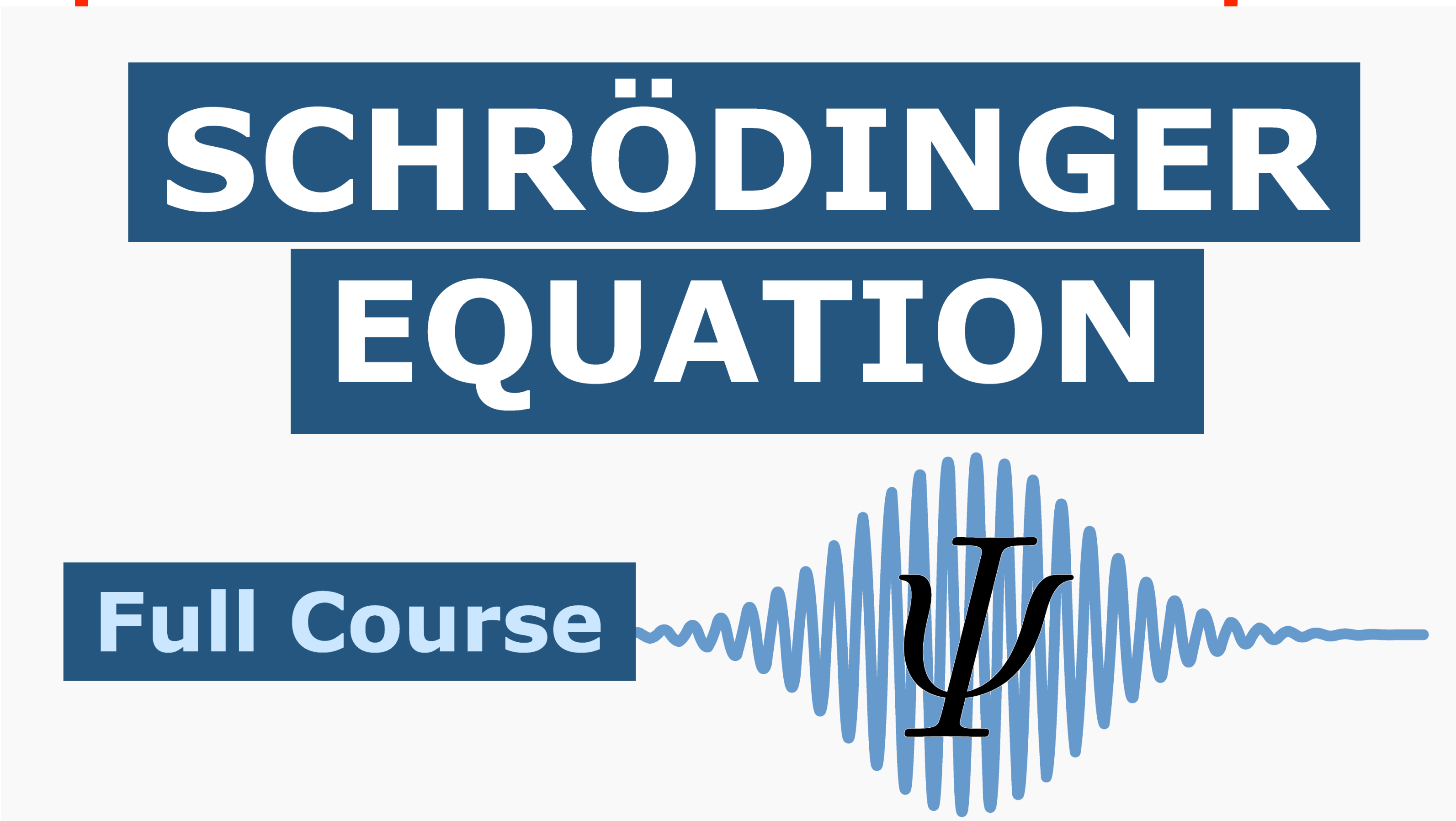
Quantum mechanics

Chapter III One dimension problem



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Postulate 1: State of a system

The state of any physical system is specified, at each time t, by a state vector $|\psi(t)\rangle$ in a Hilbert space H; $|\psi(t)\rangle$ contains (and serves as the basis to extract) all the needed information about the system. Any superposition of state vectors is also a state vector.

Postulate 2: Observables and operators

To every physically measurable quantity A, called an observable or dynamical variable, there corresponds a linear Hermitian operator A whose eigenvectors form a complete basis

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Postulate 3: Measurements and eigenvalues of operators

The measurement of an observable A may be represented formally by the action of A on a state vector $|\psi(t)\rangle$. The only possible result of such a measurement is one of the eigenvalues a_n of the operator A

Postulate 4: Probabilistic outcome of measurements

When measuring an observable A of a system in a state, the probability of obtaining one of the nondegenerate eigenvalues a_n of the corresponding operator A is given by

$$P_n(a_n) = \frac{|\langle\psi_n|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \frac{|a_n|^2}{\langle\psi|\psi\rangle},$$

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Postulate 5: Time evolution of a system

The time evolution of the state vector $|\psi(t)\rangle$ of a system is governed by the time-dependent Schrödinger equation

$$i\hbar\frac{\partial|\psi(t)\rangle}{\partial t}=\hat{H}|\psi(t)\rangle,$$

Postulate 6: The wave function of many-particle system

The total wavefunction must be antisymmetric with respect to the interchange of all coordinates of one fermion with those of another. Electronic spin must be included in this set of coordinates. The Pauli exclusion principle is a direct result of this antisymmetry principle.

Average value of a dynamical variable: The average value, $\langle A\rangle$, of a dynamical variable A, in a given state ψ of the system, is defined as

$$\langle A\rangle = \int_{-\infty}^{+\infty} \psi^*(\vec{r})\,[\hat{A}\psi(\vec{r})]\,d^3x \Big/ \int_{-\infty}^{+\infty} \psi^*(\vec{r})\psi(\vec{r})\,d^3x,$$

where the integration is over the entire region of variation of the independent variables, x, y, and z. The asterisk stands for complex conjugation.

If the wave function is normalized to unity, the required average value is given by

$$\langle A\rangle = \int_{-\infty}^{+\infty} \psi^*(\vec{r})(\hat{A}\psi(\vec{r}))\,d^3x.$$

Average value

For instance, the average value of the position operator, x, in one spatial dimension in the normalized state ψ,

$$\langle x\rangle = \int_{-\infty}^{+\infty} \psi^*(x)(\hat{x}\psi)\,dx = \int_{-\infty}^{+\infty} \psi^*(x)x\psi(x)\,dx.$$

Similarly, the expectation value of the x component of momentum, $\langle p_x\rangle$, is given by

$$\langle p_x\rangle = \int_{-\infty}^{+\infty} \psi^*(x)(\hat{p}_x\psi(x))\,dx = -i\hbar\int_{-\infty}^{+\infty} \psi^*(x)\frac{d\psi(x)}{dx}\,dx.$$

Let $\psi_1(r)$, $\psi_2(r)$ $\psi_3(r)$,. . . , be the normalized eigenfunctions of a hermitian operator A with discrete eigenvalues λ_1, λ_2, λ_3,. . . , respectively.

$$\langle A\rangle = \sum_\ell\sum_k \lambda_k c_\ell^* c_k \int_{-\infty}^{+\infty} \psi_\ell^*(\vec{r})\psi_k(\vec{r})\,d^3x = \sum_\ell\sum_k \lambda_k c_\ell^* c_k\,\delta_{\ell k} = \sum_k \lambda_k |c_k|^2$$

$$= \lambda_1|c_1|^2 + \lambda_2|c_2|^2 + \lambda_3|c_3|^2 + \dots$$

Time derivative of an operator: since an observable cannot have a definite value at a given instant of time. Therefore, it is not possible to define the time derivative of an operator in the usual way of mathematical analysis:

$$\frac{d\hat{A}(t)}{dt} = \lim_{\Delta t \to 0} \frac{\hat{A}(t+\Delta t) - \hat{A}(t)}{\Delta t}.$$

However, the expectation (average) value of the observable A, given by $\langle A \rangle$, can have a definite value at a given instant t. Therefore, for defining the time derivative of an operator, we must use its expectation value rather than the operator itself.

The time derivative of the expectation value, ⟨A⟩, of the observable, is equal to the expectation value of the time derivative of the operator A itself. That means:

$$\frac{d\langle\hat{A}\rangle}{dt} = \left\langle \frac{d\hat{A}}{dt} \right\rangle.$$

According to the formalism of quantum mechanics, we have

$$\langle\hat{A}\rangle = \int_{-\infty}^{+\infty} \psi^*(\vec{r},t)\hat{A}\psi(\vec{r},t)\,d\tau,$$

Therefore,

$$\frac{d\langle\hat{A}\rangle}{dt} = \int_{-\infty}^{+\infty} \left(\frac{\partial\psi^*}{\partial t}\hat{A}\psi + \psi^*\frac{\partial\hat{A}}{\partial t}\psi + \psi^*\hat{A}\frac{\partial\psi}{\partial t} \right) d\tau.$$

Using the time-dependent Schrödinger equations, we have

$$\frac{\partial \psi}{\partial t} = \frac{1}{i\hbar}\hat{H}\psi, \qquad \frac{\partial \psi^*}{\partial t} = -\frac{1}{i\hbar}\psi^*\hat{H}^\dagger = -\frac{1}{i\hbar}\psi^*\hat{H},$$

We get

$$\frac{d\langle \hat{A}\rangle}{dt} = \int_{-\infty}^{+\infty} \psi^* \left[\frac{\partial \hat{A}}{\partial t} + \frac{1}{i\hbar}\left(-\hat{H}\hat{A} + \hat{A}\hat{H}\right)\right] \psi \, d\tau.$$

Recollecting that

$$\frac{\partial \langle \hat{A}\rangle}{\partial t} = \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle \quad \text{where} \quad \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle = \int_{-\infty}^{+\infty} \psi^*(\vec{r},t)\frac{\partial \hat{A}}{\partial t}\psi(\vec{r},t)\, d\tau,$$

Finally,

$$\frac{d\langle \hat{A}\rangle}{dt} = \frac{\partial \langle \hat{A}\rangle}{\partial t} + \frac{1}{i\hbar}\int_{-\infty}^{+\infty} \psi^*(\vec{r},t)\left(-\hat{H}\hat{A} + \hat{A}\hat{H}\right)\psi(\vec{r},t)\, d\tau.$$

Pictures of Quantum Mechanics

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It can be written as

$$\frac{d\langle\hat{A}\rangle}{dt} = \frac{\partial\langle A\rangle}{\partial t} + \frac{1}{i\hbar}\left\langle[\hat{A},\hat{H}]\right\rangle,$$

In the case when there is no explicit dependence of the operator A on time, we have

$$\frac{d\langle\hat{A}\rangle}{dt} = \frac{1}{i\hbar}\left\langle[\hat{A},\hat{H}]\right\rangle.$$

Ehrenfest's theorem: The average values of observables in quantum mechanics obey the classical equations of motion.

$$\frac{d\langle\hat{x}\rangle}{dt} = \frac{\langle\hat{p}_x\rangle}{m}.$$

$$\frac{d\langle\hat{p}_x\rangle}{dt} = -\left\langle\frac{\partial V(x)}{\partial x}\right\rangle.$$

We also saw that under a unitary transformation between different representation, the forms of the wave function and that of the observables change, but the physical state of the system remains unaltered because the unitary operator S is time-independent.

In what follows, we shall show that it is possible to describe the time-evolution of the state vector by a time-dependent unitary operator, U(t).

U(t) is called the time-evolution operator or, simply, the evolution operator. Each of such descriptions is called a picture of quantum mechanics.

The Schrödinger picture: the state vector, $|\psi(t)\rangle$, of a quantum system depends explicitly on time, while the observables (operators of physical characteristics) of the system are time-independent.

The time evolution of the state vector is controlled by the Schrödinger equation

$$i\hbar\frac{\partial|\psi(t)\rangle}{\partial t}=\hat{H}|\psi(t)\rangle,$$

and can be represented in terms of a time evolution operator (propagator), $U(t,t_0)$, as

$$|\psi(t)\rangle=\hat{U}(t,t_0)|\psi(t_0)\rangle.$$

The condition of conservation of the norm of the wave function under this representation reads

$$\langle\psi(t)|\psi(t)\rangle = \langle\hat{U}(t,t_0)\psi(t_0)|\hat{U}(t,t_0)\psi(t_0)\rangle$$
$$= \langle\psi(t_0)|\hat{U}^\dagger(t,t_0)\hat{U}(t,t_0)|\psi(t_0)\rangle = \langle\psi(t_0)|\psi(t_0)\rangle.$$

This requires the evolution operator, $U(t,t_0)$, to be unitary:

$$\hat{U}^\dagger(t,t_0)\hat{U}(t,t_0) = \hat{U}(t,t_0)\hat{U}^\dagger(t,t_0) = \hat{I}.$$

In addition, the evolution operator also satisfies the following properties

$$\hat{U}(t,t) = \hat{I},$$
$$\hat{U}^\dagger(t,t_0) = \hat{U}^{-1}(t,t_0) = \hat{U}(t_0,t),$$
$$\hat{U}(t_k,t_j)\hat{U}(t_j,t_i) = \hat{U}(t_k,t_i), \quad t_k > t_j > t_i.$$

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The propagator can be determined as follows,

$$i\hbar\frac{\partial\hat{U}(t,t_0)}{\partial t}=\hat{H}\hat{U}(t,t_0).$$

If the Hamiltonian, H, is time independent, its solution satisfying the initial condition, $U(t_0,t_0) = I$, can be written as

$$\hat{U}(t,t_0)=e^{-\frac{i}{\hbar}(t-t_0)\hat{H}}.$$

The wave function can be written as

$$|\psi(t)\rangle=e^{-\frac{i}{\hbar}(t-t_0)\hat{H}}|\psi(t_0)\rangle.$$

We can expand the wave function $\psi(q,0)$ into a series with respect to the eigenfunctions, $\phi_m(q)$, m = 1,2,3,..., of the Hamiltonian

$$\psi(q,t_0)=\sum_m c_m\phi_m(q),$$

$$\psi(q,t)=\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{-i\hat{H}}{\hbar}(t-t_0)\right)^n\sum_m c_m\phi_m$$

$$=\sum_m c_m\phi_m\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{-iE_m^0}{\hbar}(t-t_0)\right)^n=\sum_m c_m\phi_m e^{-\frac{i}{\hbar}E_m^0(t-t_0)}.$$

The Heisenberg picture: in this picture, the state vector, $|\psi\rangle$, is time-independent, while the observables are time-dependent. This is accomplished by defining the Heisenberg state vector, $|\psi_H\rangle$, as

$$|\psi_H\rangle = \hat{U}^\dagger(t,t_0)|\psi(t)\rangle,$$

With such a definition $|\psi_H\rangle$ turns out to be time-independent

$$|\psi_H\rangle = \hat{U}^\dagger(t,t_0)|\psi(t)\rangle. = \hat{U}^{-1}(t,t_0)|\psi(t)\rangle = e^{\frac{i}{\hbar}(t-t_0)\hat{H}}|\psi(t)\rangle = |\psi(t_0)\rangle,$$

As a consequence, the state vector $|\psi_H\rangle$ gets frozen in time.

This leads to

$$\frac{d|\psi_H\rangle}{dt} = 0.$$

U represents a unitary transformation of the state vector, physical properties of a quantum system in both the the Schrödinger and the Heisenberg pictures should be the same.

