PH 101: Physics I

Module 3: Introduction to Quantum Mechanics

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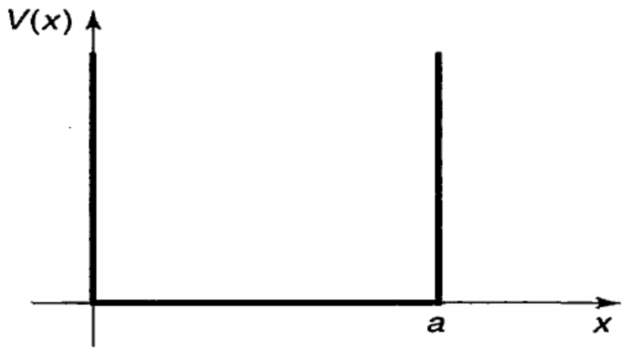
RECAP

Particle in a box (infinite square well)



$$V(x) = \begin{cases} 0, & \text{if } 0 \le x \le a, \\ \infty, & \text{otherwise} \end{cases}$$

V = 0 (particle is completely free)

Particle doesn't exist at all in the region

x > a and x < 0

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi,$$

$$\text{or} \quad \frac{d^2\psi}{dx^2} = -k^2\psi, \quad \text{where } k \equiv \frac{\sqrt{2mE}}{\hbar}.$$

Inside the well, the solutions are (the phase of *A* carries no physical significance, hence is taken as positive)

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right).$$

The time-independent Schrodinger equation has an infinite set of solutions (one for each positive integer n).

RECAP

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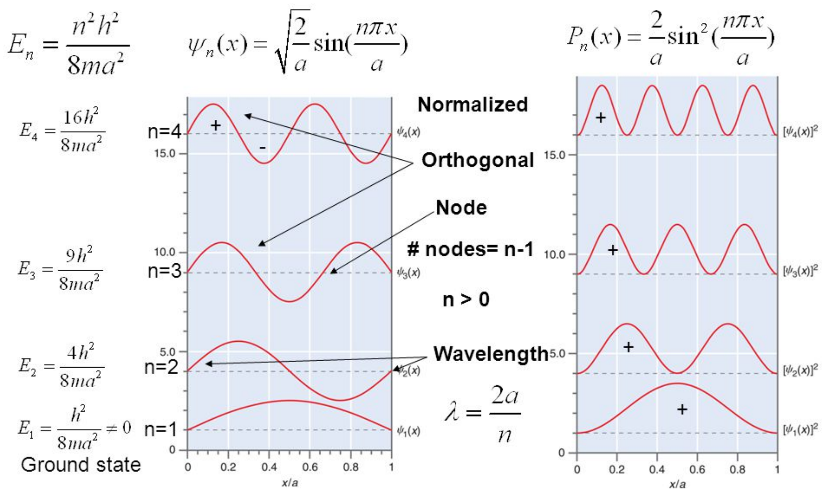


Energy: $E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}.$

Wavefunction: $\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$

Important properties of the wave function:

1. They are alternately even and odd, with respect to the center of the well: ψ_1 is even, ψ_2 is odd, ψ_3 is even, and so on.

2. As you go up in energy, each successive state has one more node (zero-crossing): ψ_1 has none (the end points don't count), ψ_2 has one, ψ_3 has two, and so on.

3. They are mutually orthogonal, in the sense tha $\int \psi_m(x)^* \psi_n(x)\, dx = 0$, whenever $m \neq n$.

To understand why this idea corresponds to orthogonality we have to understand the geometry of Hilbert space.

- In rigid bodies, we saw that there were special directions [principal directions] called $\hat{e}_1, \hat{e}_2, \hat{e}_3$ such that the moment of inertia matrix **I** which is a 3x3 matrix when acting on any one these special directions resulted in a vector which was parallel to it. In other words,

$$\mathbf{I}\,\hat{e}_j = \mathrm{I}_j\,\hat{e}_j$$

where I_j are pure numbers with $j = 1, 2, 3$. In quantum mechanics, the time independent Schrodinger equation has a similar form –

$$H\,\varphi_j(x) = \mathrm{E}_j\,\varphi_j(x)$$

where instead of the 3x3 moment of inertia matrix we have the Hamiltonian operator –

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

Geometry of Hilbert space

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

While in case of rigid bodies there are only three special vectors that have this property, in quantum mechanics it is always the case that the number of special "directions" [in this case, functions] $\varphi_j(x)$, j =1,2,3,…. are infinitely many. The space generated by the unit vectors $\hat{e}_1$, $\hat{e}_2$, $\hat{e}_3$ is the usual three dimensional space of vectors. The space generated by the functions

$\varphi_j(x)$, j =1,2,3,…. is an infinite dimensional space where the most general object is a general function of x, just as in three dimensional vector space, the most general object was a general vector in 3D. This infinitely dimensional space of functions is called a Hilbert space.

In case of rigid bodies, the three directions (unit vectors) $\hat{e}_1$, $\hat{e}_2$, $\hat{e}_3$ were linearly independent and mutually orthogonal so that any other general vector may be expressed as,

$$\vec{v} = c_1\,\hat{e}_1 + c_2\,\hat{e}_2 + c_3\,\hat{e}_3$$

Similarly we may expect that a general function $\psi(x)$ may be expressed as linear combinations of special "directions" $\varphi_j(x)$, j =1,2,3,….

$$\psi(x) = c_1\,\varphi_1(x) + c_2\,\varphi_2(x) + \;\ldots\ldots$$

Geometry of Hilbert space

The notion of unit vector, parallelism, orthogonality e.t.c. are geometrical notions. We would like to find analogous notions in the case of the Hilbert space of functions. Just as we know that $\hat{e}_1$ is perpendicular to $\hat{e}_2$ because $\hat{e}_1 . \hat{e}_2 = 0$ and we know that $\hat{e}_1$ is a unit vector because $\hat{e}_1 . \hat{e}_1 = 1$, can we make similar statements about the special functions $\varphi_1(x)$ and $\varphi_2(x)$? What does it mean for $\varphi_1(x)$ and $\varphi_2(x)$ to be mutually orthogonal? What does it mean for $\varphi_1(x)$ to be a unit vector? Answering these amounts to studying the "geometry" of the Hilbert space of functions.

One word of notation: We prefer to denote the dot product $\hat{e}_i . \hat{e}_j$ as $< \hat{e}_i \mid \hat{e}_j >$

One way to answer both these questions [dot product and unit vector] is to define the "dot product" between any two functions $\psi(x)$ and $\phi(x)$ is

$$\int_{-\infty}^{\infty} \psi^*(x)\, \phi(x)\; dx \;\equiv < \psi|\phi > = < \phi|\psi >^*$$

This means the statement that different special directions $\varphi_1(x)$ and $\varphi_2(x)$ are "mutually orthogonal" is the statement that,

$$< \varphi_1|\varphi_2 > \equiv \int_{-\infty}^{\infty} \varphi_1^*(x)\, \varphi_2(x)\; dx \;=\; 0$$

Geometry of Hilbert space

The statement that the basis function $\varphi_1(x)$ has length one (unit vector) is,

$$< \varphi_1|\varphi_1 > \equiv \int_{-\infty}^{\infty} \varphi_1^*(x)\, \varphi_1(x)\; dx \;=\; 1$$

We also recognize this as the statement that the total probability of finding the particle somewhere on the real axis is unity.

Thus once we pin down the meaning of the dot product in the Hilbert space of functions we have understood how to do geometry in this space.

