frac{1}{2}}$

Same relation is obtained by setting

$$V = \frac{\hbar^2 x^2}{2ma^2} = \frac{m\omega^2 x^2}{2}$$

(b) $\psi_1(x) = Bxexp(-x^2/2a^2)$

Differentiate twice and multiply by $-\hbar^2/2m$

$$\left(-\frac{\hbar^2}{2m}\right)\frac{d^2\psi_1}{dx^2}=\frac{B\hbar^2x^3exp(x^2/a)}{2ma^4}+\frac{3\hbar^2exp(-x^2/2a^2)}{2ma^2}$$

Substitute

$Bxexp(-x^2/2a^2)=\psi_1$ and $a=\left(\frac{\hbar}{m\omega}\right)^{\frac{1}{2}}$ and rearrange to get

$$\left(-\frac{\hbar^2}{2m}\right)\frac{d^2\psi_1}{dx^2}+\left(\frac{m\omega^2}{2}\right)\psi_1=\left(\frac{3\hbar\omega}{2}\right)\psi_1$$

(c) $E=\frac{3\hbar\omega}{2}$

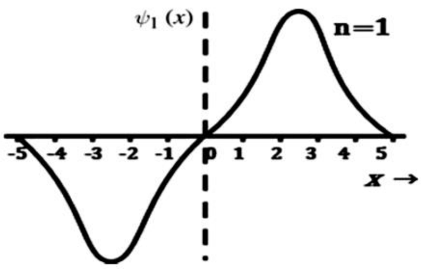


Fig: ψ_1 for SHO