For instance, consider the average value of time-independent observable, A_s, in the Schrödinger picture

$$\begin{aligned}\langle\hat{A}_S\rangle &= \left\langle\psi(t)\left|\hat{A}_S\right|\psi(t)\right\rangle = \left\langle\hat{U}(t,t_0)\psi_H\left|\hat{A}_S\right|\hat{U}(t,t_0)\psi_H\right\rangle \\ &= \left\langle\psi_H\left|\left(\hat{U}^\dagger(t,t_0)\hat{A}_S\hat{U}(t,t_0)\right)\right|\psi_H\right\rangle\end{aligned}$$

The requirement of the unchanged average value of A in both the pictures gives

$$\hat{A}_H(t) = \hat{U}^\dagger(t,t_0)\hat{A}_S(t_0)\hat{U}(t,t_0) = e^{\frac{i}{\hbar}(t-t_0)\hat{H}}\hat{A}_S(t_0)e^{-\frac{i}{\hbar}(t-t_0)\hat{H}}.$$

The Heisenberg's equation of motion for an observable is obtained by simply differentiating it with respect to time

$$\begin{aligned}
\frac{d\hat{A}_H}{dt} &= \frac{i}{\hbar}e^{\frac{i}{\hbar}(t-t_0)\hat{H}}\hat{H}\hat{A}_S e^{-\frac{i}{\hbar}(t-t_0)\hat{H}} - \frac{i}{\hbar}e^{\frac{i}{\hbar}(t-t_0)\hat{H}}\hat{A}_S\hat{H}e^{-\frac{i}{\hbar}(t-t_0)\hat{H}} \\
&= \frac{i}{\hbar}\left(\left\{e^{\frac{i}{\hbar}(t-t_0)\hat{H}}\hat{H}e^{-\frac{i}{\hbar}(t-t_0)\hat{H}}\right\}\left\{e^{\frac{i}{\hbar}(t-t_0)\hat{H}}\hat{A}_S e^{-\frac{i}{\hbar}(t-t_0)\hat{H}}\right\}\right. \\
&\quad \left. -\left\{e^{\frac{i}{\hbar}(t-t_0)\hat{H}}\hat{A}_S e^{-\frac{i}{\hbar}(t-t_0)\hat{H}}\right\}\left\{e^{\frac{i}{\hbar}(t-t_0)\hat{H}}\hat{H}e^{-\frac{i}{\hbar}(t-t_0)\hat{H}}\right\}\right) \\
&= \frac{i}{\hbar}\left(\hat{H}_H\hat{A}_H - \hat{A}_H\hat{H}_H\right).
\end{aligned}$$

Therefore, the Heisenberg's equation of motion can be written as

$$\frac{d\hat{A}_H}{dt} = \frac{1}{i\hbar}\left[\hat{A}_H, \hat{H}\right]$$

Interaction picture: In this picture, both the state vector, $|\psi_I(t)\rangle$, and the observables depend explicitly on time.

In the cases when the total Hamiltonian, H, can be separated into a time-independent part, H_0, and a time-dependent part, W(t) (interaction Hamiltonian), the state vector, $|\psi_I(t)\rangle$, is defined through

$$|\psi_I\rangle = \hat{U}_0^\dagger(t,t_0)|\psi(t)\rangle = \hat{U}_0^{-1}(t,t_0)|\psi(t)\rangle \equiv e^{\frac{i}{\hbar}(t-t_0)\hat{H}_0}|\psi(t)\rangle,$$

where $|\psi(t)\rangle$ is the state vector in the Schrödinger picture.

The equation of motion for the state vector is obtained as follows.

Defining an observable, $A_I(t)$, in the interaction picture by

$$\hat{A}_I(t) = e^{\frac{i}{\hbar}(t-t_0)\hat{H}_0}\hat{A}e^{-\frac{i}{\hbar}(t-t_0)\hat{H}_0},$$

where A is the corresponding observable in the Schrödinger's, and following the same calculations as in the case of Heisenberg's picture, we arrive at the following equation of motion for an observable in the interaction picture

$$i\hbar\frac{d\hat{A}_I}{dt} = \left[\hat{A}_I, \hat{H}_0\right].$$

We see that, in this picture, the time evolution of the state vector is governed by the time-dependent interaction Hamiltonian $W_I(t)$ only, while the time variation of an observable is controlled only by the time-independent part.

Differentiating $|\psi_I\rangle$ with respect to time, we obtain

$$\frac{\partial|\psi_I\rangle}{\partial t}=\frac{i}{\hbar}e^{\frac{i}{\hbar}(t-t_0)\hat{H}_0}\hat{H}_0|\psi(t)\rangle+e^{\frac{i}{\hbar}(t-t_0)\hat{H}_0}\frac{\partial|\psi(t)\rangle}{\partial t}.$$

For $|\psi(t)\rangle$ in the Schrödinger's picture, and a bit of algebra we obtain

$$i\hbar\frac{\partial|\psi_I(t)\rangle}{\partial t}=\hat{W}_I(t)|\psi_I(t)\rangle,$$

where

$$\hat{W}_I(t)\ =\ e^{\frac{i}{\hbar}(t-t_0)\hat{H}_0}\hat{W}(t)e^{-\frac{i}{\hbar}(t-t_0)\hat{H}_0}$$

is the time-dependent part of the total Hamiltonian in the interaction picture.

The properties of wave function

The wave function must be single-valued.

It must be continuous in the entire region of its arguments (that is, of the independent variables).

It must be finite everywhere.

The wave function must also be square-integrable, which requires the wave function to vanish at spatial infinity:

$$\lim_{(x,y,z)\to\pm\infty} \psi(x,y,z,t) = 0.$$

Stationary Schrödinger equation

The time evolution of the wave function, $\psi(r,t)$, representing the state of a quantum mechanical system is governed by the following partial differential equation:

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}=-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi(\vec{r},t)+V(\vec{r})\psi(\vec{r},t),$$

Solutions to the Schrödinger equation with time-independent potentials, V(r), can be found by employing the method of separation of variables; well known from the theory of differential equations.

$$\psi(\vec{r},t)=\phi(\vec{r})f(t).$$

The Schrödinger equation then leads to

$$i\hbar \frac{1}{f}\frac{df}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\phi(\vec{r})}\vec{\nabla}^2\phi(\vec{r}) + V(\vec{r}).$$

The left-hand side is a function of time, whereas the right-hand side depends only on spatial variables, x, y and z. Therefore, for this equality to hold, both the left-hand side and the right-hand side must be equal to a constant (same for both the sides).

Let us call it E. As a consequence, we get a system of two ordinary differential equations:

$$i\hbar \frac{1}{f}\frac{df}{dt} = E \quad \Rightarrow \quad \frac{df}{dt} = -\frac{i}{\hbar}E f(t),$$

The first of these equations, can be readily integrated to yield

$$f(t) = e^{-\frac{i}{\hbar}Et}.$$

and the second one is

$$-\frac{\hbar^2}{2m}\frac{1}{\phi(\vec{r})}\vec{\nabla}^2\phi(\vec{r}) + V(\vec{r}) = E \;\Rightarrow\; -\frac{\hbar^2}{2m}\vec{\nabla}^2\phi(\vec{r}) + V(\vec{r})\phi(\vec{r}) = E\phi(\vec{r}).$$

This differential equation satisfied by ϕ(r) is called the time-independent Schrödinger equation (TISE) and its solution depends on the form of the potential V(r).

In view of the standard conditions (to be satisfied by the overall wave function ϕ(r,t)), a given specific form of V(r) imposes specific boundary conditions on ϕ(r).

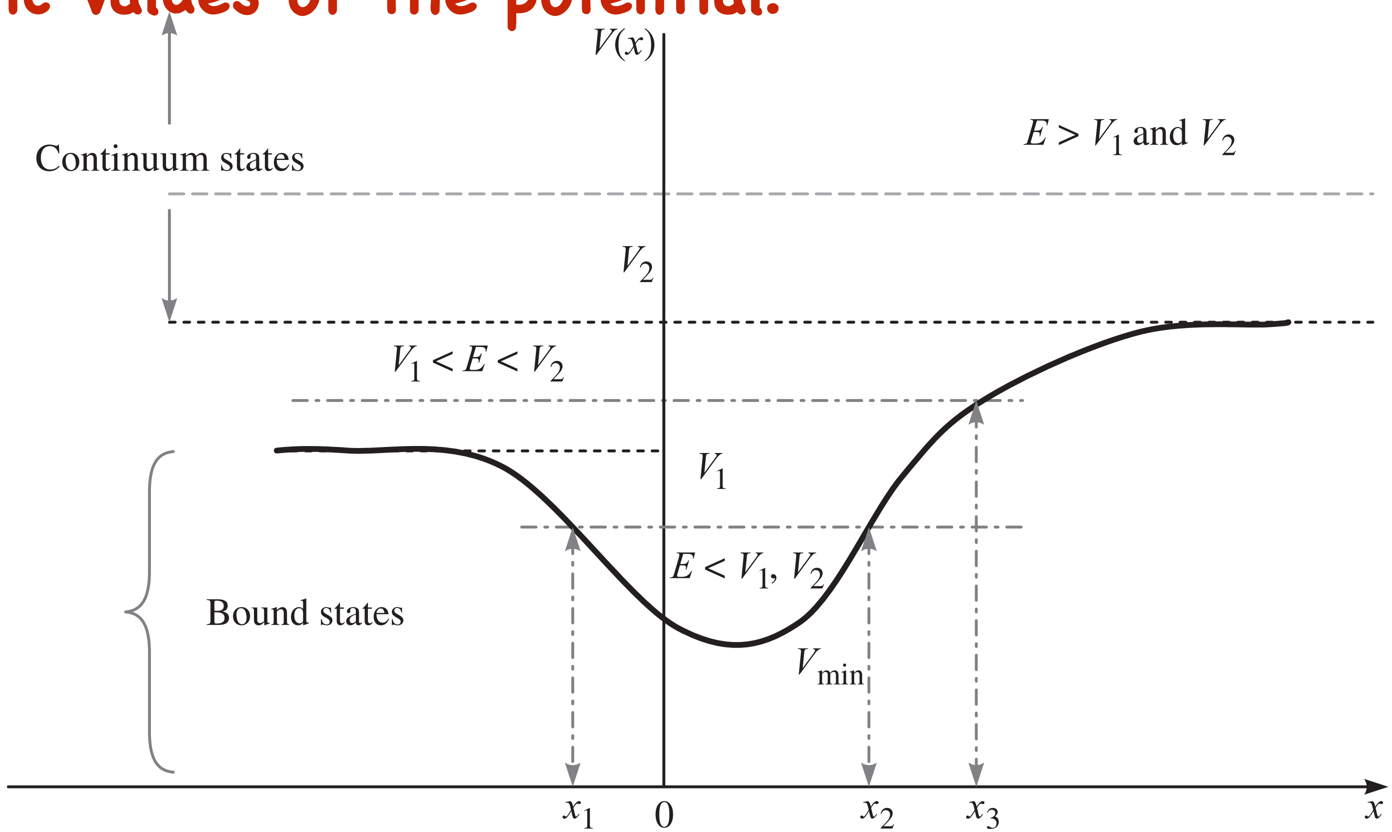
The TISE in one spatial dimension takes the form:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi(x)}{\partial x^2}+V(x)\phi(x)=E\phi(x),$$

where x $\in$ (−∞,+∞) is the independent variable. The nature and the properties of the solutions to this equation depend on the interrelationship between the total energy, E, of the particle and the potential V (x).

Consider an arbitrary form of the potential V (x), which is general enough to allow for the illustration of all the desired features. Without any loss of generality, the potential has been assumed to remain finite at spatial infinities: $\lim_{x\to-\infty}V(x)=V_1 \quad \lim_{x\to+\infty}V(x)=V_2$

and it has a minimum V_{min} at some point. The character of the energy states of the particle is completely determined by the energy E of the particle in comparison with the asymptotic values of the potential.



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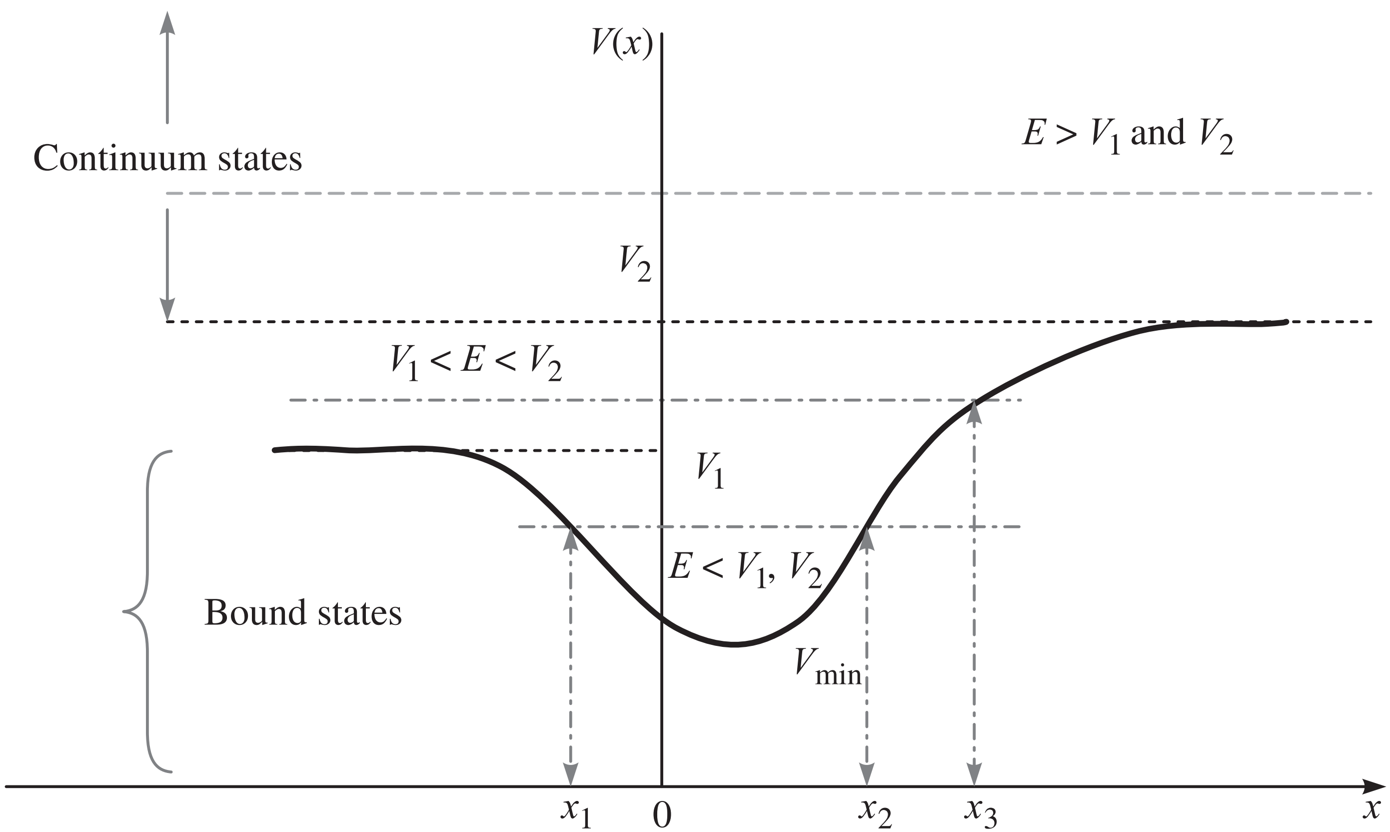
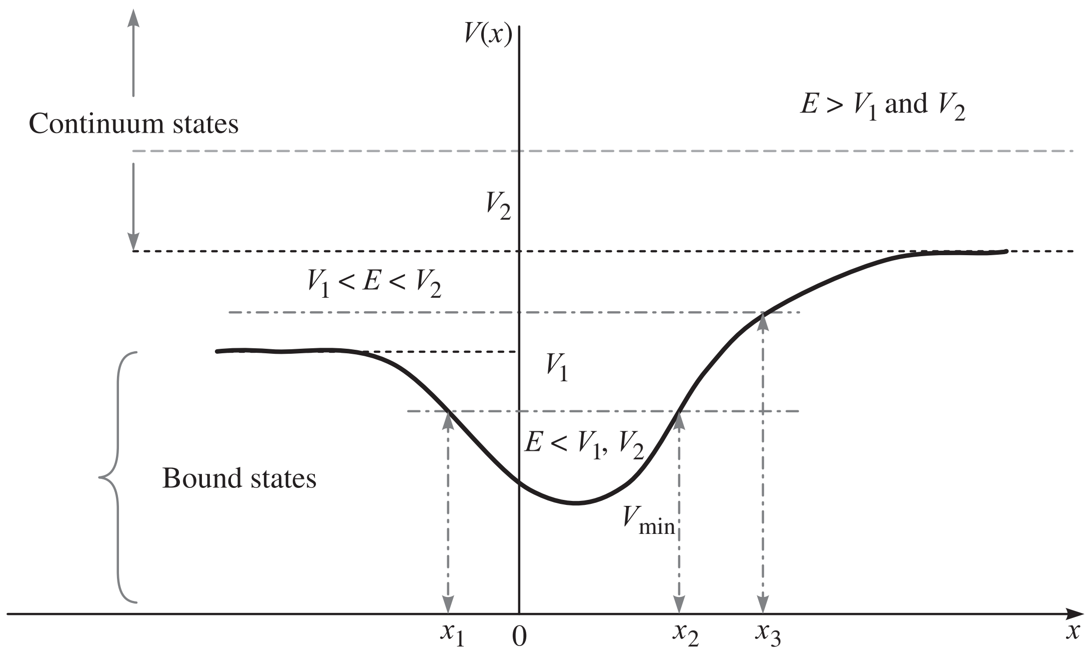
Bound states: Bound states occur whenever the particle is confined (or bound) at all energies to move within a finite and limited region of space.



Scattering states: If the total energy of the particle is either greater than V_1 and less than V_2 or greater than both V_1 and V_2, the particle's motion is not confined to a finite region of space and the states of the particle, corresponding to these ranges of the total energy, are called scattering states.