Just as a general vector in three dimensions may be written in terms of the principal directions of the rigid body as,

$$\vec{\mathrm{v}} = c_1\;\hat{e}_1 + c_2\;\hat{e}_2 + c_3\;\hat{e}_3$$

and using orthogonality of these unit vectors we may write,

$$c_1 = \;\hat{e}_1.\vec{\mathrm{v}}\;,\; c_2 = \;\hat{e}_2.\vec{\mathrm{v}}\;,\; c_3 = \;\hat{e}_3.\vec{\mathrm{v}}$$

or, $$c_j = \;\hat{e}_j.\vec{\mathrm{v}} \;\;\equiv < \hat{e}_j\,|\vec{\mathrm{v}} >$$

Geometry of Hilbert space

In Hilbert space a general function has the expansion in terms of the basis functions,

$$\psi(x) = c_1\,\varphi_1(x) + c_2\,\varphi_2(x) + \ldots\ldots \qquad [1]$$

and the coefficients are similarly given as,

$$c_j \equiv <\varphi_j|\psi> = \int_{-\infty}^{\infty} \varphi_j^*(x)\psi(x)\; dx$$

HW: Prove this by multiplying [1] above on both sides by $\varphi_j^*(x)$ and integrate with respect to x and use the orthogonality and normalization of the basis functions $\varphi_j(x)$.

$$\begin{aligned}
\textit{Proof}:\ \int \psi_m(x)^*\psi_n(x)\,dx &= \frac{2}{a}\int_0^a \sin\left(\frac{m\pi}{a}x\right)\sin\left(\frac{n\pi}{a}x\right)\,dx \\
&= \frac{1}{a}\int_0^a \left[\cos\left(\frac{m-n}{a}\pi x\right) - \cos\left(\frac{m+n}{a}\pi x\right)\right]dx \\
&= \left\{\frac{1}{(m-n)\pi}\sin\left(\frac{m-n}{a}\pi x\right) - \frac{1}{(m+n)\pi}\sin\left(\frac{m+n}{a}\pi x\right)\right\}\Bigg|_0^a \\
&= \frac{1}{\pi}\left\{\frac{\sin[(m-n)\pi]}{(m-n)} - \frac{\sin[(m+n)\pi]}{(m+n)}\right\} = 0.
\end{aligned}$$

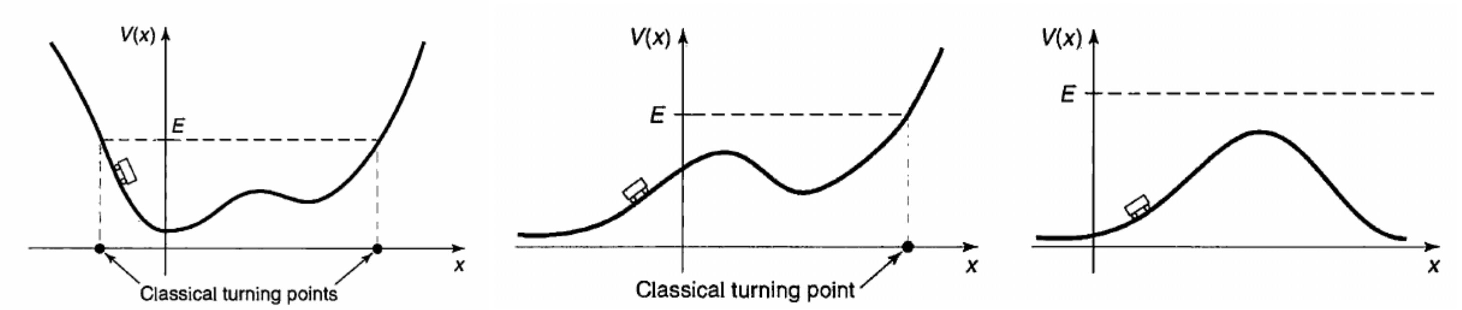
We can combine orthogonality and normalization into a single statement:

$$\int \psi_m(x)^*\psi_n(x)\,dx = \delta_{mn},$$

where δ_{mn} (the so-called **Kronecker delta**) is defined in the usual way,

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

Bound and scattering states



(a) (b)

In classical mechanics a one-dimensional time-independent potential can give rise to two rather different kinds of motion. If V(x) rises higher than the particle's total energy (E) on either side (fig.(a)), then the particle is "stuck" in the potential well—it rocks back and forth between the turning points, but it cannot escape of its own. We call this a bound state. If, on the other hand, E exceeds V(x) on one side (or both), then the particle comes in from "infinity," slows down or speeds up under the influence of the potential, and returns to infinity (fig. (b)). (It can't get trapped in the potential unless there is some mechanism, such as friction, to dissipate energy, but again, we're not talking about that.) We call this a scattering state.

Some potentials admit only bound states (for instance, the harmonic oscillator); some allow only scattering states (a potential hill with no dips in it, for example); some permit both kinds, depending on the energy of the particle.

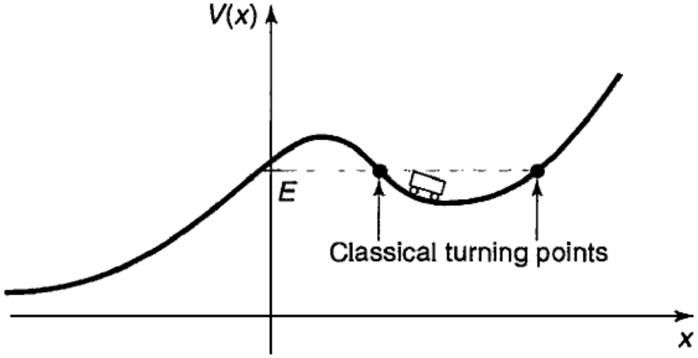
Bound and scattering states in Quantum Mechanics

The two kinds of solutions to the Schroedinger equation correspond precisely to bound and scattering states. The only thing that matters is the potential at infinity (fig. (c)):

$$\begin{cases} E < [V(-\infty) \quad \text{and } V(+\infty)] \Rightarrow & \text{bound state,} \\ E > [V(-\infty) \quad \text{or} \quad V(+\infty)] \Rightarrow & \text{scattering state.} \end{cases}$$

In "real life" most potentials go to zero at infinity, in which case the criterion simplifies even further:

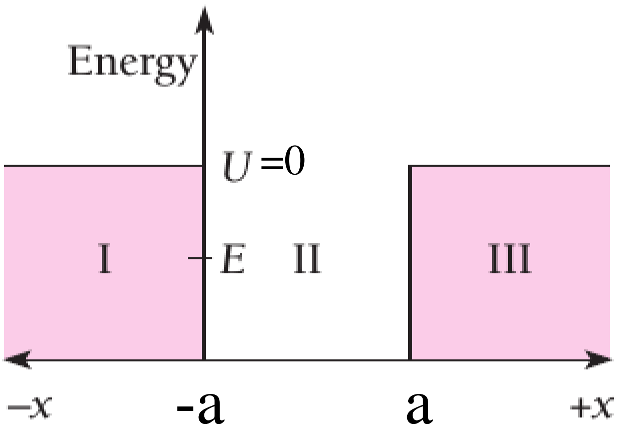
$$\begin{cases} E < 0 \Rightarrow & \text{bound state,} \\ E > 0 \Rightarrow & \text{scattering state.} \end{cases}$$



(c)

Particle in a finite square well

Figure shows a potential well with square corners that is U high and L wide and contains a particle whose energy E is less than U.



Classical: According to classical mechanics, when the particle strikes the sides of the well, it bounces off without entering regions I and III. Quantum: In quantum mechanics, the particle also bounces back and forth, but now it has a certain probability of penetrating into regions I and III even though E< U.

For bound states $E < 0$, hence we can write $E = -\epsilon$, where ϵ is +ve.