Important properties of bound state energy levels and the wave functions in one dimension:

1. The bound state energy levels of a system in one spatial dimension are discrete and nondegenerate.

2. In general, the nth bound state wave function, $\phi_n(x)$, in one spatial dimension has n nodes (that is, $\phi_n(x)$ vanishes n times), if n = 0 corresponds to the ground state and (n – 1) nodes if n = 1 corresponds to the ground state.

The Free Particle Solution

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A free particle represents a typical example of a stationary state that corresponds to an unbounded motion (scattering state) both along the positive and the negative x directions. In this case, the external potential is absent, that is, V(x) = 0, and the TISE reads

$$-\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} = E\phi(x) \quad \Rightarrow \quad \frac{d^2\phi(x)}{dx^2} + k^2\phi(x) = 0,$$

where

$$k^2 = \frac{2mE}{\hbar^2}, E > 0.$$

This equation has two linearly independent solutions:

$$\phi_{(+)}(x) = e^{ikx}, \quad \phi_{(-)}(x) = e^{-ikx}.$$

The general stationary state solution is the linear superposition given by

$$\psi(x,t) = A_{(+)} e^{i(kx-\omega t)} + A_{(-)} e^{-i(kx+\omega t)},$$

where $A_{(+)}$ and $A_{(-)}$ are arbitrary, in general complex, constants. If we use the de Broglie formula, the solution can be written as

$$\psi(x,t) = A_{(+)}\, e^{\frac{i}{\hbar}(px-Et)} + A_{(-)}\, e^{-\frac{i}{\hbar}(px+Et)}.$$

The first term in the above equation represents a particle traveling to the right (positive x direction) and the second term represents a particle traveling to the left.

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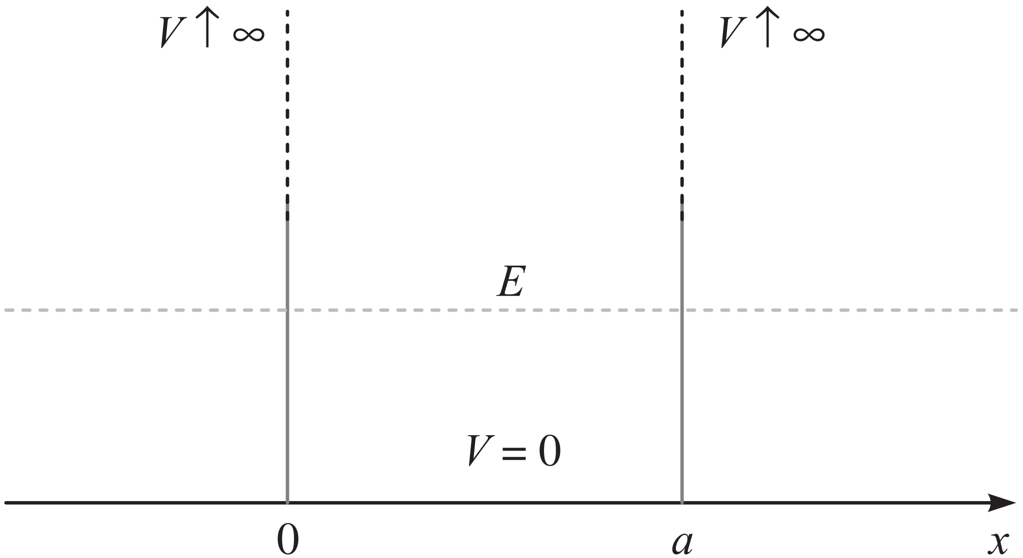
Three problems about the solution of free particle:

1. Firstly, the probability densities corresponding to either solutions are constant that is, they depend neither on x nor on t.
2. The second difficulty is in an apparent discrepancy between the speed of the wave and the speed of the particle it is supposed to represent. $v_p = \frac{\omega}{k} = \frac{E}{\hbar k} = \frac{\hbar k}{2m}$. $v = \frac{p}{m} = \frac{\hbar k}{m} = 2v_p$.
3. The third difficulty is that the free particle wave function cannot be normalized:

$$\int_{-\infty}^{+\infty} |\psi(x,t)|^2 \, dx = |A_\pm|^2 \int_{-\infty}^{+\infty} dx \ \rightarrow \ \infty.$$

Asymmetric infinite square well potential.



Mathematically this is given by the following expression:

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

An Infinite Potential Well

Since the motion of the particle is confined inside the well, quantum mechanically, it corresponds to the case of a bound state problem.

Since the particle cannot penetrate the regions $x<0$ and $x>a$, the wave function of the particle must be zero in these regions: $\phi=0$ for $x<0$ and $x>a$.

The time-independent Schrödinger equation

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

for the given case can be written as

$$\frac{\phi''}{\phi}=-\frac{2m}{\hbar^2}\left(E-V\right),$$

An Infinite Potential Well

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Inside the well, V = 0, and the solution is given by the linear combination

$$\phi(x) = A\ \sin(kx) + B\ \cos(kx),$$

where A and B are arbitrary constants and

$$k^2 = \frac{2mE}{\hbar^2}.$$

According to the standard conditions, the wave function has to be continuous across the boundaries and we must have

$$\phi \equiv 0 \text{ for } x = 0 \text{ and } x = a.$$

The first boundary condition leads to

$$B = 0.$$

The second boundary condition yields

$$\sin(ka) = 0, \quad \Rightarrow \quad k_n = \frac{n\pi}{a}, \; n = 1, 2, 3, ...$$

Therefore, we conclude that the boundary conditions can be satisfied only for the discrete values of energy

$$E_n = \frac{n^2\hbar^2\pi^2}{2ma^2}, \; n = 1, 2, 3, \ldots,$$

Thus, a particle, trapped inside an infinite potential well, can have only discrete set of energy eigenvalues. The corresponding eigenfunctions are

$$\phi_n(x) = B_n \, \sin\left(\frac{n\pi}{a}x\right).$$

The constant B_n is determined by the normalization condition

$$|B_n|^2 \int_{-\infty}^{+\infty} \phi_n^*(x)\phi_n(x)dx = |B_n|^2 \int_0^a \sin^2\left(\frac{\pi x}{a}n\right)dx = 1.$$

The result is

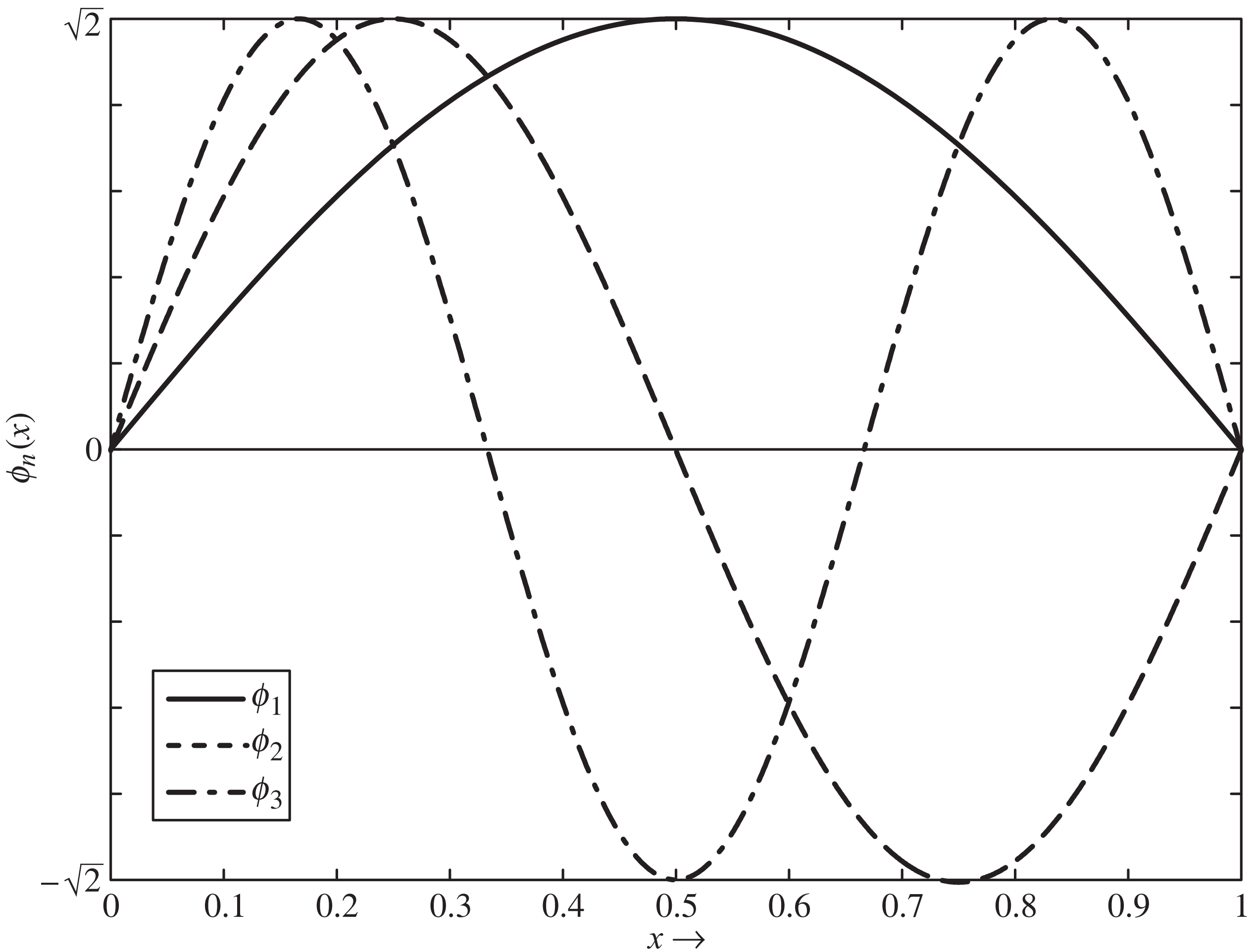
$$B_n = \sqrt{\frac{2}{a}}.$$

Therefore, the normalized eigenfunctions and the corresponding energies are

$$\psi_n(x,t) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}n\right), \quad E_n = \frac{n^2\hbar^2\pi^2}{2ma^2}, \quad n = 1, 2, 3, \ldots \ .$$

An Infinite Potential Well

The wave function



An Infinite Potential Well

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We thus got an infinite sequence of discrete energy levels corresponding to the positive integer values of the quantum number n.

The ground state corresponds to n = 1 with energy

$$E_1 = \hbar^2 \pi^2 / (2ma^2)$$

The states with quantum numbers n > 1 are called the excited states. Their energies are equal to n^2 times the ground state energy.

The full stationary state solutions are

$$\psi_n(x,t) = \sqrt{\frac{2}{a}}\,\sin\left(\frac{\pi x}{a}n\right)e^{-i\frac{n^2\pi^2\hbar}{2ma^2}t}.$$

Note that, in view of the linearity of the Schrödinger equation, the most general stationary state solution for the given case can be written as

$$\psi(x,t) = \sum_{n=1}^{\infty} c_n\sqrt{\frac{2}{a}}\,\sin\left(\frac{\pi x}{a}n\right)e^{-i\frac{n^2\pi^2\hbar}{2ma^2}t},$$

where c_n are arbitrary constants. Let us enumerate the important properties of the obtained solutions. These properties are quite general and hold good for most of the potentials encountered in quantum mechanics.

An Infinite Potential Well

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1. The eigenfunction $\phi_n(x)$ has(n−1) nodes (zero-crossing).

2. These functions are alternately symmetric and antisymmetric with respect to the centre of the well.

3. None of the energy levels is degenerate, that is, each energy level corresponds to a unique eigenfunction.

4. The eigenfunctions corresponding to different energy eigenvalues are orthogonal:

$$\int_{-\infty}^{+\infty} \phi_m^*(x)\phi_n(x)dx = \int_0^a \phi_m^*(x)\phi_n(x)dx = \delta_{mn},$$

where δ_{mn} is the Kronecker delta:

$$\delta_{mn} = \begin{cases} 1 & \text{if} \quad m = n \\ 0 & \text{if} \quad m \neq n. \end{cases}$$

The eigenfunctions$\{\phi_n(x)\}$,n=1,2,3,...constitute a complete set in the sense that an arbitrary function f (x) can be expanded as a linear combination of these functions:

$$f(x) = \sum_{n=1}^{\infty} c_n \phi_n(x) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} c_n \sin\left(\frac{\pi x}{a} n\right),$$

where the coefficients c_n are calculated as

$$c_n = \int_0^a \phi_n^*(x) f(x) dx.$$

Note that, the ground state corresponds to n = 1 instead of n = 0. The reason behind it lies in Heisenberg's uncertainty relation between the position and momentum

If the particle has zero total energy, it will be at rest inside the well and we can, in principle, precisely determine its position and momentum simultaneously at a given instant of time.

Furthermore, since our particle is localized inside the well of width a, according to the uncertainty relation, there is a zero-point energy $\hbar^2 / 8ma^2$

Discontinuous Potentials

If $V(x)$ is finite and continuous everywhere, we can expect the solutions of the TISE to be finite, continuous and differentiable.

It is evident from the physical interpretation of the wave function that it has to be continuous everywhere irrespective of the fact whether or not the potential has discontinuity.

However, the differentiability of the wave function is not guaranteed in advance and hence, must be examined.

The potential has a finite jump (discontinuity), say, at x = 0:

$$V(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ V_0 > 0 & \text{for} \quad x \geq 0. \end{cases}$$

The wave function has to be continuous across x = 0. To check the continuity of the first derivative, we first replace the potential V (x) by a smoothened potential $V_\varepsilon(x)$ in the interval $x \in [-\varepsilon, +\varepsilon]$ such that

$$\lim_{\varepsilon \to 0} V_\varepsilon(x) = V_0.$$

Here $\varepsilon \ll 1$ is an infinitesimal positive parameter.

Integrating the time-independent Schrödinger equation in this interval over x, we obtain

$$\left(\frac{d\phi}{dx}\right)_{+\varepsilon}-\left(\frac{d\phi}{dx}\right)_{-\varepsilon}=-\frac{2mE}{\hbar^2}\int_{-\varepsilon}^{+\varepsilon}\phi(x)\,dx+\frac{2mE}{\hbar^2}\int_{-\varepsilon}^{+\varepsilon}V(x)\phi(x)\,dx.$$

If we take the limit $\varepsilon \to 0$, we get

$$\Delta\left(\frac{d\phi}{dx}\right)=-\frac{2mE}{\hbar^2}\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{+\varepsilon}\phi(x)\,dx+\frac{2mE}{\hbar^2}\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{+\varepsilon}V(x)\phi(x)\,dx.$$

The first term on the right-hand side is zero because $\phi(x)$ is continuous across $x = 0$ and hence, the integral goes to zero as ε becomes zero.

The second term is also zero because

$$\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{+\varepsilon} V(x)\phi(x)\,dx. = V_0 \lim_{\varepsilon\to 0}\int_{-\varepsilon}^{+\varepsilon} \phi(x)\,dx = 0.$$

As a result, we arrive at

$$\left(\frac{d\phi}{dx}\right)_{+\varepsilon} = \left(\frac{d\phi}{dx}\right)_{-\varepsilon}$$

Thus, if the potential has a finite jump at a point, the wave function and its first derivative are continuous at the point of discontinuity. That is, the wave function is differentiable at the points of finite discontinuity of the potential.

Discontinuous Potentials

The potential V(x) is infinite in a region: in this case, the particle cannot penetrate through the infinite barrier and the probability of finding the particle inside the barrier is zero. Therefore, the wave function must vanish everywhere in the region of infinite potential.

The potential becomes infinite at a point (that is, has a singularity at a point). We can model this situation by assuming

$$V(x) = -\alpha\,\delta(x - x_0)$$

The wave function will be continuous at $x = x_0$.

Discontinuous Potentials

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In order to verify the continuity of the first derivative, we once again integrate the corresponding TISE in the vicinity of the point $x=x_0$. We get

$$\left(\frac{d\phi}{dx}\right)_{+\varepsilon} - \left(\frac{d\phi}{dx}\right)_{-\varepsilon} = -\frac{2m\alpha}{\hbar^2}\int_{-\varepsilon}^{+\varepsilon} \delta(x-x_0)\phi(x)\,dx = -\frac{2m\alpha}{\hbar^2}\phi(x_0).$$

Thus, the first derivative of the wave function is not continuous across the point of singularity.

Instead, it has a finite jump of

$$(-2m\alpha/\hbar^2)\phi(x_0)$$

at $x=x_0$

A particle of mass, m and total energy –E (E>0), is subject to the potential given by

$$V(x) = -\alpha\delta(x),$$

here α is a positive constant and δ(x) is the Dirac delta function.

For x<0 and x>0, V(x)=0 and we have

$$\frac{d^2\phi}{dx^2} - \frac{2m|E|}{\hbar^2}\phi = 0.$$

Since the standard conditions require the wave function to vanish for x→±∞, we have

Delta Potential

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$$\phi(x) = \begin{cases} Ae^{kx} & \text{for} \quad x < 0 \\ Be^{-kx} & \text{for} \quad x > 0, \end{cases}$$

where

$$k = \sqrt{2m|E|}/\hbar$$

and A and B are real but arbitrary constants. The continuity of $\phi(x)$ at x = 0 yields

$$A = B.$$

The potential is infinite at x = 0. Therefore, as discussed earlier, the first derivative of the wave function will be discontinuous and we shall have

$$\left(\frac{d\phi}{dx}\right)_{+\varepsilon} - \left(\frac{d\phi}{dx}\right)_{-\varepsilon} = -\frac{2m\alpha}{\hbar^2}\int_{-\varepsilon}^{+\varepsilon} \delta(x)\phi(x)\,dx = -\frac{2m\alpha}{\hbar^2}\phi(0).$$

If we take the limit $\varepsilon \to 0$ and put A=B, we obtain

$$-2kA = -\frac{2m\alpha}{\hbar^2}\phi(0) = -\frac{2m\alpha}{\hbar^2}A \quad \Rightarrow \quad k = \frac{m\alpha}{\hbar^2}.$$

We thus see that there is only one bound state for the particle in this case whose energy is

$$E = -\frac{m\alpha^2}{2\hbar^2}$$

The normalization of the wave function reads

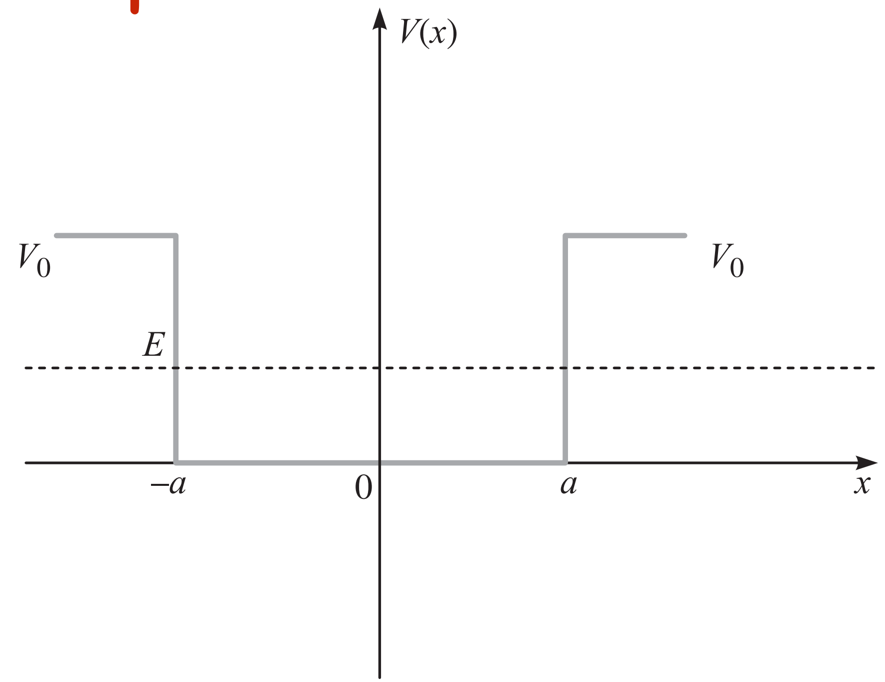
$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = A^2 \int_{-\infty}^{0} e^{2kx} dx + A^2 \int_{0}^{+\infty} e^{-2kx} dx = \frac{A^2}{k} = 1.$$

The normalized wave function is thus given by

$$\phi(x) = \begin{cases} \sqrt{k}e^{kx} & \text{for} \quad x < 0, \\ \sqrt{k}e^{-kx} & \text{for} \quad x > 0. \end{cases} \qquad \text{or,} \qquad \phi(x) = \sqrt{\frac{m\alpha}{\hbar^2}}\, e^{-\frac{m\alpha}{\hbar^2}|x|}.$$

Finite Square Well Potential

Consider the motion of a quantum particle in a finite potential well



$$V(x) = \begin{cases} 0, & \text{if} \quad |x| \leq a \\ V_0, & \text{if} \quad |x| > a \,. \end{cases}$$

We are required to solve the TISE with this potential for the bound states, when the total energy, E, of the particle is less than V_0 and determine the eigenfunctions and the corresponding energy eigenvalues.

Parity operator: Consider the operation of space inversion in which we change the space variables from r = {x, y, z} to -r = {−x, −y, −z}.

As a result, a function ψ(r) goes into ψ(-r). If ψ(-r) =ψ(r), the function ψ(r) is said to be symmetric (even) or, equivalently, a function with even parity. On the other hand, if ψ(-r) =−ψ(r), the function ψ(r) is said to be **anti-symmetric** (odd) or, equivalently, a function with odd parity. The transformation of a function ψ(r) under space inversion can be written in operator form as

$$\psi(-\vec{r}) = \hat{\mathscr{P}}\psi(\vec{r}),$$

Symmetric Potential

The bound state wave functions of a particle moving in a one-dimensional symmetric potential have definite parity, that is, they are either even or odd.

Consider now the TISE for the symmetric potential:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\phi(x)=E\phi(x).$$

Let us now perform the spatial inversion by replacing x with -x. Then

$$\hat{\mathscr{P}}\phi(x)\rightarrow\phi(-x) \qquad \hat{\mathscr{P}}V(x)\rightarrow V(-x).$$

Symmetric Potential

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Since V(−x) = V(x), the Hamiltonian commutes with the parity operator and we get

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\phi(-x)=E\phi(-x).$$

Thus, we see that thus stationary Schrödinger equation for the symmetric potential is satisfied by $\phi_1(-x) = \phi_1(x)$ as well as $\phi_2(-x) = -\phi_2(x)$.

The former, denoted as $\phi_s(x)$, is called the symmetric wave function and has even parity, while the latter, denoted as $\phi_a(x)$, is called the anti-symmetric wave function and has odd parity.

The entire range of x from $-\infty$ to $+\infty$ can be divided into three regions:

$-a \le x \le a$ (Region I), $x < -a$ (Region II), $x > a$ (Region III).

The general TISE reads

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

The TISE and the corresponding solutions in these regions can be written as:

Region I:

$$\phi_1''+k_1^2\phi_1=0, \qquad k_1^2=\frac{2mE}{\hbar^2},$$

$$\phi_1=A_1\cos(k_1x)+B_1\sin(k_1x).$$

Region II:

$$\phi_2'' - k_2^2\phi_2 = 0, \qquad k_2^2 = \frac{2m(V_0 - E)}{\hbar^2},$$

$$\phi_2 = A_2\, e^{k_2 x} + B_2\, e^{-k_2 x}.$$

Region III:

$$\phi_3'' - k_2^2\phi_3 = 0,$$

$$\phi_3 = A_3\, e^{k_2 x} + B_3\, e^{-k_2 x}.$$

In the aforementioned equations, the prime stands for the ordinary derivative with respect to x, and A_j and B_j (j = 1, 2, 3) are arbitrary constants to be determined by the boundary conditions.

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Boundary conditions:

1. The full solution of the TISE must be square-integrable.

$$\phi(x)=\begin{cases}\phi_2=A_2\,e^{k_2x}, & x<-a\\ \phi_1=A_1\cos(k_1x)+B_1\sin(k_1x), & -a\le x\le a\\ \phi_3=B_3\,e^{-k_2x}. & x>a\end{cases}$$

2. the solutions belonging to different regions in x must be continuous and differentiable at the boundaries x=±a, that is,

$$\phi_1(-a)=\phi_2(-a),\phi_1'(-a)=\phi_2'(-a),\phi_1(a)=\phi_3(a)$$

$$\phi_1'(a)=\phi_3'(a)$$

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These conditions lead to

$$A_2\, e^{-k_2 a} = A_1 \cos(k_1 a) - B_1 \sin(k_1 a),$$

$$k_2 A_2\, e^{-k_2 a} = k_1 A_1 \sin(k_1 a) + k_1 B_1 \cos(k_1 a),$$

$$B_3\, e^{-k_2 a} = A_1 \cos(k_1 a) + B_1 \sin(k_1 a),$$

$$-k_2 B_3\, e^{-k_2 a} = -k_1 A_1 \sin(k_1 a) + k_1 B_1 \cos(k_1 a).$$

They can be combined as

$$(A_2 + B_3)\, e^{-k_2 a} = 2A_1 \cos(k_1 a),$$

$$k_2 (A_2 + B_3)\, e^{-k_2 a} = 2k_1 A_1 \sin(k_1 a).$$

$$(A_2 - B_3)\, e^{-k_2 a} = -2B_1 \sin(k_1 a),$$

$$k_2 (A_2 - B_3)\, e^{-k_2 a} = 2k_1 B_1 \cos(k_1 a).$$

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If $A_2 + B_3 \neq 0$ and $A_1 \neq 0$, then

$$k_2 = k_1 \tan(k_1 a).$$

Therefore,

$$B_1 \sin(k_1 a) = -\frac{k_1}{k_2} B_1 \cos(k_1 a) = -B_1 \frac{k_1^2}{k_2^2} \sin(k_1 a),$$

so,

$$B_1 \left(1 + \frac{k_2^2}{k_1^2}\right) = 0, \quad \Rightarrow \quad B_1 = 0.$$

It yields,

$$A_2 = B_3.$$

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Taking all these results into account, we get that the full solution, corresponding to the case when $A_2 + B_3 \neq 0$ and $A_1 \neq 0$, is

$$\phi(x) = \begin{cases} A_2\, e^{k_2 x} & \text{for} \quad x < -a \\ A_1 \cos(k_1 x) & \text{for} \quad -a \leq x \leq a \\ A_2\, e^{-k_2 x} & \text{for} \quad x > a, \end{cases}$$

where A_1 and A_2 are arbitrary constants. It is not difficult to check that the given solution is a symmetric solution, that is, $\phi(-x) = \phi(x)$, and hence has positive parity.

The boundary conditions, lead to a transcendental equation, for the determination of the energies of the bound states.

Since the potential is symmetric in x: $V(-x) = V(x)$, there is another solution to the TISE which is anti-symmetric.

If $A_2 - B_3 \neq 0$ and $B_1 \neq 0$, we get

$$-k_1 \cot(k_1 a) = k_2.$$

and

$$A_1 \cos(k_1 a) = \frac{k_1}{k_2} A_1 \sin(k_1 a) = -A_1 \frac{k_1^2}{k_2^2} \cos(k_1 a),$$

It leads to

$$A_1 \left(1 + \frac{k_2^2}{k_1^2}\right) = 0, \quad \Rightarrow \quad A_1 = 0.$$

Therefore,

$$A_2 = -B_3$$

Taking all these results into account, we get that the antisymmetric solution,

$$\phi(x) = \begin{cases} A_2\, e^{k_2 x} & \text{for} \quad x < -a \\ B_1 \sin(k_1 x) & \text{for} \quad -a \le x \le a \\ -A_2\, e^{-k_2 x} & \text{for} \quad x > a, \end{cases}$$

It is not difficult to check that the given solution is an anti-symmetric solution, that is, $\phi(-x) = -\phi(x)$, and hence has negative parity.

Finite Square Well Potential

The equations about the k_1 and k_2 are transcendental equations and cannot be solved analytically. However, they can be solved graphically as described here. Let us introduce new variables

$$\xi = k_1 a = \sqrt{\frac{2mE}{\hbar^2}}\, a, \qquad \eta = k_2 a = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}\, a.$$

Clearly, the following holds

$$\xi^2 + \eta^2 = R^2, \qquad R^2 = \frac{2ma^2V_0}{\hbar^2}.$$

The transcendental equations will become

$$\xi \tan(\xi) = \eta,$$
$$-\xi \cot(\xi) = \eta.$$

Let ξ_n be the n[th] root of the transcendental equations. If we introduce the notation

$$\xi_n^2 = (k_1\, a)^2 = \frac{2ma^2 E_n}{\hbar^2},$$

then

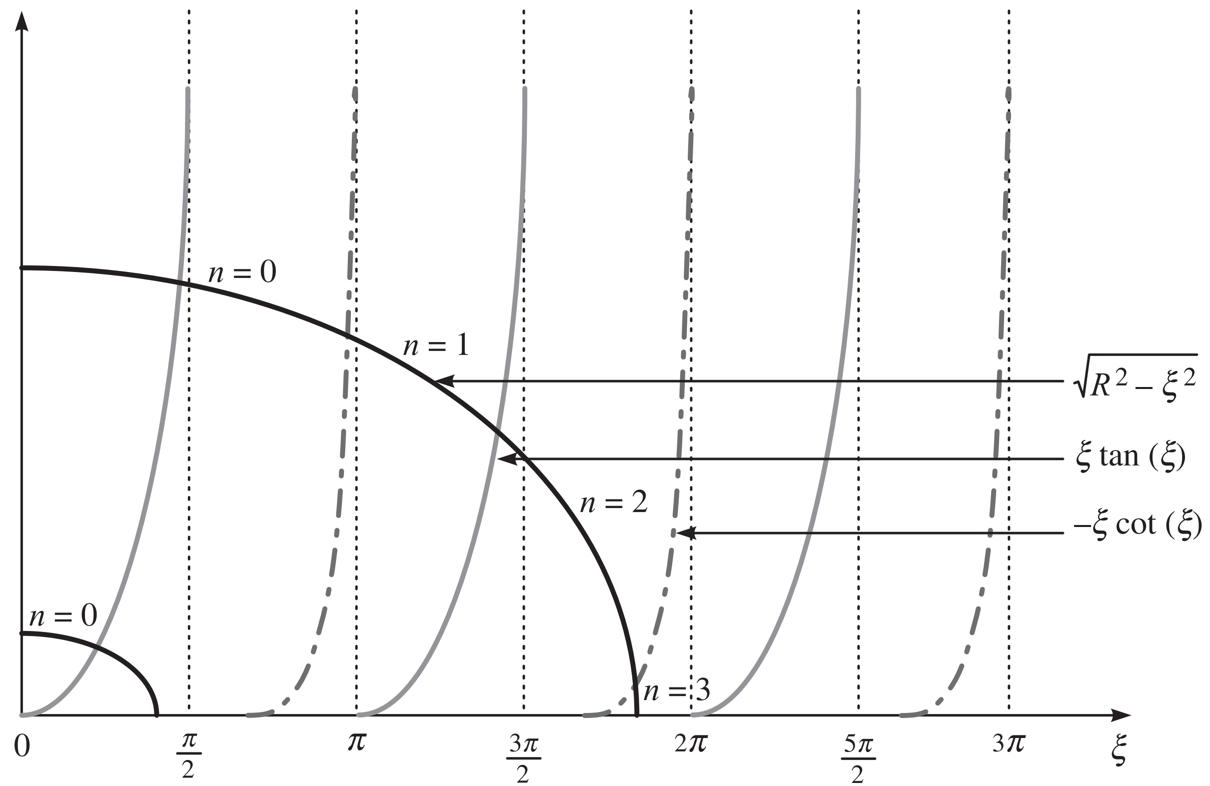
$$\eta = \sqrt{R^2 - \xi_n^2}$$

and the transcendental equations take the form

$$\xi_n \tan \xi_n = \sqrt{R^2 - \xi_n^2}. \qquad \text{(For even parity states)}$$

$$-\,\xi_n \cot \xi_n = \sqrt{R^2 - \xi_n^2}. \qquad \text{(For odd parity states)}$$

The left-hand sides contain trigonometric functions, while the right-hand sides represent a circle of radius R. The solutions are given by the points where the circle intersects the functions $\xi_n \tan\xi_n$ and $-\xi_n \cot\xi_n$.



Finite Square Well Potential

The solutions form a discrete set. Figure contains the results of the solution of the equations for two values of the radius, R=1 and R=2, which correspond to

$$V_0 a^2 = \hbar^2/2m \quad \text{and} \quad V_0 a^2 = 2\hbar^2/m,$$

The intersection of the small circle (R = 1) with the curve $\xi_n \tan\xi_n$ yields only one bound state, n = 0. The intersection of the larger circle (R = 2) with $\xi_n \tan \xi_n$ yields two bound states, n = 0,2, and its intersection with $-\xi_n \cot\xi_n$ yields two other bound states, n = 1,3. Hence, for R = 2, the system in all will have four bound states.

This analysis shows that the number of solutions depends on the value of R, which in turn depends on the depth of the well, V_0, and the width 2a of the well.

Clearly, the deeper and wider the well, the greater the number of points of intersection of the curves and hence, greater will be the number of bound states of the particle inside the well.