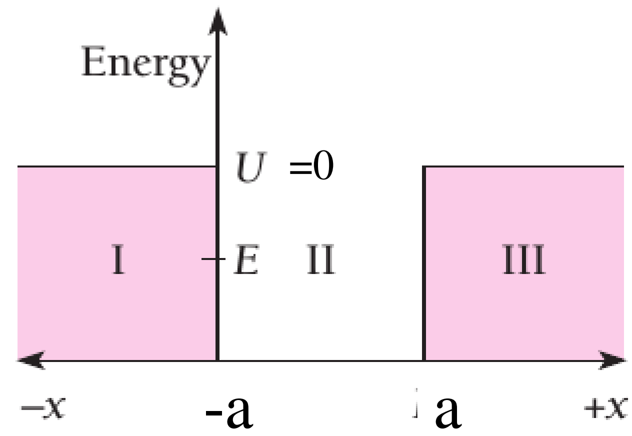
The time independent Schroedinger equation can be written as ;

$$\psi''(x) + \frac{2m}{\hbar^2}[E - U(x)]\psi(x) = 0$$

$$\psi''(x) - \frac{2m}{\hbar^2}[\epsilon + U(x)]\psi(x) = 0$$

Particle in a finite square well

$$\psi''(x) - \frac{2m}{\hbar^2}[\epsilon + U(x)]\psi(x) = 0$$



Region I and III:

Here $U(x) = 0$.

Hence, $\psi_1'' - k^2\psi_1 = 0$ $\psi_3'' - k^2\psi_3 = 0$ where, $k^2 = \frac{2m\epsilon}{\hbar^2}$

$$\psi_1 = A_1 e^{kx} + A_2 e^{-kx} \quad (x < -a)$$

$$\psi_3 = B_1 e^{kx} + B_2 e^{-kx} \quad (x > a)$$

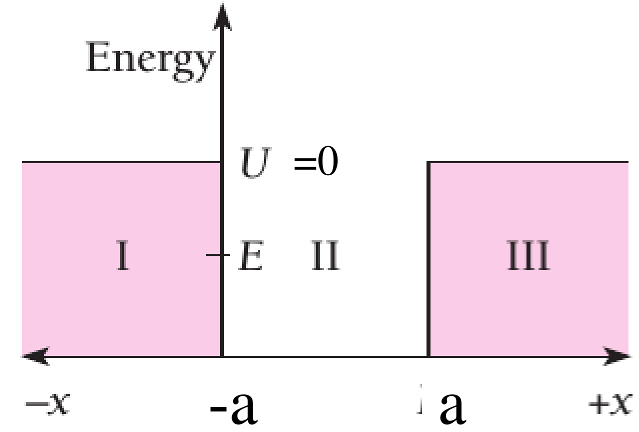
The condition $\psi \to 0$ as $x \to \pm\infty$ demands that $A_2 = 0, \quad B_1 = 0$

We can now write $A_1 = A$ and $B_2 = B$

$\therefore \quad \psi_1 = Ae^{kx} \quad (x < -1)$ $\qquad \psi_3 = Be^{-kx} \quad (x > a)$

Particle in a finite square well

$$\psi''(x) - \frac{2m}{\hbar^2}[\epsilon + U(x)]\psi(x) = 0$$



Region II:

Here $U(x) = -U_0$

$$\psi_2'' + \frac{2m}{\hbar^2}(U_0 - \epsilon)\psi_2 = 0 \Rightarrow \psi_2'' + q^2\psi_2 = 0$$

where $q^2 = \frac{2m}{\hbar^2}(U_0 - \epsilon)$

The general solution for this kind of equation is :

$$\psi_2 = C sin\ qx + D cos\ qx$$

We will evaluate C and D from the boundary conditions.

ψ and $d\psi/dx = \psi'$ is continuous across the boundaries.

$$\psi_1|_{x=-a} = \psi_2|_{x=-a}$$

$$\psi_1'|_{x=-a} = \psi_2'|_{x=-a}$$

$$k = q\frac{C\ cos\ qa + D\ sin\ qa}{D\ cos\ qa - C\ sin\ qa}$$

$$CD = -CD$$

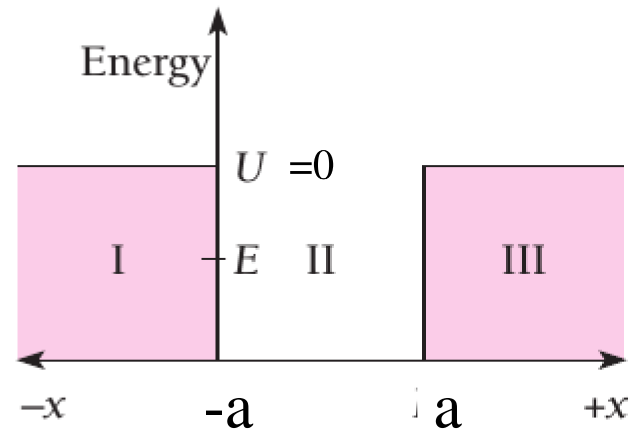
$$\psi_2|_{x=a} = \psi_3|_{x=a}$$

$$\psi_2'|_{x=a} = \psi_3'|_{x=a}$$

$$-k = q\frac{C\ cos\ qa - D\ sin\ qa}{D\ cos\ qa + C\ sin\ qa}$$

Particle in a finite square well

$\psi''(x) - \frac{2m}{\hbar^2}[\epsilon + U(x)]\psi(x) = 0$



Region II:

Here $U(x) = -U_0$

$CD = -CD$ This is possible if (i) $C = 0, \quad D \neq 0$ or (ii) $C \neq 0, \quad D = 0$

Hence there are two classes of solutions.

1st Class:

If $C = 0, \quad D \neq 0$ then $\psi_2 = D\ cos\ qx$ and $k = q\ tan\ qa \Rightarrow ka = qa\ tan\ qa$

This is transcendental equation.

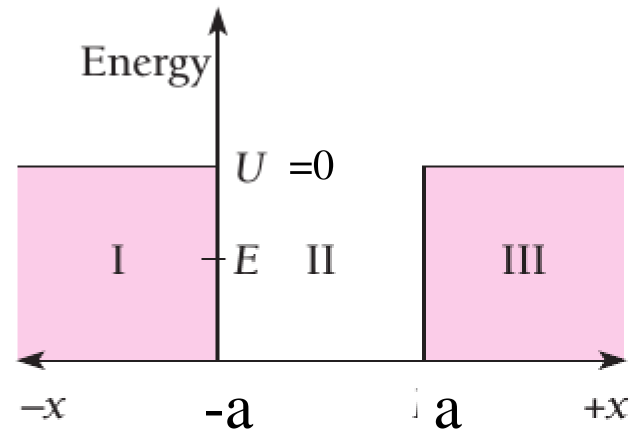
2nd Class:

If $C \neq 0, \quad D = 0$ then $\psi_2 = C\ sin\ qx$ and $k = -q\ cot\ qa \Rightarrow ka = -qa\ cot\ qa$

This is also a transcendental equation.

Particle in a finite square well

$\psi''(x) - \frac{2m}{\hbar^2}[\epsilon + U(x)]\psi(x) = 0$



Region II:

Here $U(x) = -U_0$

$ka = qa\ tan\ qa$ $\qquad$ $ka = -qa\ cot\ qa$

Let's introduce two new variables $\lambda = qa$ and $\mu = ka$ which are positive quantities.

$\mu = \lambda\ tan\ \lambda$ for 1st class solution.

$\mu = -\lambda\ cot\ \lambda = \lambda\ tan\ (\lambda + \pi/2)$ for 2nd class solution.

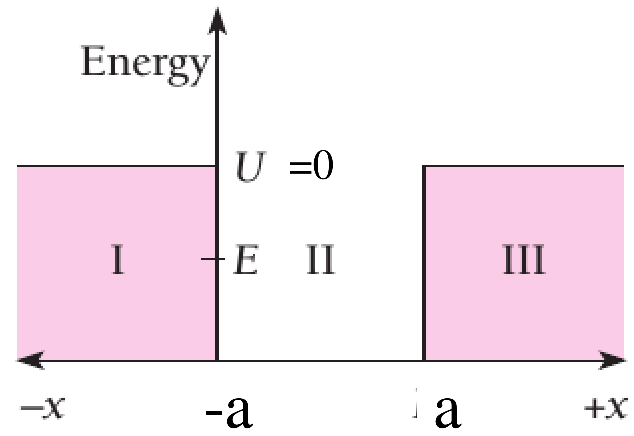
Note that $\lambda^2 + \mu^2 = (k^2 + q^2)a^2$

$\Rightarrow \lambda^2 + \mu^2 = \frac{2m}{\hbar^2}U_0 a^2 = R^2$, where $R = \sqrt{\frac{2m}{\hbar^2}U_0 a^2}$

This represents an equation of circle with radius $R = \sqrt{\frac{2m}{\hbar^2}U_0 a^2}$

Particle in a finite square well

$\psi''(x) - \frac{2m}{\hbar^2}[\epsilon + U(x)]\psi(x) = 0$



Region II:

Here $U(x) = -U_0$

$$\mu = \lambda \; tan \; \lambda \qquad \text{for 1st class solution.}$$

$$\mu = -\lambda \; cot \; \lambda = \lambda \; tan \; (\lambda + \pi/2) \qquad \text{for 2nd class solution.}$$

$$\lambda^2 + \mu^2 = \frac{2m}{\hbar^2} U_0 a^2 = R^2, \text{ where } R = \sqrt{\frac{2m}{\hbar^2} U_0 a^2}$$

R depends on $U_0 a^2$ (i.e. the strength of the potential and the range)

$U_0 a^2 = \hbar^2/2m, \qquad \lambda^2 + \mu^2 = 1^2$

$U_0 a^2 = 4\hbar^2/2m, \qquad \lambda^2 + \mu^2 = 2^2$

$U_0 a^2 = 12\hbar^2/2m, \qquad \lambda^2 + \mu^2 = 3.45^2$

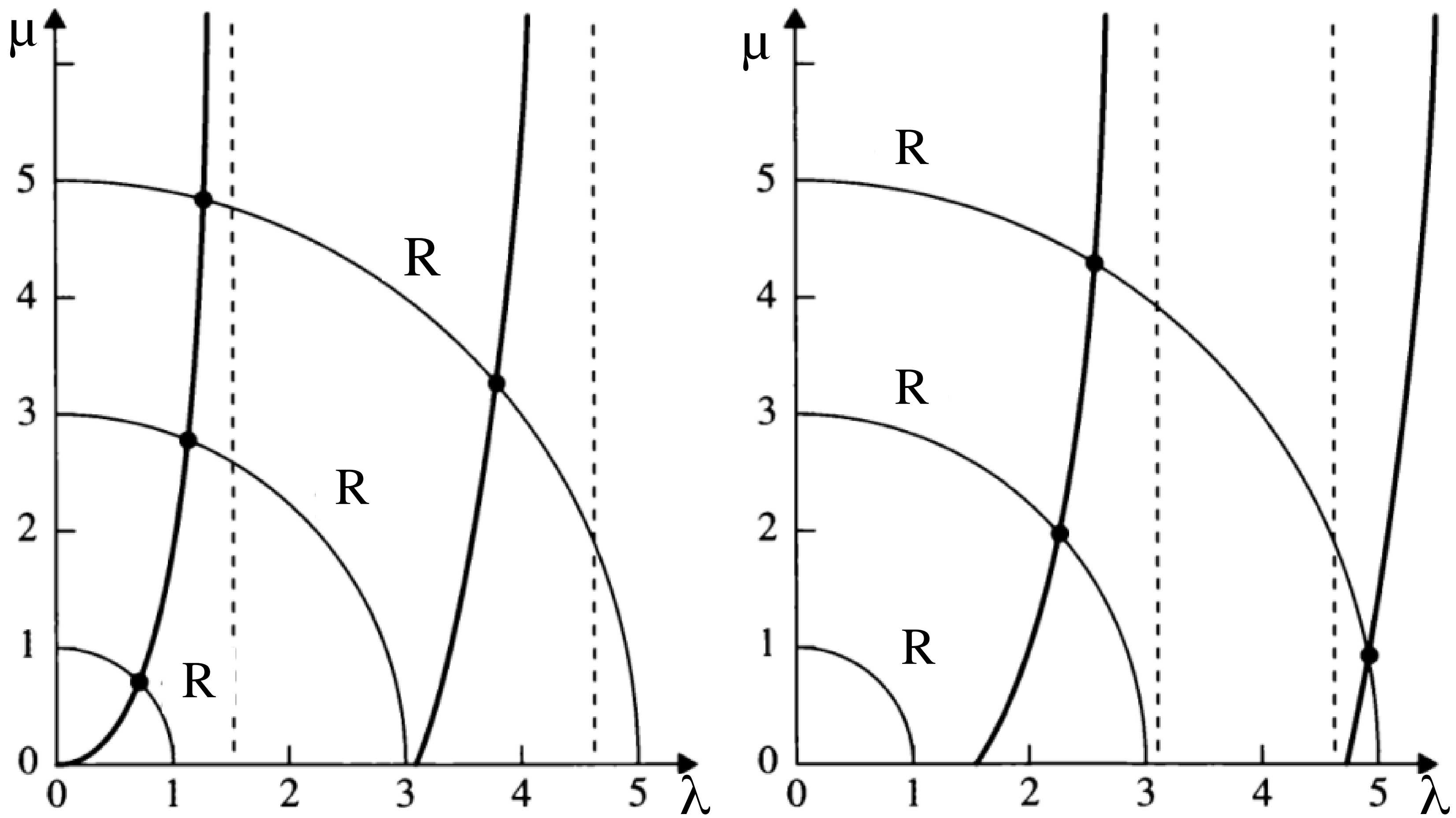
Particle in a finite square well

Now the energy levels can be obtained by looking at the intersections of the curve

$\lambda \; tan \; \lambda \; vs. \lambda$ and the circe of known radii.

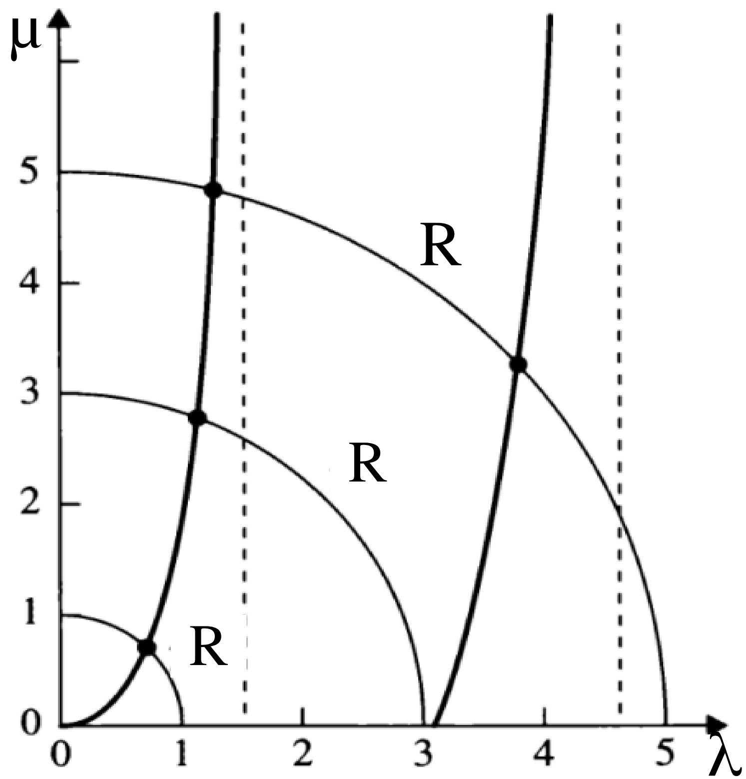
$\lambda \; tan \; (\lambda + \pi/2) \; vs. \lambda$ and the circe of known radii.