Thus, there is always at least one bound state (that is, one intersection) no matter how small V_0 is.

A closer look at previous figure shows that when

$$0 < R < \frac{\pi}{2}, \quad \text{that is,} \quad 0 < V_0 < \frac{\pi^2\hbar^2}{8ma^2},$$ one solution n=0

$$\frac{\pi}{2} < R < \pi, \quad \text{that is,} \quad \frac{\pi^2\hbar^2}{8ma^2} < V_0 < \frac{\pi^2\hbar^2}{2ma^2},$$ two solutions n=0,1

$$\pi < R < \frac{3\pi}{2}, \quad \text{that is,} \quad \frac{\pi^2\hbar^2}{2ma^2} < V_0 < \frac{9\pi^2\hbar^2}{8ma^2},$$ three solutions n=0,1,2

$$\frac{3\pi}{2} < R < 2\pi, \quad \text{that is,} \quad \frac{9\pi^2\hbar^2}{8ma^2} < V_0 < \frac{2\pi^2\hbar^2}{ma^2},$$ four solutions n=0,1,2,3

Finite Square Well Potential

In general, for a given V_0, the width, $w_0 = 2a$, of the well that allows for n bound states is determined by

$$R = \frac{n\pi}{2},$$

and equals

$$w_0 = \frac{\pi^2 \hbar^2}{2mV_0} n^2.$$

In the limiting case of $ma^2V_0 \to \infty$ for a given a, the radius of the circle becomes infinite and the intersections occur at

$$\tan(k_1 a) = \infty \quad \Rightarrow \quad k_1 a = \pi\frac{2n+1}{2}, n = 0, 1, 2, 3, ...$$

$$-\cot(k_2 a) = \infty \quad \Rightarrow \quad k_2 a = n\pi, n = 1, 2, 3, ...$$

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If we combine the two, we obtain

$$k_1 a = \frac{n\pi}{2} \quad \Rightarrow \quad \frac{2mE_n}{\hbar^2} = \frac{n^2\pi^2}{4a^2}.$$

Finally, we arrive at

$$E_n = \frac{n^2\pi^2\hbar^2}{8ma^2}.$$

Thus, we recover the energy spectrum of the infinite potential well.

When $E < V_0$, the regions $x < -a$ and $x > a$ are classically forbidden for the particle in the sense that it cannot penetrate into these regions.

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Consider x>a. The solution of the TISE in this region is φ(x)~ exp(-k_2x). Let us define

$$\phi(x) = \frac{\phi(0)}{e} = e^{-k_2\eta},$$

where x = η is the point where the wave function falls by a factor of 1/e. Then, we have

$$\eta = \frac{1}{k_2} = \frac{\hbar}{\sqrt{2m(V_0 - E)}}.$$

η is called the penetration depth, that is, the distance to which the particle can penetrate into the classically forbidden region. Hence, the probability of finding the particle inside the forbidden regions on either side of the finite potential well is in principle non-zero.

Consider the one-dimensional simple harmonic oscillator characterized by the potential energy

$$V(x)=\frac{1}{2}m\omega^2x^2,$$

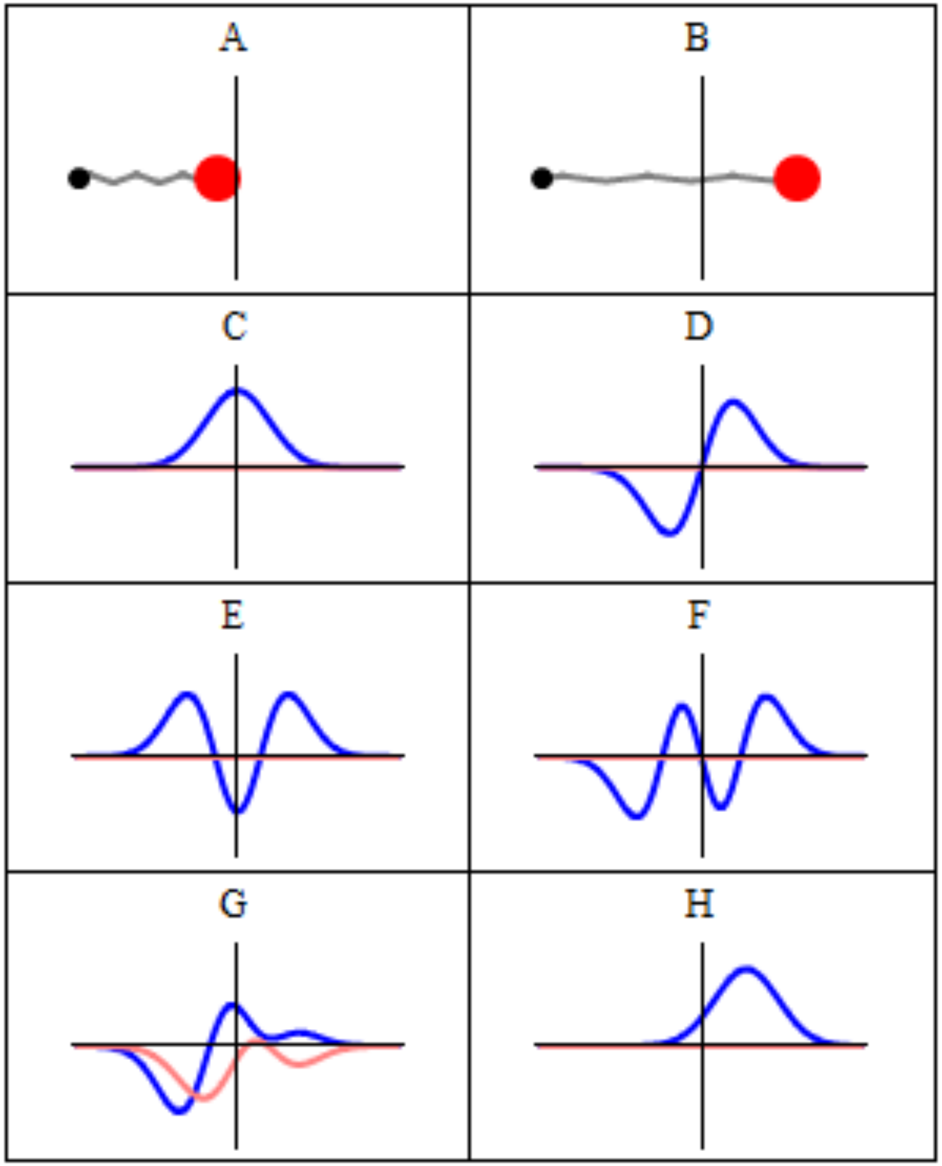
where m is the mass and ω is the angular frequency of the oscillator, which is assumed to be constant.

The corresponding TISE is

$$-\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2}+\frac{1}{2}m\omega^2x^2\phi(x)=E\phi(x),$$

which can be rewritten as

$$\phi''(x)+\frac{2m}{\hbar^2}\left[E-\frac{1}{2}m\omega^2x^2\right]\phi(x)=0,$$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where the prime stands for the ordinary derivative with respect to x. Let us introduce the following abbreviations

$$\lambda = \frac{2mE}{\hbar^2}, \quad \alpha = \frac{m\omega}{\hbar}.$$

Then the TISE becomes

$$\phi'' + [\lambda - \alpha^2 x^2]\phi = 0.$$

This is a second order ordinary differential equation with variable coefficients. Therefore, in order to have an idea about the behavior of the solution at large values of x, let

$$\alpha x \gg 1$$

so that we can neglect the term $\lambda\phi$ in comparison with the term $\alpha^2 x^2 \phi$.

We then have

$$\phi'' - \alpha^2 x^2 \phi = 0.$$

The solution of this equation is

$$\phi(x) = e^{-\alpha x^2/2}$$

for large x. Therefore, we look for the solution of original equation in the form

$$\phi(x) = e^{-\alpha x^2/2} f(x),$$

for large x. Therefore, we look for the solution of original equation in the form

$$\phi' = (-\alpha x f + f')e^{-\alpha x^2/2},$$
$$\phi'' = [(-\alpha f - \alpha x f' + f'') + \alpha^2 x^2 f - \alpha x f']e^{-\alpha x^2/2}.$$

we arrive at the following differential equation for the function f(x)

$$f'' - 2\alpha x f' + (\lambda - \alpha) f = 0.$$

Introducing the dimensionless variable

$$\xi = \sqrt{\alpha} x,$$

we get

$$\frac{d}{dx} = \sqrt{\alpha}\frac{d}{d\xi}, \quad \frac{d^2}{dx^2} = \alpha\frac{d^2}{d\xi^2}.$$

As a result, the equation about TISE can be rewritten as

$$f'' - 2\xi f' + \left(\frac{\lambda}{\alpha} - 1\right) f = 0,$$

where prime stands for ordinary derivative with respect to ξ.

We look for the series solution in the following form

$$f(x) = \sum_{k=\nu}^{\infty} a_k \xi^k,$$

where the value of ν will be determined later. We have

$$\sum_{k=\nu}^{\infty}\left[k(k-1)a_k\xi^{k-2} - 2ka_k\xi^k + \left(\frac{\lambda}{\alpha}-1\right)a_k\xi^k\right] = 0.$$

Writing the series on the left-hand side in the order of increasing powers of ξ , we obtain

$$\nu(\nu-1)a_\nu\xi^{\nu-2} + \nu(\nu+1)a_{\nu+1}\xi^{\nu-1} + (\nu+1)(\nu+2)a_{\nu+2}\xi^\nu$$

$$-2\nu a_\nu\xi^\nu + \left(\frac{\lambda}{\alpha}-1\right)a_\nu\xi^\nu + \ldots = 0.$$

For this equation to hold good, the coefficient before each power of ξ must be equal to zero. We have

$$\nu(\nu-1)=0 \quad \Rightarrow \quad \nu=0,1,$$

$$\nu(\nu+1)=0 \quad \Rightarrow \quad \nu=0,-1.$$

The value -1 of ν is not acceptable because, in that case, the above series will start with the term $\sim\xi^{-1}$ that blows up at $\xi=0$. Hence, ν can take only two values 0 and 1.

Equating the coefficient of ξ^{ν} equal to zero, we arrive at the recursion relation for the coefficients of the series

$$a_{\nu+2} = \frac{2\nu - \left(\frac{\lambda}{\alpha} - 1\right)}{(\nu+1)(\nu+2)} a_\nu.$$

Consequently, we shall have two possible solutions for f (ξ):

$$f_1(\xi) \sim a_0 + a_2\xi^2 + a_4\xi^4 + a_6\xi^6 + ...,$$

and

$$f_2(\xi) \sim a_1\xi + a_3\xi^3 + a_5\xi^5 + ...,$$

Let us take the first of the solutions that starts with $\nu = 0$ and see how it behaves for large values of ξ.

For that, let us determine the behavior of the ratio $a_{\nu+2}/a_{\nu}$ for $\nu \to \infty$. We have

$$\lim_{\nu\to\infty}\frac{a_{\nu+2}}{a_\nu}=\lim_{\nu\to\infty}\frac{\nu\left(2-\frac{\left(\frac{\lambda}{\alpha}-1\right)}{\nu}\right)}{\nu^2(1+1/\nu)(1+2/\nu)}=\frac{2}{\nu}.$$

For comparison, consider the series

$$e^{\xi^2}=\sum_{\sigma=0}^{\infty}b_\sigma\xi^\sigma=1+\frac{\xi^2}{1!}+\frac{\xi^4}{2!}+\frac{\xi^6}{3!}+\ldots+\frac{\xi^\sigma}{\frac{\sigma}{2}!}+\frac{\xi^{\sigma+2}}{\left(\frac{\sigma}{2}+1\right)!}+\ldots$$

For this exponential series,

$$\lim_{\sigma\to\infty}\frac{b_{\sigma+2}}{b_\sigma}=\lim_{\sigma\to\infty}\frac{\frac{\sigma}{2}!}{\left(\frac{\sigma}{2}+1\right)!}=\lim_{\xi\to\infty}\frac{\frac{\sigma}{2}!}{\left(\frac{\sigma}{2}+1\right)\frac{\sigma}{2}!}\approx\frac{2}{\sigma}.$$

Therefore, for large values of ξ , the series from TISE behaves as the exponential series. Consequently, for large values of ξ , the function f (ξ) blows up because

$$f(\xi) \approx e^{-\frac{\xi^2}{2}} \cdot e^{\xi^2} \sim e^{\frac{\xi^2}{2}}.$$

It does not satisfy the boundary conditions and hence, cannot be the acceptable solution.

For this to happen, the series has to be truncated at some term, say n^{th} term. In that case, the numerator in recursion relation for the coefficients would be zero for ν = n.

As a consequence, we get

$$2n - \frac{\lambda}{\alpha} - 1 = 0, \quad \Rightarrow \quad \frac{\lambda}{\alpha} = 2n + 1.$$

Substituting the values of λ and α, we obtain

$$\frac{2mE_n}{\hbar^2} = \frac{m\omega}{\hbar}(2n+1).$$

It leads to the quantization of energy of the harmonic oscillator:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, 3, \ldots$$

Note that this formula for the quantized energy of the oscillator differs from the one obtained in the old quantum theory

$$E_n = n\hbar\omega, \quad n = 0, 1, 2, 3, \ldots$$

Let us go back to our problem of finding the solutions to the differential equation. Evidently, the solutions satisfying the standard conditions can now be written as

$$\phi_n(\xi) = N_n e^{-\xi^2/2} H_n(\xi),$$

where N_n is the normalization constant and $H_n(\xi)$ is the polynomial of degree n. These polynomials for different n values are known as Hermite polynomials. The coefficient is given by

$$a_n = \frac{2(n-2)+1-(2n+1)}{n(n-1)} a_{n-2} = -\frac{4}{n(n-1)} a_{n-2}.$$

Therefore, we have

$$a_{n-2} = -\frac{n(n-1}{4} a_n \equiv -\frac{n(n-1)}{1 \times 2^2} a_n.$$

Similarly, we can compute

$$a_{n-4} = -\frac{(n-2)(n-1)}{8} a_{n-2} = \frac{n(n-1)(n-2)(n-3)}{1 \times 2 \times 2^2} a_n,$$

and so on and so forth. As a result, the polynomial will be given by

$$H_n(\xi) = a_n \left[\xi^n - \frac{n(n-1)}{1 \times 2^2} \xi^{n-2} + \frac{n(n-1)(n-2)(n-3)}{1 \times 2 \times 2^2} \xi^{n-4} - \ldots \right].$$

If we put

$$a_n = 2^n, n = 0, 1, 2, 3, ...,$$

we obtain the formulae for the polynomials of the corresponding degree. A few of these are given here for illustration:

$$H_0(\xi) = 1, \qquad H_1(\xi) = 2\xi,$$
$$H_2(\xi) = 4\xi^2 - 2, \qquad H_3(\xi) = 8\xi^3 - 12\xi,$$
$$H_4(\xi) = 16\xi^4 - 48\xi^2 + 12, \qquad H_5(\xi) = 32\xi^5 - 160\xi^3 + 120\xi.$$

Rodriguez's formula for the Hermite polynomials:

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

Recurrence formula for Hermite polynomials:

$$H_{n+1}(\xi) = 2\xi H_n(\xi) - 2n H_{n-1}(\xi).$$

The normalization coefficients

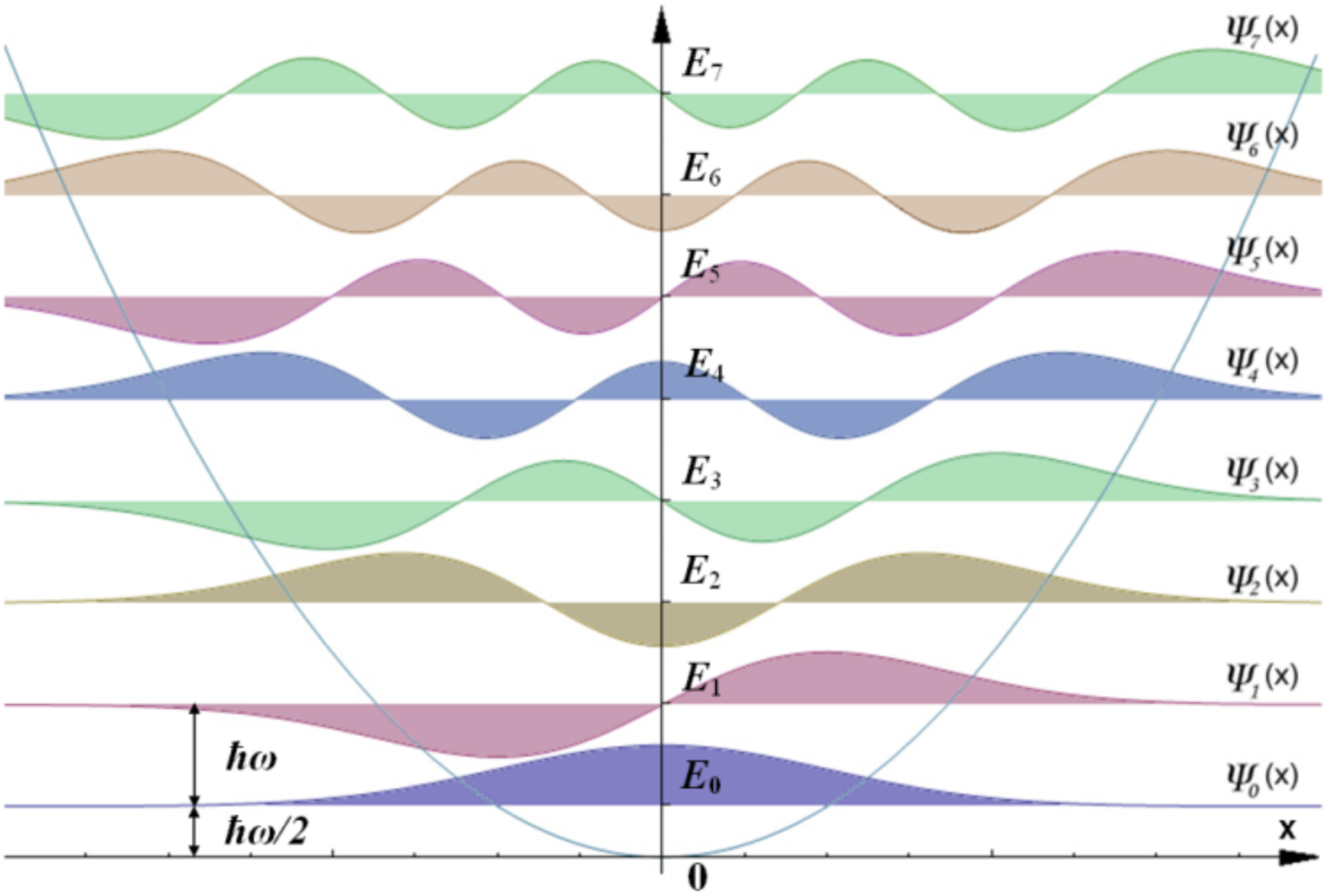
$$\int_{-\infty}^{+\infty} |\phi_n(\xi)|^2 d\xi = (-1)^n \frac{N_n^2}{\sqrt{\alpha}} \int_{-\infty}^{+\infty} e^{-\xi^2} e^{\xi^2} \frac{d^n e^{-\xi^2}}{d\xi^n} H_n(\xi)\, d\xi$$

$$= (-1)^n \frac{N_n^2}{\sqrt{\alpha}} \int_{-\infty}^{+\infty} \frac{d^n e^{-\xi^2}}{d\xi^n} H_n(\xi)\, d\xi.$$

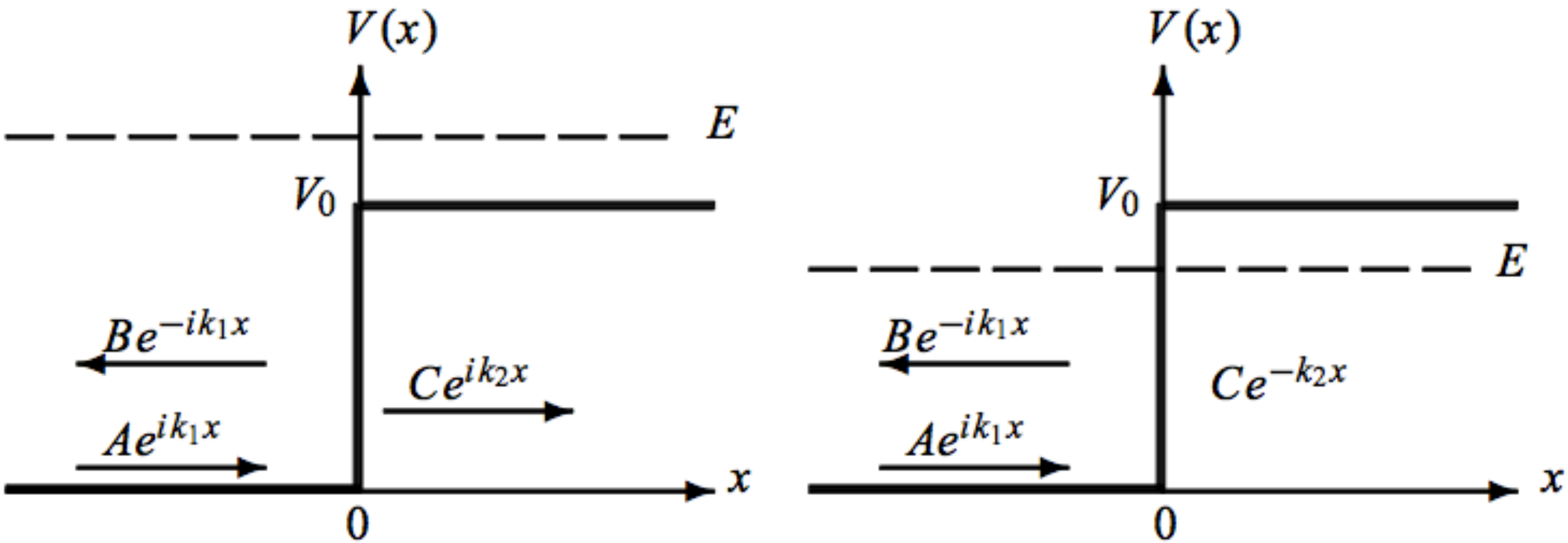
Finally

$$N_n = \sqrt{\frac{\alpha^{1/2}}{2^n n! \pi^{1/2}}}.$$

One-dimensional Harmonic Oscillator



Step Potential



A free particle of mass, m, and total energy, E, is incident from $x \to -\infty$、 on a potential step given by

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

where $V_0 > E$ is a positive constant.

Step Potential

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The given potential divides the entire region $-\infty < x < +\infty$ into two halves:

$x < 0$, where the potential is zero

$x > 0$, where the potential has a constant value V_0.

We will call them Region 1 and Region 2, respectively.

In region 1,

$$\frac{d^2\phi}{dx^2} + \frac{2mE}{\hbar^2}\phi = 0$$

has the following general solution

$$\phi(x) = Ae^{ik_1 x} + Be^{-ik_1 x}, \qquad k_1^2 = 2mE/\hbar^2$$

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As a result,

$$\psi_1(x,t) = Ae^{i(kx-\frac{E}{\hbar}t)} + Be^{-i(kx+\frac{E}{\hbar}t)}$$

The first term of this solution represents the incident particle moving along the positive x-axis, while the second term represents the particle reflected by the potential barrier and moving along the negative x-axis.

In region 2,

$$\frac{d^2\phi}{dx^2} - \frac{2m(V_0-E)}{\hbar^2}\phi = 0.$$

Its general solution is

$$\phi(x) = Ce^{-k_2x} + De^{k_2x}, \qquad k_2^2 = 2m(V_0-E)/\hbar^2$$

Step Potential

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Since the wave function must tend to zero at spatial infinities ($x \to \pm\infty$), we must put

$$D = 0,$$

otherwise the solution will diverge. Therefore, the stationary state solution in the second region can be written as

$$\psi_2(x,t) = Ce^{-k_2 x - i(E/\hbar)t}.$$

Since the potential has only a finite jump at x = 0, both the wave functions (ϕ_1 and ϕ_2) and their first-order derivatives must be continuous at x = 0. We thus have

$$A + B = C,$$

$$ik_1(A - B) = -k_2 C.$$

There is a small problem here because we have only two equations but three constants to be determined. Let us first determine the coefficients B and C in terms of the constant A.

$$1+\frac{B}{A}=\frac{C}{A},$$

$$1-\frac{B}{A}=\frac{ik_2}{k_1}\frac{C}{A}.$$

Solving these equations for C/A, we get

$$C=\frac{2k_1}{k_1+ik_2}A.$$

$$B=\frac{k_1-ik_2}{k_1+ik_2}A.$$

Now, without any loss of generality, we might assume that the incident particle's wave function (a wave packet) is normalized in such a way that A = 1. Then the required wave function is

$$\phi(x) = \begin{cases} e^{i(k_1 x - \omega t)} + \dfrac{k_1 - ik_2}{k_1 + ik_2} e^{-i(k_1 x + \omega t)} & x < 0 \\ \dfrac{2k_1}{k_1 + ik_2} e^{-(k_2 x + i\omega t)} & x > 0 \end{cases}$$

where,

$$\omega = E/\hbar.$$

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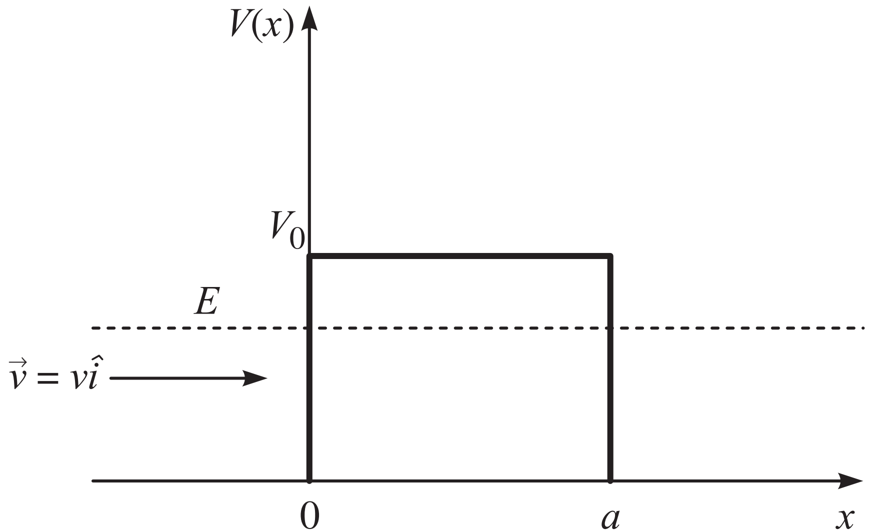
Barrier penetration – tunneling: a micro-particle incident on one side of a potential barrier of height V_0 with a total energy $E < V_0$ can pass through the barrier and appear on the other side.

This phenomenon does not have any classical analogue and represents a purely quantum mechanical effect and has been confirmed experimentally. Consider an external potential field given by

$$V(x) = \begin{cases} V_0, & \text{for } \ 0 \leq x \leq a, \\ 0, & \text{otherwise.} \end{cases}$$

The case with the total energy $E < V_0$ corresponds to tunneling and we take up this case.

For the solution of the problem, we divide the entire region $-\infty<x<+\infty$ into three parts: $-\infty<x<0$ (Region 1), $0<x<a$ (Region 2) and $a<x<+\infty$ (Region 3). The one-dimensional potential barrier has width a and height V_0.



Region 1:

$$\phi_1'' + k_1^2 \phi_1 = 0, \qquad k_1^2 = \frac{2mE}{\hbar^2},$$

$$\phi_1 = A\, e^{ik_1 x} + B\, e^{-ik_1 x},$$

where A and B are arbitrary complex constants. Here the first term in the solution corresponds to the incident particle propagating along the positive x direction, while the second term describes the particle reflected from the potential and propagating along the negative x direction.

Region 2:

$$\phi_2'' - k_2^2 \phi_2 = 0, \qquad k_2^2 = \frac{2m(V_0 - E)}{\hbar^2},$$

$$\phi_2 = C\, e^{k_2 x} + D\, e^{-k_2 x},$$

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Region 1:

$$\phi_1'' + k_1^2 \phi_1 = 0, \qquad k_1^2 = \frac{2mE}{\hbar^2},$$

$$\phi_1 = A\, e^{ik_1 x} + B\, e^{-ik_1 x},$$

Region 2:

$$\phi_2'' - k_2^2 \phi_2 = 0, \qquad k_2^2 = \frac{2m(V_0 - E)}{\hbar^2},$$

$$\phi_2 = C\, e^{k_2 x} + D\, e^{-k_2 x},$$

Region 3:

$$\phi_3'' + k_1^2 \phi_3 = 0,$$

$$\phi_3 = F\, e^{ik_1 x}.$$

Here, F is an arbitrary complex constant and the solution represents the transmitted particle traveling along the positive x direction. Note that, because of the fact that the potential vanishes beyond x = a, there is no any reflected particle in this region and hence, we have taken only the forward propagating plane wave as solution.

Boundary conditions: The wave functions $\phi_1(x)$, $\phi_2(x)$ and $\phi_3(x)$ have to be continuous in the entire region of x, as required by the standard conditions. The first derivatives of the wave functions with respect to x will also be continuous everywhere. These boundary conditions then yield

$$A + B = C + D,$$

$$(A - B) = -\frac{i k_2}{k_1}(C - D),$$

and

$$C e^{k_2 a} + D e^{-k_2 a} = F e^{ik_1 a},$$

$$C e^{k_2 a} - D e^{-k_2 a} = \frac{i k_1}{k_2} F e^{ik_1 a}.$$

If we add up above equation, we get

$$2C e^{k_2 a} = F e^{ik_1 a}\left(1 + \frac{i k_1}{k_2}\right).$$

Hence

$$C = \frac{F}{2} e^{ik_1 a}\left(1 + \frac{i k_1}{k_2}\right) e^{-k_2 a}.$$

Similarly, if we subtract them

$$2D\,e^{-k_2 a} = F\,e^{ik_1 a}\left(1 - \frac{i\,k_1}{k_2}\right),$$

and therefore,

$$D = \frac{F}{2}\,e^{ik_1 a}\left(1 - \frac{i\,k_1}{k_2}\right)\,e^{k_2 a}.$$

Finally, the relation between A, B, and F are

$$1 + \frac{B}{A} = \frac{F}{2A}\,e^{ik_1 a}\left[\left(1 + \frac{i\,k_1}{k_2}\right)\,e^{-k_2 a} + \left(1 - \frac{i\,k_1}{k_2}\right)\,e^{k_2 a}\right]$$

$$= \frac{F}{A}\,e^{ik_1 a}\left[\frac{e^{k_2 a} + e^{-k_2 a}}{2} - \frac{i\,k_1}{k_2}\,\frac{\left(e^{k_2 a} - e^{-k_2 a}\right)}{2}\right]$$

$$= \frac{F}{A}\,e^{ik_1 a}\left[\cosh(k_2 a) - \frac{i\,k_1}{k_2}\,\sinh(k_2 a)\right].$$

and

$$1-\frac{B}{A}=\frac{F}{2A}e^{ik_1a}\left[\left(-\frac{ik_2}{k_1}+1\right)e^{-k_2a}+\left(\frac{ik_2}{k_1}+1\right)e^{k_2a}\right]$$
$$=\frac{F}{A}e^{ik_1a}\left[\frac{e^{k_2a}+e^{-k_2a}}{2}+\frac{ik_2}{k_1}\frac{\left(e^{k_2a}-e^{-k_2a}\right)}{2}\right]$$
$$=\frac{F}{A}e^{ik_1a}\left[\cosh(k_2a)+\frac{ik_2}{k_1}\sinh(k_2a)\right].$$

Therefore

$$2=\frac{F}{A}e^{ik_1a}\left[2\cosh(k_2a)+i\left(\frac{k_2}{k_1}-\frac{k_1}{k_2}\right)\sinh(k_2a)\right].$$

$$2\frac{B}{A}=-i\frac{F}{A}e^{ik_1a}\left(\frac{k_2}{k_1}+\frac{k_1}{k_2}\right)\sinh(k_2a).$$

The reflection coefficient is defined as

$$\mathscr{R} = \frac{\text{Reflected particle flux density}}{\text{Incident particle flux density}} = \frac{J_R}{J_I} = \frac{v_1|B|^2}{v_1|A|^2} = \frac{|B|^2}{|A|^2}.$$

It is given by

$$\mathscr{R} = \frac{\left(\frac{k_2^2+k_1^2}{k_2 k_1}\right)^2 \sinh^2(k_2 a)}{\left[4\cosh^2(k_2 a) + \left(\frac{k_2^2-k_1^2}{k_1 k_2}\right)^2 \sinh^2(k_2 a)\right]}.$$

The transmission coefficient, on the other hand, is defined as

$$\mathscr{T} = \frac{\text{Transmitted particle flux density}}{\text{Incident particle flux density}} = \frac{J_T}{J_I} = \frac{|F|^2}{|A|^2}.$$

and

$$\mathscr{T} = \frac{4}{\left[4\cosh^2(k_2 a) + \left(\frac{k_2^2-k_1^2}{k_1 k_2}\right)^2 \sinh^2(k_2 a)\right]}.$$

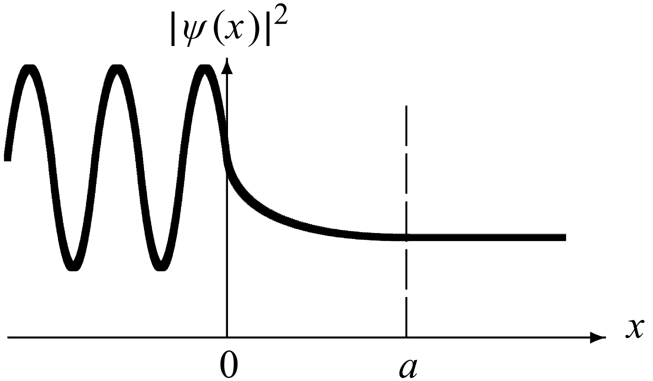
Further, making use of the well-known formula $\cosh^2 x - \sinh^2 x = 1$, we can rewrite the reflection and the transmission coefficients as

$$\mathscr{R} = \frac{\mathscr{T}}{4}\left(\frac{k_1^2 + k_2^2}{k_2 k_1}\right)^2 \sinh^2(k_2 a),$$

$$\mathscr{T} = \frac{1}{\left[1 + \frac{1}{4}\left(\frac{k_1^2+k_2^2}{k_2 k_1}\right)^2 \sinh^2(k_2 a)\right]}$$

Clearly, the transmission probability is finite. Therefore, we conclude that the probability that a quantum particle could penetrate a classically impenetrable barrier is non-zero.