Graphical solutions:

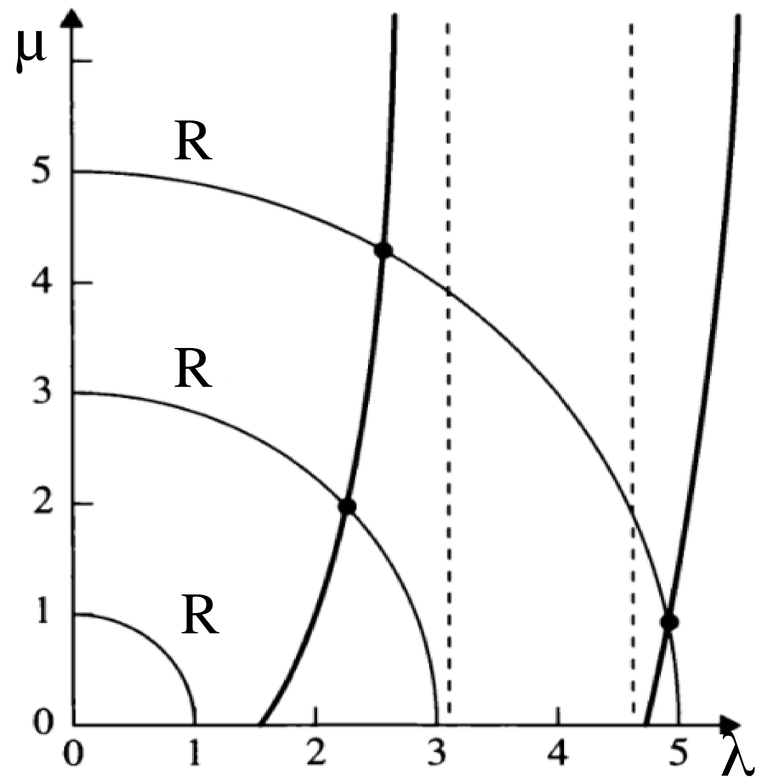


Particle in a finite square well

1st class



2nd class



(i) For $R < \pi/2$ or $\sqrt{\frac{2m}{\hbar^2} U_0 a^2} < \pi/2$ or $U_0 a^2 < \frac{\pi^2\hbar^2}{8m}$

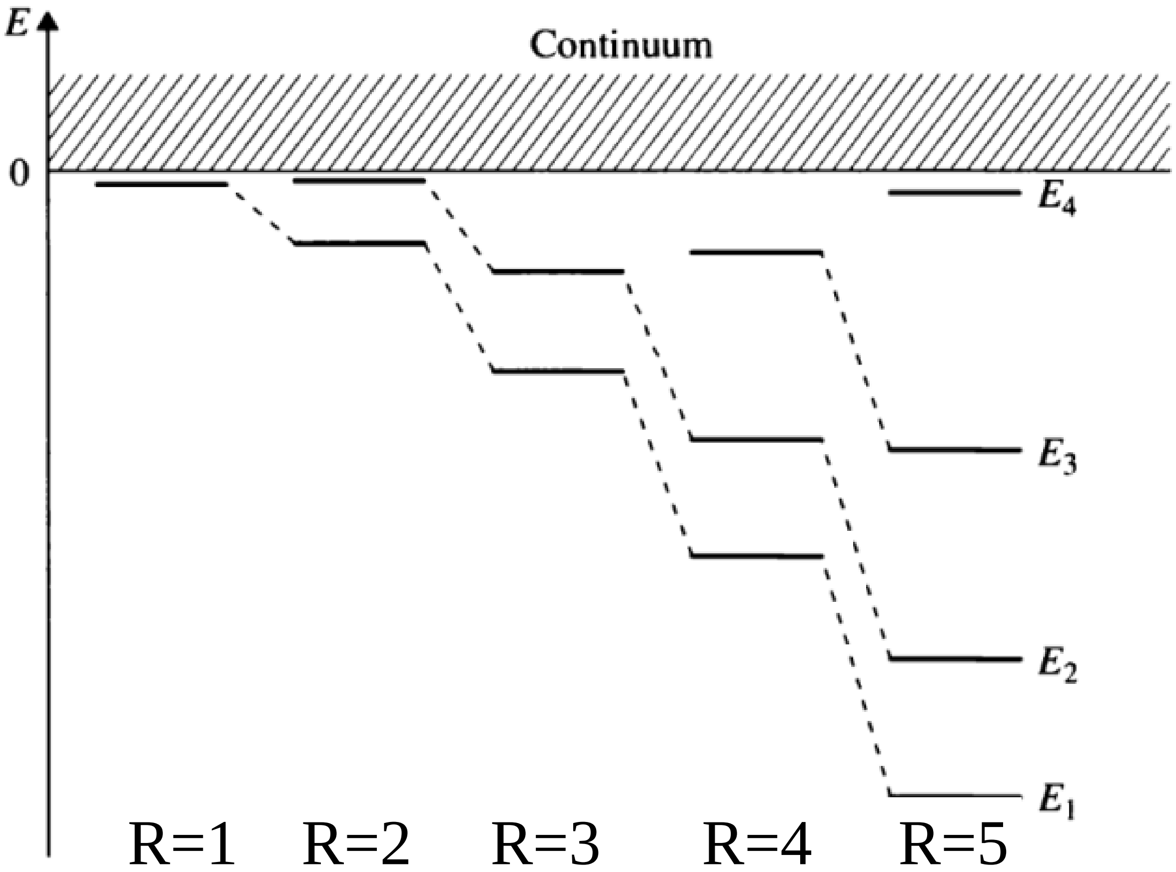
there is only one bound state. i.e. for $0 < U_0 a^2 < \frac{\pi^2\hbar^2}{8m}$, there is one energy level belonging to the 1st class.

(ii) For $\pi/2 < R < \pi$ or $\pi^2/4 < \frac{2m}{\hbar^2} U_0 a^2 < \pi^2$ or $\frac{\pi^2\hbar^2}{8m} U_0 a^2 < \frac{\pi^2\hbar^2}{2m}$

There are two bound states,one belonging to 1st class and the other belonging to the 2nd class.

(iii) As $U_0 a^2$ increases more energy levels appear successively for the 1st and 2nd class.

Particle in a finite square well



Once we get the intersection points we get the value of μ and λ.

From these values we can obtain the energy eigen values and the wave functions.

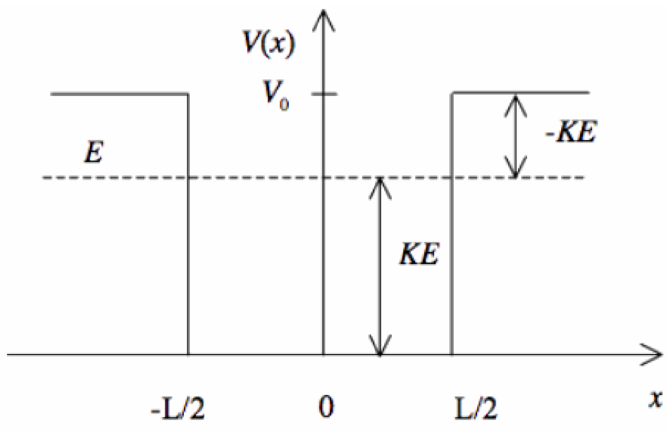
The wave functions are very similar to the particle in a box case. However, it has finite probability to tunnel which decays exponentially.

Particle in a finite square well

Consider a particle in the potential

$$V(x) = \begin{cases} V_0 & x < -\frac{L}{2} \\ 0 & -\frac{L}{2} \leq x \leq \frac{L}{2} \\ V_0 & x > \frac{L}{2} \end{cases}$$

$V_0 > 0$



- $E > V_0$ – unbound states, total energy E continuous (not quantized)
- $E < V_0$ – bound states, expect discrete states

- $-\frac{L}{2} \leq x \leq \frac{L}{2}$ (Region I):

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x) \;\Rightarrow\; \psi''(x) = -k^2\psi(x) \quad \boxed{k^2 = \frac{2mE}{\hbar^2} > 0}$$

solutions: $\psi_I(x) = A\sin kx + B\cos kx$

- $x > \frac{L}{2}$ (Region II):

  Note: in region II $E = KE + PE = KE + V_0 < V_0 \;\Rightarrow\; KE < 0$!

  $$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V_0\psi(x) = E\psi(x)$$

  $$\Rightarrow\; \psi''(x) = \alpha^2\psi(x)$$

  $$\boxed{\alpha^2 = \frac{2m(V_0 - E)}{\hbar^2} > 0}$$

  solutions $\psi_{II}(x) = Ce^{-\alpha x} + De^{\alpha x}$

  C, D – arbitrary constants

  $\Rightarrow$ put $D = 0$, otherwise $\psi(x)$ not square integrable (blows up at large +ve x)

- $x < -\frac{L}{2}$ (Region III):

  solutions $\psi_{III}(x) = Fe^{-\alpha x} + Ge^{\alpha x}$ (like in region II)

  F, G – arbitrary constants

  $\Rightarrow$ put $F = 0$, otherwise $\psi(x)$ not square integrable (blows up at large -ve x)

Particle in a finite square well

The boundary conditions are

$$\psi \text{ and } d\psi/dx \text{ continuous at} -L/2 \text{ and } +L/2$$

In order to solve for the wave functions, we are going to exploit the following property related to the given form of potential:

If $V(x)$ is an even function, $V(-x) = V(x)$, then $\psi(x)$ can always be taken to be either even or odd, that is, if $\psi(x)$ satisfies the time-independent Schrödinger equation for a given E, so too does $\psi(-x)$, and hence also the even and odd linear combinations $\psi(x) \pm \psi(-x)$.

So, we can assume with no loss of generality that the solutions are either even or odd. The advantage of this is that we need only impose the boundary conditions on one side (say, $+L/2$); the other side is then automatic, since $\psi(-x) = \pm\, \psi(x)$.

Particle in a finite square well

- The potential is symmetric w.r.t. to $x = 0 \;\Rightarrow\;$ expect symmetric (even-parity) and antisymmetric (odd-parity) states
- Consider even-parity solutions only: $\psi_I(x) = B\cos kx$

  Apply general conditions on ψ at $x = L/2$:

  - ψ continuous at $x = L/2$: $\Rightarrow \;\psi_I(L/2) = \psi_{II}(L/2)$
    $\Rightarrow \; B\cos(kL/2) = C\exp(-\alpha L/2)$
  - ψ' continuous at $x = L/2$: $\Rightarrow \;\psi'_I(L/2) = \psi'_{II}(L/2)$
    $\Rightarrow \; -Bk\sin(kL/2) = -C\alpha\exp(-\alpha L/2)$

  No new constraints at $x = -L/2$ since we consider symmetric solutions only.

- divide them side-by-side: $\Rightarrow \; \boxed{\tan\frac{kL}{2} = \frac{\alpha}{k}}$

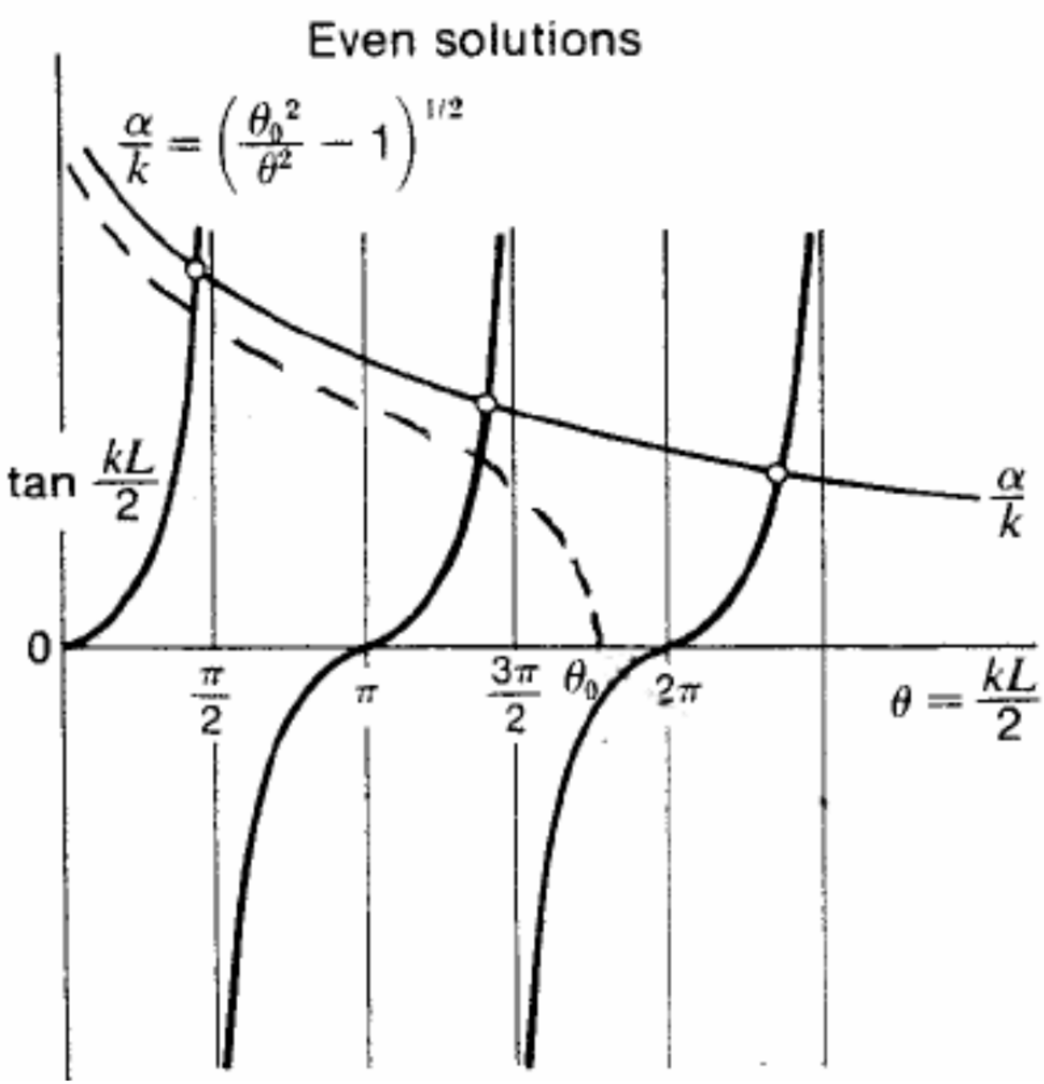
  introduce $\theta = \frac{kL}{2} \;\Rightarrow\;$ LHS: $y(\theta) = \tan\theta$

  and $\theta_0 = \frac{k_0 L}{2}$ – const. where $k_0^2 = \frac{2mV_0}{\hbar^2} > 0$

  $\Rightarrow$ RHS: $y(\theta) = \frac{\alpha}{k} = \sqrt{\frac{k_0^2}{k^2} - 1} = \sqrt{\frac{V_0 - E}{E}} = \sqrt{\frac{\theta_0^2}{\theta^2} - 1}$

Particle in a finite square well

The even-parity solutions are determined when the curve $y = \tan\theta$ intersects the curve $y = \frac{\alpha}{k}$. $\theta = \frac{kL}{2}$