This barrier penetration effect is usually called the tunneling effect and has important physical implications. The radioactive decay and charge transport in electronic devices are typical examples of the quantum mechanical tunneling effect.



$E < V_0$

Using the expressions for k_1 and k_2 in terms of the physical parameters, we have

$$\left(\frac{k_1^2+k_2^2}{k_2 k_1}\right)^2 = \left(\frac{V_0}{\sqrt{E(V_0-E)}}\right)^2 = \frac{V_0^2}{E(V_0-E)}.$$

Therefore, we can rewrite the expressions for the reflection and transmission coefficients as

$$\mathscr{R} = \mathscr{T}\frac{V_0^2}{4E(V_0-E)}\ \sinh^2\left(\frac{a}{\hbar}\sqrt{2m(V_0-E)}\right),$$

$$\mathscr{T} = \frac{1}{1+\frac{1}{4}\frac{V_0^2}{E(V_0-E)}\ \sinh^2\left(\frac{a}{\hbar}\sqrt{2m(V_0-E)}\right)}.$$

Let us consider the case when the energy of the incident particle is much smaller than the height of the barrier $E \ll V_0$. Then, we have

$$\frac{a}{\hbar}\sqrt{2m(V_0-E)} = \frac{a\sqrt{2mV_0}}{\hbar}\sqrt{1-\frac{E}{V_0}} \gg 1,$$

and we can write

$$\sinh\left(\frac{a}{\hbar}\sqrt{2m(V_0-E)}\right)\sim\frac{1}{2}e^{\frac{a\sqrt{2mV_0}}{\hbar}\sqrt{1-\frac{E}{V_0}}}=\frac{1}{2}\,e^{(a/\hbar)\sqrt{2m(V_0-E)}}.$$

Therefore, in the low energy limit, the transmission coefficient is given by

$$\mathscr{T}=\frac{16E}{V_0}\left(1-\frac{E}{V_0}\right)\,e^{-(2a/\hbar)\sqrt{2m(V_0-E)}}.$$

Also, when $E \sim V_0$, it is not difficult to deduce the following expressions for the reflection and transmission coefficients:

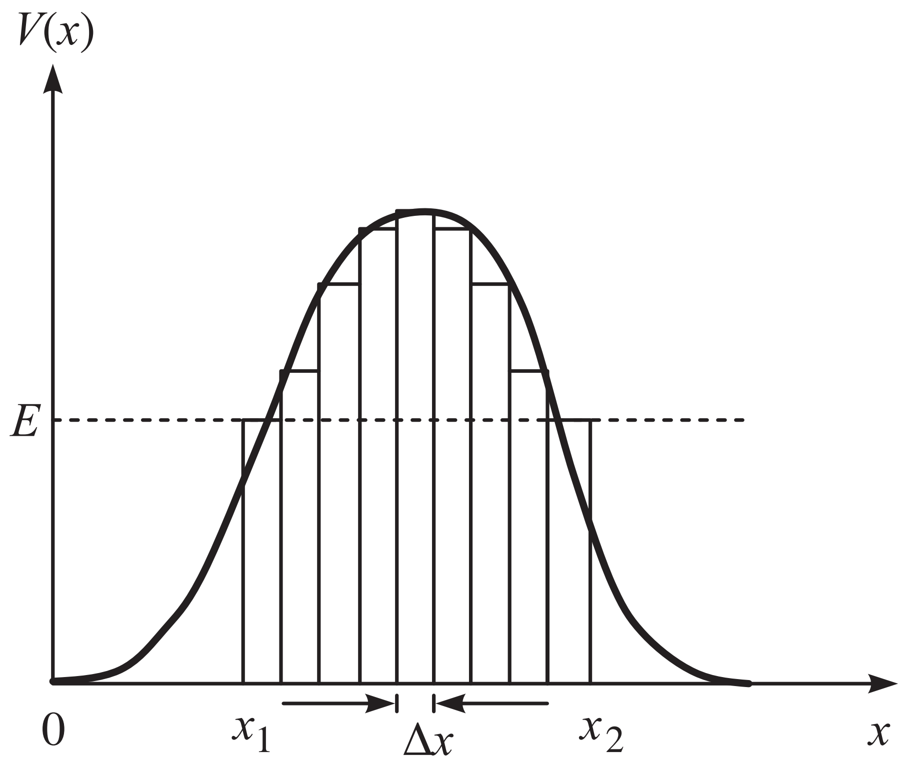
$$\mathscr{R}=\left(1+\frac{2\hbar^2}{ma^2V_0}\right)^{-1},$$

$$\mathscr{T}=\left(1+\frac{ma^2V_0}{2\hbar^2}\right)^{-1}.$$

We, thus, see that even if the energy of the particle is much smaller than the barrier height, there is a finite probability that the particle can tunnel through the barrier and appear on the other side of it. Classically, such a phenomenon is not possible.

The region $0 < x < a$ is forbidden for a particle with energy less than the barrier height V_0. Quantum mechanically, such tunneling effect is permissible and the apparent paradox arising out of it can be resolved with the help of Heisenberg's uncertainty principle.

Note that in the given example we considered the constant value for the potential barrier. In a more general case, the potential barrier is not a constant but can be a function of x: V = V (x)



An approximate formula for the transmission coefficient can be derived by dividing the classically forbidden region between the turning points x_1 and x_2 into N (N large enough to approximate the curve V (x)) small rectangular sequence of barriers, each of width Δx.

In each of these rectangular barriers, we can assume the potential to be constant. Then for each of them, the transmission coefficient can be written as:

$$\mathscr{T}_i \sim \exp\left[-\frac{2\Delta x_i}{\hbar}\sqrt{2m(V(x_i)-E)}\right],$$

The transmission coefficient for the entire potential is then given by the following limit:

$$\mathscr{T} \approx \exp\left[-\frac{2}{\hbar}\lim_{\Delta x_i \to 0}\sum_{i=1} f(x_i)\,\Delta x_i\right],$$

where

$$f(x_i) = \sqrt{2m(V(x_i) - E)}.$$

As a result, we obtain

$$\mathscr{T} \approx \exp\left[-\frac{2}{\hbar}\int_{x_1}^{x_2} dx\sqrt{2m(V(x) - E)}\right].$$

Note that the aforementioned approximate analysis is valid and gives satisfactory results only if the potential is a smooth and slowly varying function of x.

Potential Barrier and Tunneling

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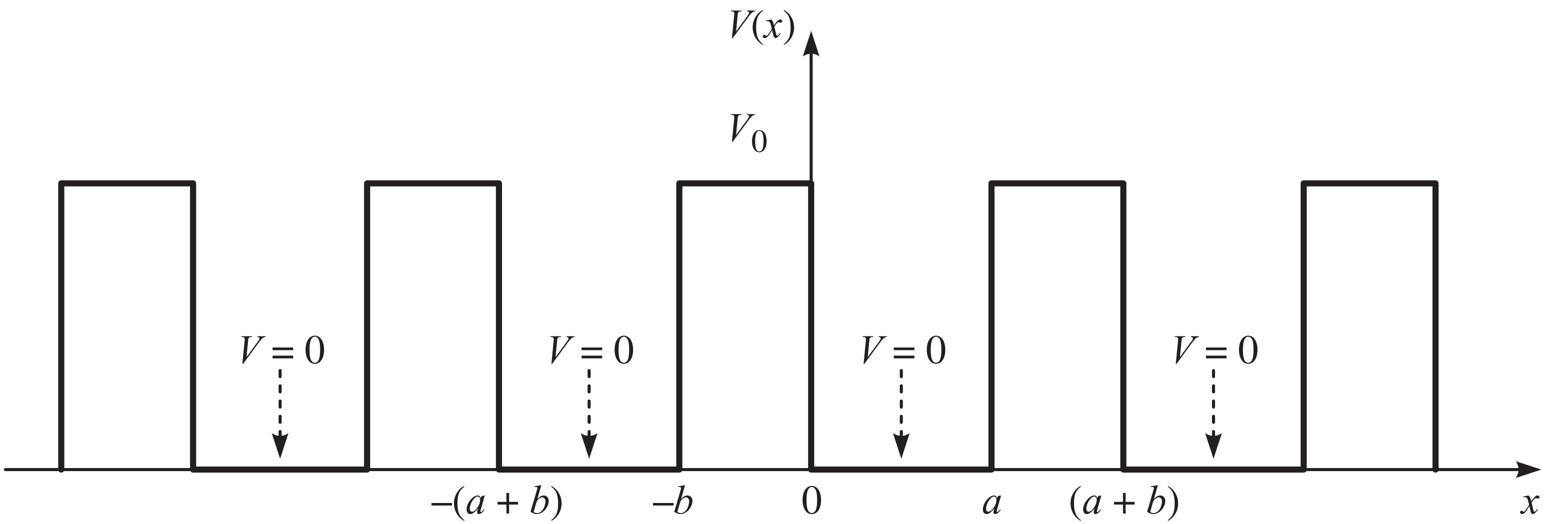
A typical periodic potential is shown



As shown, the potential is zero over a distance a, peaks at $V(x) = V_0$ over a distance b and then repeats itself. It is evident that

$$V(x+c) = V(x).$$

where c = a + b is the period. Since the potential is a periodic function of x with a period c, the Schroedinger equation is invariant under space translations

$$x \to x + nc, \quad n = 0, \pm 1, \pm 2, \pm 3, \ldots$$

This invariance imposes certain restriction on the form of the allowable solution of the Schroedinger equation. To determine this restriction, let us introduce an operator D, called the space translation operator, which while acting on a function f (x) shifts it horizontally along the x direction over a distance c:

$$\hat{D} f(x) = f(x + c).$$

For instance, acting on the potential function V(x), it shifts the entire potential over a distance c: DV (x) = V(x + c). Repeated applications this operator leads to

$$\hat{D}f(x) = f(x+c), \hat{D}^2 f(x) = f(x+2c), \hat{D}^3 f(x) = f(x+3c), \ldots, \hat{D}^n f(x) = f(x+nc).$$

Considering now the following

$$(\hat{D}\hat{H})\psi(x) = \hat{D}(\hat{H}\psi) = \hat{D}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x)$$

$$= \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x+c)\right)\psi(x+c)$$

$$= \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x+c)$$

$$= \hat{H}\left(\hat{D}\psi(x)\right) = \left(\hat{H}\hat{D}\right)\psi(x).$$

In obtaining the above result we have used the fact that

$$\frac{\partial}{\partial(x+c)} = \frac{\partial}{\partial x}\frac{\partial x}{\partial(x+c)} = \frac{\partial}{\partial x}.$$

Therefore,

$$\hat{H}\left(\hat{D}\psi(x)\right) = \left(\hat{H}\hat{D}\right)\psi(x) = \left(\hat{D}\hat{H}\right)\psi(x) = E\left(\hat{D}\psi(x)\right),$$

This, in turn means that, if the energy spectrum is non-degenerate, ψ (x + c) and ψ (x) must represent the same state of the system. Therefore, ψ (x + c) can differ from ψ (x) only by a constant factor:

$$\psi(x+c) = \alpha\,\psi(x),$$

where α is a constant of magnitude unity.

$$\alpha = \exp\left(\frac{2\pi i\ell}{n}\right), \qquad \ell = 0, 1, 2, 3, \ldots$$

Defining now

$$\kappa = \frac{2\pi\ell}{n\,c},$$

we arrive at

$$\psi(x+nc) = e^{i\kappa c}\psi(x).$$

Now, any function $\psi(x)$, satisfying the above condition, can be written as

$$\psi(x) = e^{i\kappa x}u_\kappa(x),$$

where $u_\kappa(x)$ is a periodic function of x of period c: $u_\kappa(x + c) = u_\kappa(x)$. To ensure that it is really so, we write

$$\psi(x+c) = e^{i\kappa\,(x+c)} u_\kappa(x+c) = e^{i\kappa c} e^{i\kappa x} u_\kappa(x+c).$$

Therefore, if $u_\kappa(x + c) = u_\kappa(x)$,

$$\psi(x+c) = e^{i\kappa(x+c)} u_\kappa(x+c) = e^{i\kappa c} e^{i\kappa x} u_\kappa(x) = e^{i\kappa c} \psi(x).$$

The above result is a fundamental result for condensed matter physics and it is known as Bloch's theorem.

It states that any solution to the Schroedinger equation, with a periodic potential of period c, must have this form.

Consider now the case of a particle (mass m and total energy $E < V_0$) subject to the above periodic potential. If we introduce

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

$$k_2^2 = \frac{2m(V_0 - E)}{\hbar^2},$$

the solutions of the TISE in the relevant regions can be written as

$$\psi(x) = A\cos(k_1 x) + B\sin(k_1 x), \quad (0 < x < a),$$

$$\psi(x) = C\cosh(k_2 x) + D\sinh(k_2 x), \quad (-b < x < 0),$$

They must be chosen such that both $\psi(x)$ and $\psi'(x)$ are continuous at the boundaries, where the potential has a finite jump, and abide by Bloch's theorem.

At x = 0, we have

$$A = C,$$

$$k_1 B = k_2 D.$$

Furthermore, using the Bloch theorem (with n = 1), we get

$$\psi(a) = e^{iKc}\,\psi(-b),$$

$$\psi'(a) = e^{iKc}\,\psi'(-b),$$

$$K = \frac{2\pi\ell}{(a+b)}.$$

The boundary conditions lead to

$$A\cos(k_1 a) + B\sin(k_1 a) = e^{iKc}\left[C\cosh(k_2 b) - D\sinh(k_2 b)\right],$$

$$-k_1 A\sin(k_1 a) + k_1 B\cos(k_1 a) = e^{iKc}\left[-k_2 C\sinh(k_2 b) + k_2 D\cosh(k_2 b)\right].$$

The algebraic equations can be written as a matrix equation:

$$\mathscr{M} X = 0,$$

where

$$X = (A\ B\ C\ D)^T$$

is a column matrix and

$$\mathscr{M} = \begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & k_1 & 0 & -k_2 \\ \cos(k_1 a) & \sin(k_1 a) & -e^{iKc}\cosh(k_2 b) & e^{iKc}\sinh(k_2 b) \\ -k_1\sin(k_1 a) & k_1\cos(k_1 a) & k_2 e^{iKc}\sinh(k_2 b) & -k_2 e^{iKc}\cosh(k_2 b) \end{pmatrix}$$

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For the non-trivial solutions the determinant of the matrix, must be zero:

$$|\mathscr{M}| = \begin{vmatrix} 1 & 0 & -1 & 0 \\ 0 & k_1 & 0 & -k_2 \\ \cos(k_1 a) & \sin(k_1 a) & -e^{iKc}\cosh(k_2 b) & e^{iKc}\sinh(k_2 b) \\ -k_1\sin(k_1 a) & k_1\cos(k_1 a) & k_2 e^{iKc}\sinh(k_2 b) & -k_2 e^{iKc}\cosh(k_2 b) \end{vmatrix} = 0.$$

Finally,

$$(k_1^2 - k_2^2)\sinh(k_2 b)\sin(k_1 a) - 2k_1 k_2\cosh(k_2 b)\cos(k_1 a) + k_1 k_2\left[e^{iKc} + e^{-iKc}\right] = 0.$$

It yields the following transcendental equation for the determination of the energy eigenvalues

$$\frac{(k_2^2 - k_1^2)}{2k_1 k_2}\sinh(k_2 b)\sin(k_1 a) + \cosh(k_2 b)\cos(k_1 a) = \cos[K(a+b)].$$

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As a result of the numerical solution, one gets the values of k_1 using which one can calculate the energy eigenvalues as

$$E = \frac{\hbar^2 k_1^2}{2m}.$$

Note that, for practical purposes, the above transcendental equation can be simplified by imposing some reasonable restrictions on the model parameters.

Assume that the width of the potential tends to zero while the height tends to infinity such that $V_0 b$ remains constant. In such a limit

$$\lim_{b\to 0} \sinh(k_2 b) = k_2 b, \qquad \lim_{b\to 0} \cos(k_2 b) = 1.$$

Here, we have gone to the leading order in the Taylor expansions of the hyperbolic trigonometric functions on the left-hand side, and simply let b = 0 on the right-hand side. We obtain

$$\frac{(k_2^2 - k_1^2)}{2k_1} b \sin(k_1 a) + \cos(k_1 a) = \cos[Ka].$$

We then find it convenient to define the dimensionless quantity,

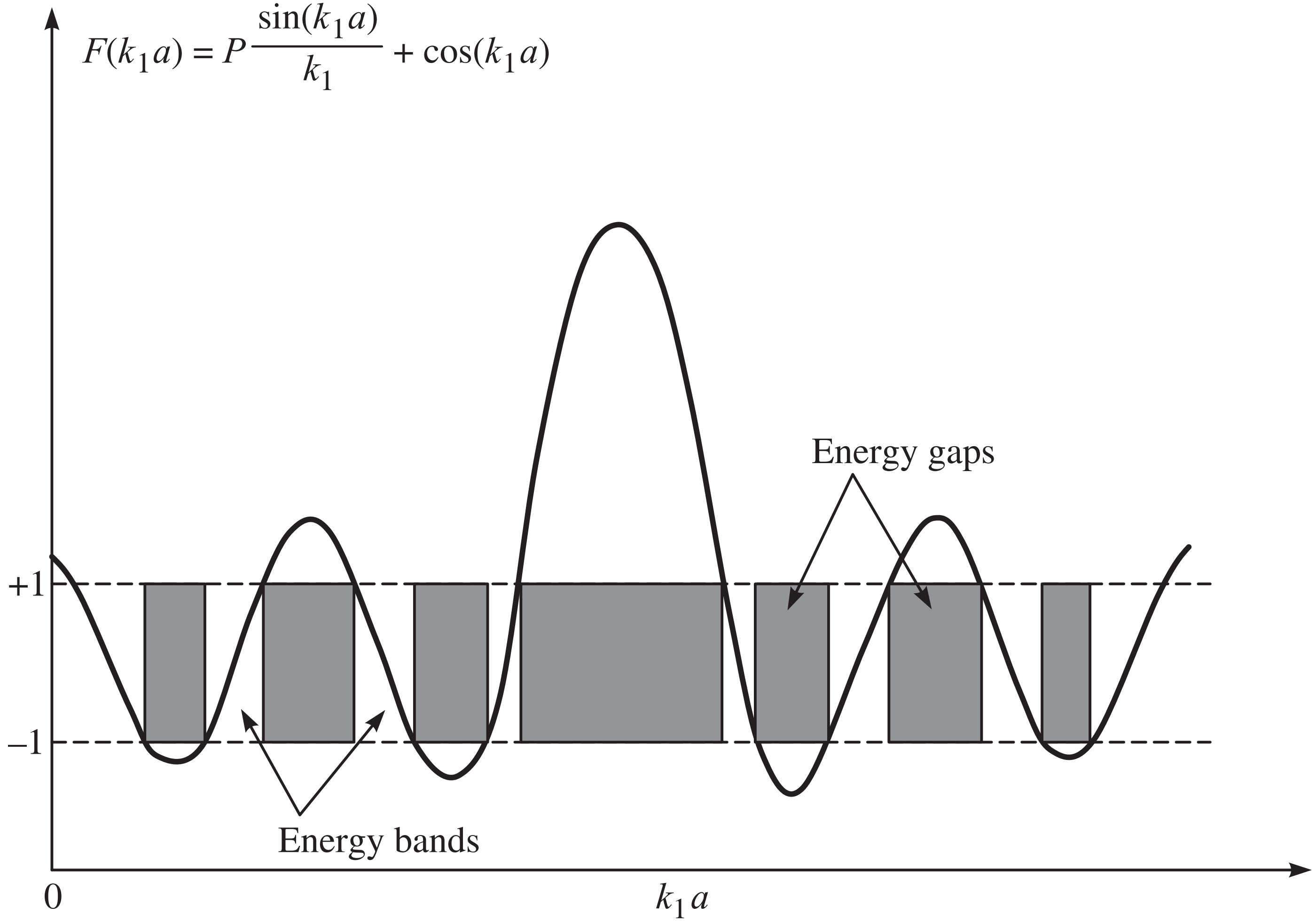
$$P = \frac{mV_0 ba}{2},$$

which determines the effective strength of the potential. Then we have

$$F(k_1 a) = \cos[Ka],$$

where

$$F(k_1 a) = P\frac{\sin(k_1 a)}{k_1} + \cos(k_1 a).$$



1. Find the value of the commutator

$$\hat{A} = [\hat{p}_x^2, (\hat{x}\hat{p}_y - \hat{y}\hat{p}_x)],$$

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1. Find the value of the commutator

$$\hat{A} = [\hat{p}_x^2, (\hat{x}\hat{p}_y - \hat{y}\hat{p}_x)],$$

Solution: Using the properties of the commutator of operators

$$[\hat{A}, \hat{B} + \hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}],$$

$$[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B},$$

$$[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C},$$

we get

$$[\hat{p}_x^2, (\hat{x}\hat{p}_y - \hat{y}\hat{p}_x)] = [\hat{p}_x^2, \hat{x}\hat{p}_y] - [\hat{p}_x^2, \hat{y}\hat{p}_x]$$

$$= \hat{p}_x[\hat{p}_x, \hat{x}\hat{p}_y] + [\hat{p}_x, \hat{x}\hat{p}_y]\hat{p}_x - \hat{p}_x[\hat{p}_x, \hat{y}\hat{p}_x] - [\hat{p}_x, \hat{y}\hat{p}_y]\hat{p}_x$$

$$= \hat{p}_x\hat{x}[\hat{p}_x, \hat{p}_y] + \hat{p}_x[\hat{p}_x, \hat{x}]\hat{p}_y + \hat{x}[\hat{p}_x, \hat{p}_y]\hat{p}_x + [\hat{p}_x, \hat{x}]\hat{p}_y\hat{p}_x$$

$$- \hat{p}_x\hat{y}[\hat{p}_x, \hat{p}_x] - \hat{p}_x[\hat{p}_x, \hat{y}]\hat{p}_x - \hat{y}[\hat{p}_x, \hat{p}_y]\hat{p}_x - [\hat{p}_x, \hat{y}]\hat{p}_y\hat{p}_x$$

$$= -i\hbar(\hat{p}_x\hat{p}_y + \hat{p}_y\hat{p}_x) = -2i\,\hat{p}_x\hat{p}_y\hbar$$

$$[\hat{x}_j, \hat{p}_k] = i\hbar\delta_{jk}, \; j,k = 1,2,3.$$

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2.Consider a particle of mass m confined to move in one spatial dimension in the region $0 < x < a$. Let the particle be in a state described by the wave function $\psi_1(x,t) = \sin(\pi x/a) \exp(-i\omega t)$, where ω is a constant. Find the average values of the position and momentum operators in this state.

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Solution: First, let us check whether the wave function of the particle is normalized or not. We have

$$\int_0^a |\psi_1(x,t)|^2 \, dx = \frac{a}{2}.$$

The average value of the position operator and momentum will be given by

$$\langle \hat{x} \rangle = \int_0^a \hat{x} |\psi(x,t)|^2 \, dx = a/2. \qquad \langle \hat{p}_x \rangle = \int_0^a \psi^*(x,t) \left(-i\hbar \frac{d}{dx} \right) \psi(x,t) \, dx = 0.$$

3.Consider a particle of mass m confined to move in a one-dimensional infinite potential well of width a. Let, at t = 0, the particle be in a state described by the wave function $\psi(x,t) = \sin^3(\pi x/a)$. If the energy of the particle is measured, what values will be obtained and with what probabilities? What will be the average value of energy in this state?

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Solution: We shall show that the eigenfunctions and the corresponding eigenvalues of the Hamiltonian, for a particle of mass m moving in a 1D infinite potential well of width a, are given by

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin(n\pi x/a), \quad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}, \quad n = 1, 2, 3, \ldots$$

The wave function of the particle at t = 0 can be written as

$$\psi(x) = \frac{3}{4}\sin(\pi x/a) - \frac{1}{4}\sin(3\pi x/a) = \frac{3\sqrt{a}}{4\sqrt{2}}\phi_1(x) - \frac{\sqrt{a}}{4\sqrt{2}}\phi_3(x),$$

Normalization constant

$$\int_0^a |\psi(x)|^2\,dx = \frac{9a}{32}\int_0^a |\phi_1(x)|^2\,dx + \frac{a}{32}\int_0^a |\phi_3(x)|^2\,dx$$

$$-\frac{6a}{32}\int_0^a \phi_1(x)\phi_3(x)\,dx = \frac{9a}{32} + \frac{a}{32} = \frac{5a}{16},$$

As a result, the normalized wave function at t = 0 is

$$\phi(x) = \frac{4}{\sqrt{5a}}\frac{3\sqrt{a}}{4\sqrt{2}}\phi_1(x) - \frac{4}{\sqrt{5a}}\frac{\sqrt{a}}{4\sqrt{2}}\phi_3(x) = \frac{3}{\sqrt{10}}\phi_1(x) - \frac{1}{\sqrt{10}}\phi_3(x).$$

Therefore, when energy is measured on the system, the values that can result are

$$E_1 = \frac{\pi^2\hbar^2}{2ma^2} \qquad \text{and} \qquad E_3 = \frac{9\pi^2\hbar^2}{2ma^2}.$$

Now the probability of getting E_1 and E_3 are

$$P_1 = |\langle\phi_1 \mid \phi\rangle|^2 = \frac{9}{10}, \qquad P_3 = |\langle\phi_3 \mid \phi\rangle|^2 = \frac{1}{10}.$$

The average value of energy in the state is

$$\langle E\rangle = P_1E_1 + P_3E_3 = \frac{9}{10} \times \frac{\pi^2\hbar^2}{2ma^2} + \frac{1}{10} \times \frac{9\pi^2\hbar^2}{2ma^2} = \frac{9\pi^2\hbar^2}{10ma^2}.$$

Exercise

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4. A particle in an infinite symmetrical potential well of width a ($-a/2 \le x \le a/2$) is initially ($t = 0$) in a state with the wave function

$$\psi(x,0) = A\left(1 - \frac{x^2}{a^2}\right),$$

where A is an arbitrary real constant. Find the wave function $\psi(x,t)$ at $t > 0$.

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4. A particle in an infinite symmetrical potential well of width 2a (-a≤ x ≤ a) is initially (t = 0) in a state with the wave function

$$\psi(x,0) = A\left(1 - \frac{x^2}{a^2}\right),$$

where A is an arbitrary real constant. Find the wave function ψ(x,t) at t > 0.

Solution: First, we normalize the wave function to find A. We have

$$\int_{-a}^{+a} |\psi(x,t)|^2 dx = A^2 \int_{-a}^{+a} \left(1 - 2\frac{x^2}{a^2} + \frac{x^4}{a^4}\right) dx$$

$$= A^2\left(2a - \frac{4a}{3} + \frac{2a}{5}\right) = A^2\frac{16a}{15} = 1.$$

This gives the constant A as

$$A = \frac{\sqrt{15}}{4\sqrt{a}}.$$

The general solution at t > 0 is given by the linear combination

$$\psi(x,t) = \sum_n c_n \phi_n(x)\, e^{-\frac{i}{\hbar}E_n t},$$

where $\phi_n(x)$ are the normalized time independent solutions of the corresponding TISE.

$$\phi_n(a;x) = \sqrt{\frac{1}{a}} \begin{cases} \cos\frac{n\pi x}{2a} & \text{for } n = 1,3,5\ldots \\ \sin\frac{n\pi x}{2a} & \text{for } n = 2,4,6\ldots \end{cases}$$

Exercise

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For odd n, the coefficients c_n are

$$c_{1n} = A\sqrt{\frac{1}{a}}\int_{-a}^{a}\cos\frac{n\pi x}{2a}dx - \frac{A}{a^2}\sqrt{\frac{1}{a}}\int_{-a}^{a}x^2\cos\frac{n\pi x}{2a}dx = I_1 + I_2$$

$$I_1 = \frac{\sqrt{15}}{n\pi}\sin\left(\frac{n\pi}{2}\right) \qquad I_2 = \sqrt{15}\left[\frac{1}{n\pi} - \frac{8}{n^3\pi^3}\right]\sin\left(\frac{n\pi}{2}\right)$$

For even n, the coefficients c_n are

$$c_{2n} = A\sqrt{\frac{1}{a}}\int_{-a}^{a}\sin\frac{n\pi x}{2a}dx - \frac{A}{a^2}\sqrt{\frac{1}{a}}\int_{-a}^{a}x^2\sin\frac{n\pi x}{2a}dx$$

In this case, both the integrals are zero because the integrands are odd functions of x.

Therefore, the expansion coefficients are given by

$$c_n = \sqrt{15}\left[\frac{2}{n\pi} - \frac{8}{n^3\pi^3}\right]\sin\left(\frac{n\pi}{2}\right)$$

As a consequence, the wave function at $t > 0$ is given by the following linear combination

$$\psi(x,t) = \sum_n \sqrt{15}\left[\frac{2}{n\pi} - \frac{8}{n^3\pi^3}\right]\sin\left(\frac{n\pi}{2}\right)\phi_n(x)e^{-i(n^2\pi^2\hbar/8ma^2)t}, \quad n = 1,\ 3,\ 5,\ldots$$

5.At t=0, a particle of mass m, free to move inside an infinite potential well with walls at x = 0 and x = a, is in a state that is a linear superposition of the ground state and the first excited state

$$\psi(x,0) = \frac{1}{\sqrt{2}}\left[\phi_1(x) + \phi_2(x)\right] = \frac{1}{\sqrt{a}}\left[\sin\left(\frac{\pi x}{a}\right) + \sin\left(\frac{2\pi x}{a}\right)\right],$$

Find the wave function at any t > 0. Check whether the continuity equation holds good for this state or not.

5.At t=0, a particle of mass m, free to move inside an infinite potential well with walls at x = 0 and x = a, is in a state that is a linear superposition of the ground state and the first excited state

$$\psi(x,0)=\frac{1}{\sqrt{2}}\left[\phi_1(x)+\phi_2(x)\right]=\frac{1}{\sqrt{a}}\left[\sin\left(\frac{\pi x}{a}\right)+\sin\left(\frac{2\pi x}{a}\right)\right],$$

Find the wave function at any t > 0. Check whether the continuity equation holds good for this state or not.

Solution: The wave function of the particle at t > 0 will be

$$\psi(x,t)=\frac{1}{\sqrt{a}}\left[\sin\left(\frac{\pi x}{a}\right)e^{-i\frac{E_1}{\hbar}t}+\sin\left(\frac{2\pi x}{a}\right)e^{-i\frac{E_2}{\hbar}t}\right]$$

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The probability density is calculated to be

$$\rho(x,t) = \frac{1}{a}\left[\sin^2\left(\frac{\pi x}{a}\right) + \sin^2\left(\frac{2\pi x}{a}\right)\right]$$

$$+\frac{2}{a}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)\cos\left[\frac{(E_1 - E_2)}{\hbar}t\right].$$

The probability current density j_x is therefore given by

$$j_x = \frac{\hbar}{2mi}\left[\psi^*(x,t)\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi(x,t)\right]$$

$$= \frac{2\pi\hbar}{ma^2}\sin\left(\frac{\pi x}{a}\right)\cos\left(\frac{2\pi x}{a}\right)\sin\left[\frac{(E_1 - E_2)}{\hbar}t\right]$$

$$-\frac{\pi\hbar}{ma^2}\sin\left(\frac{2\pi x}{a}\right)\cos\left(\frac{\pi x}{a}\right)\sin\left[\frac{(E_1 - E_2)}{\hbar}t\right].$$

Therefore,

$$\frac{\partial \rho(x,t)}{\partial t} = \frac{3\pi^2\hbar}{ma^3}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)\sin\left[\frac{(E_1-E_2)}{\hbar}t\right].$$

$$\frac{\partial j_x}{\partial x} = -\frac{3\pi^2\hbar}{ma^3}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)\sin\left[\frac{(E_1-E_2)}{\hbar}t\right].$$

and

$$\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial j_x}{\partial x} = 0.$$