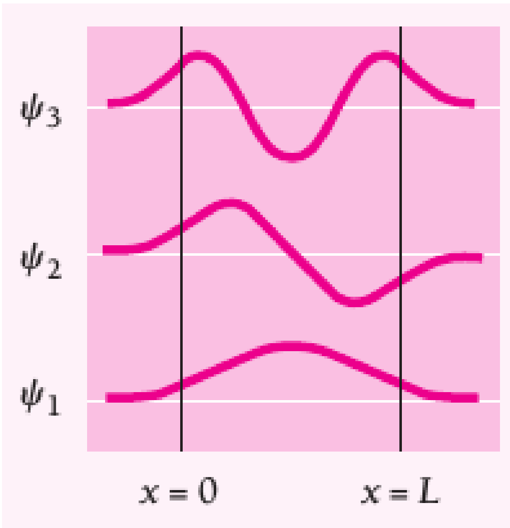


- The intersection points determine k and hence $E = \frac{\hbar^2 k^2}{2m}$.
- When $E \ll V_0$
  $\Rightarrow \frac{\alpha}{k} = \sqrt{\frac{\theta_0^2}{\theta^2} - 1} \propto \frac{1}{\theta}$
  (solid line)
- When $E \nearrow V_0$
  $\Rightarrow \theta \nearrow \theta_0$
  $\Rightarrow \frac{\alpha}{k} = \sqrt{\frac{\theta_0^2}{\theta^2} - 1} \searrow 0$
  (dashed line)

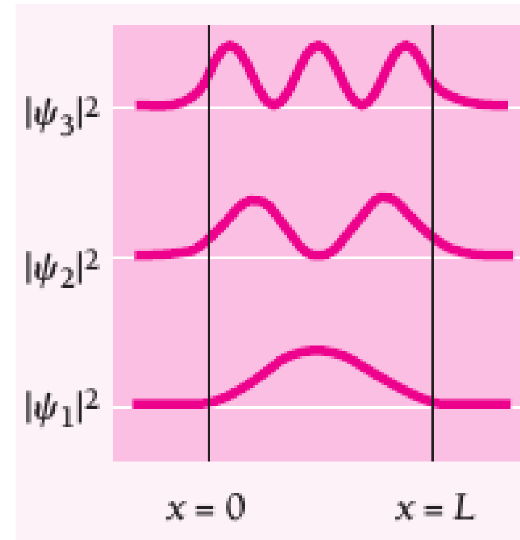
$\Rightarrow$ bound states with discrete (quantized) energy

Particle in a finite square well

Wavefunction



Probability density



Because the wavelengths that fit into the well are longer than for an infinite well of the same width, the corresponding particle momenta are lower (we recall that λ= hp). Hence the energy levels E_n are lower for each n than they are for a particle in an infinite well.

Energy levels are not equally spaced.

There is no concept of zero energy. The ground state energy is called the quantum zero-point energy

A particle without the energy to pass over a potential barrier may still tunnel through it. This is known as tunneling effect.

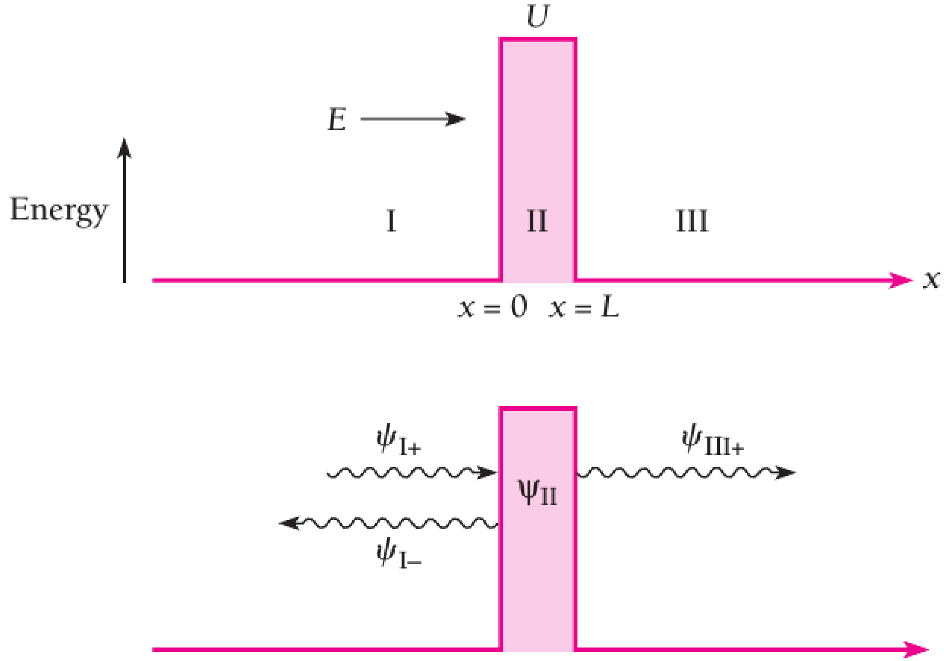
Particle in a finite square well -> Particle in infinite well

In the limit of $U \to \infty$, $R \to \infty$ this problem will approach the particle in an infinite well problem.

Tunneling Effect:

Approximate transmission probability

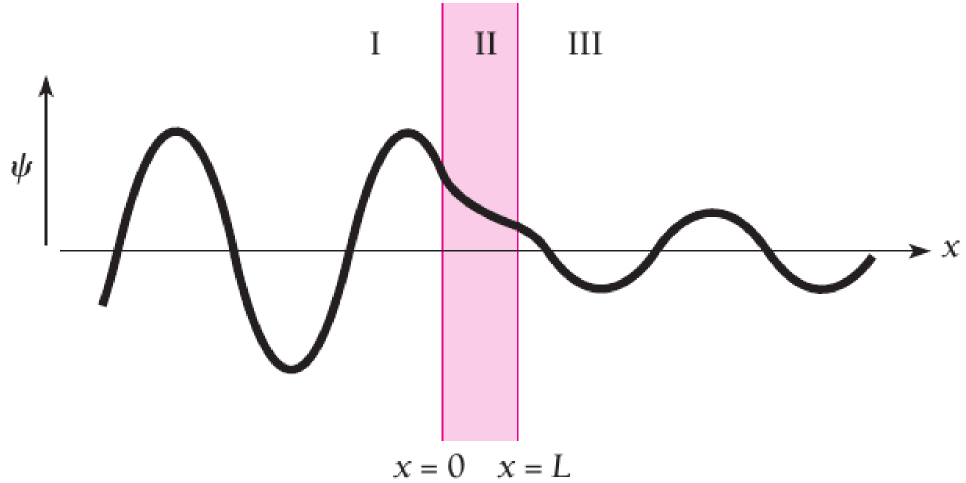
$$T = e^{-2k_2 L}$$



where

$$k_2 = \frac{\sqrt{2m(U - E)}}{\hbar}$$

and L is the width of the barrier.



Tunneling Effect:

Electrons with energies of 1.0 eV and 2.0 eV are incident on a barrier 10.0 eV high and 0.50 nm wide. (*a*) Find their respective transmission probabilities. (*b*) How are these affected if the barrier is doubled in width?

Solution

(*a*) For the 1.0-eV electrons

$$
\begin{aligned}
k_2 &= \frac{\sqrt{2m(U - E)}}{\hbar} \\
&= \frac{\sqrt{(2)(9.1 \times 10^{-31}\ \text{kg})[(10.0 - 1.0)\ \text{eV}](1.6 \times 10^{-19}\ \text{J/eV})}}{1.054 \times 10^{-34}\ \text{J} \cdot \text{s}} \\
&= 1.6 \times 10^{10}\ \text{m}^{-1}
\end{aligned}
$$

Since $L = 0.50$ nm $= 5.0 \times 10^{-10}$ m, $2k_2L = (2)(1.6 \times 10^{10}\ \text{m}^{-1})(5.0 \times 10^{-10}\ \text{m}) = 16$, and the approximate transmission probability is

$$T_1 = e^{-2k_2L} = e^{-16} = 1.1 \times 10^{-7}$$

One 1.0-eV electron out of 8.9 million can tunnel through the 10-eV barrier on the average. For the 2.0-eV electrons a similar calculation gives $T_2 = 2.4 \times 10^{-7}$. These electrons are over twice as likely to tunnel through the barrier.

(*b*) If the barrier is doubled in width to 1.0 nm, the transmission probabilities become

$$T_1' = 1.3 \times 10^{-14} \qquad T_2' = 5.1 \times 10^{-14}$$

Evidently T is more sensitive to the width of the barrier than to the particle energy here.

Harmonic Oscillator

Harmonic motion takes place when a system of some kind vibrates about an equilibrium configuration. The system may be an object supported by a spring or floating in a liquid, a diatomic molecule, an atom in a crystal lattice.

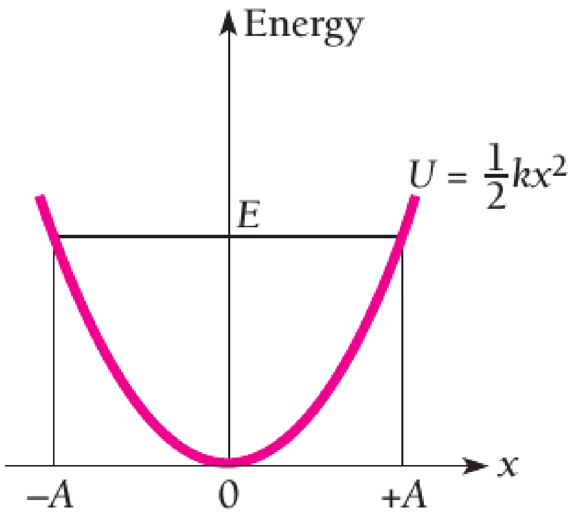
The condition for harmonic motion is the presence of a restoring force that acts to return the system to its equilibrium configuration when it is disturbed.

The inertia of the masses involved causes them to overshoot equilibrium, and the system oscillates indefinitely if no energy is lost.

In the special case of simple harmonic motion, the restoring force F on a particle of mass m is linear; that is, F is proportional to the particle's displacement x from its equilibrium position and in the opposite direction.

Thus $$F = -kx$$

$$U(x) = -\int_0^x F(x)\, dx = k\int_0^x x\, dx = \frac{1}{2}kx^2$$

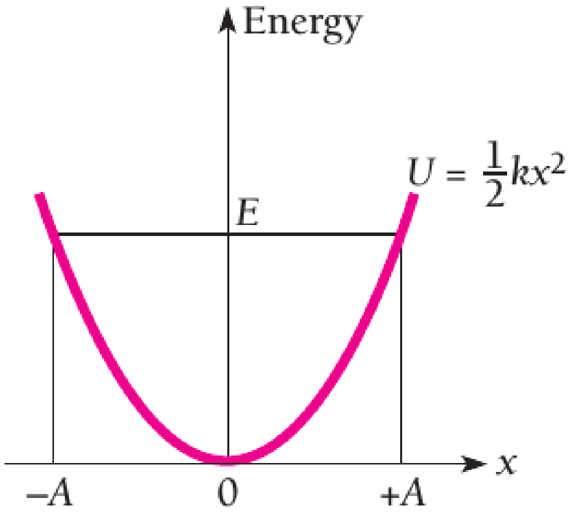


$$-kx = m\frac{d^2x}{dt^2}$$

$$\frac{d^2x}{dt^2} + \frac{k}{m}x = 0$$

Harmonic Oscillator

Such a parabolic potential is of great importance in quantum physics as well as in classical physics, since it can be used to approximate an arbitrary continuous potential W(x) in the vicinity of a stable equilibrium position at x=0.



Any function $W(x)$ can be expanded using the Taylor series expansion about $x = a$ as

$$W(x) = W(a) + (x-a)W'(a) + \frac{1}{2}(x-a)^2W''(a) + ...$$

Here $W'(a) = \frac{dW}{dx}|_{x=a}$ and $W''(a) = \frac{d^2W}{dx^2}|_{x=a}$

Since W has a minimum at $x = a$,

$W'(a) = 0$ and $W''(a) = +ve$

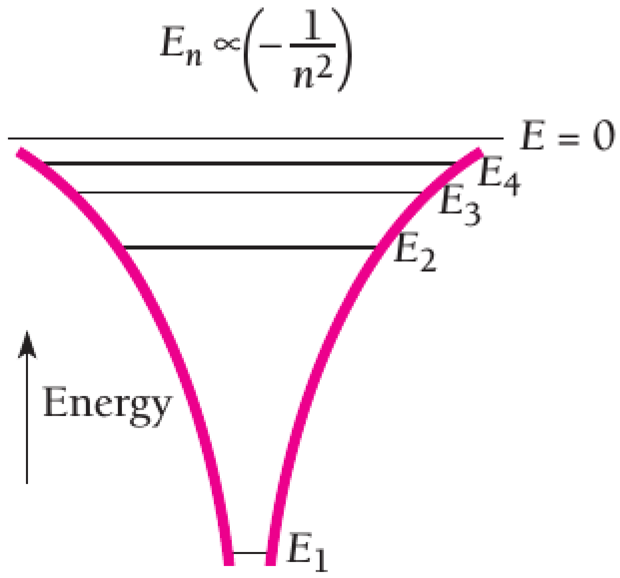
$\therefore W(x) = W(a) + \frac{1}{2}(x-a)^2W''(a)$, ignoring the higher order terms.

Now considering a as origin we have

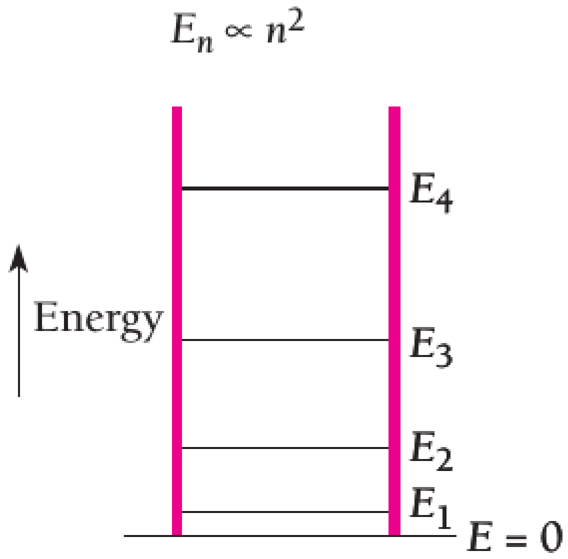
$W(x) = cont. + \frac{1}{2}x^2W''(0) \sim \frac{1}{2}x^2k$, where $k = W''(0)$

$$W(x) = \frac{1}{2}kx^2$$

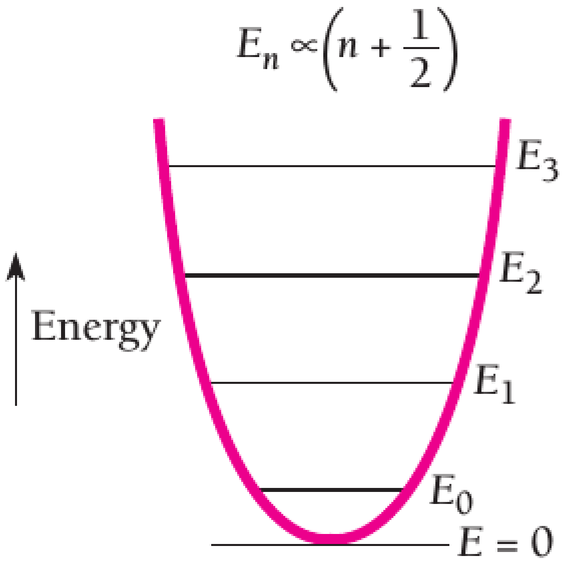
Comparison



Hydrogen Atom



Particle in a box



Harmonic oscillator