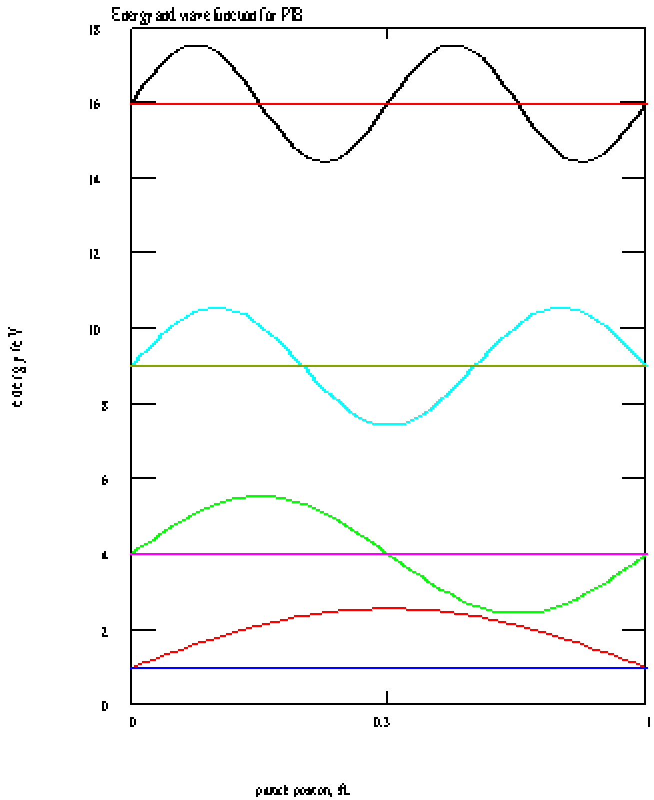
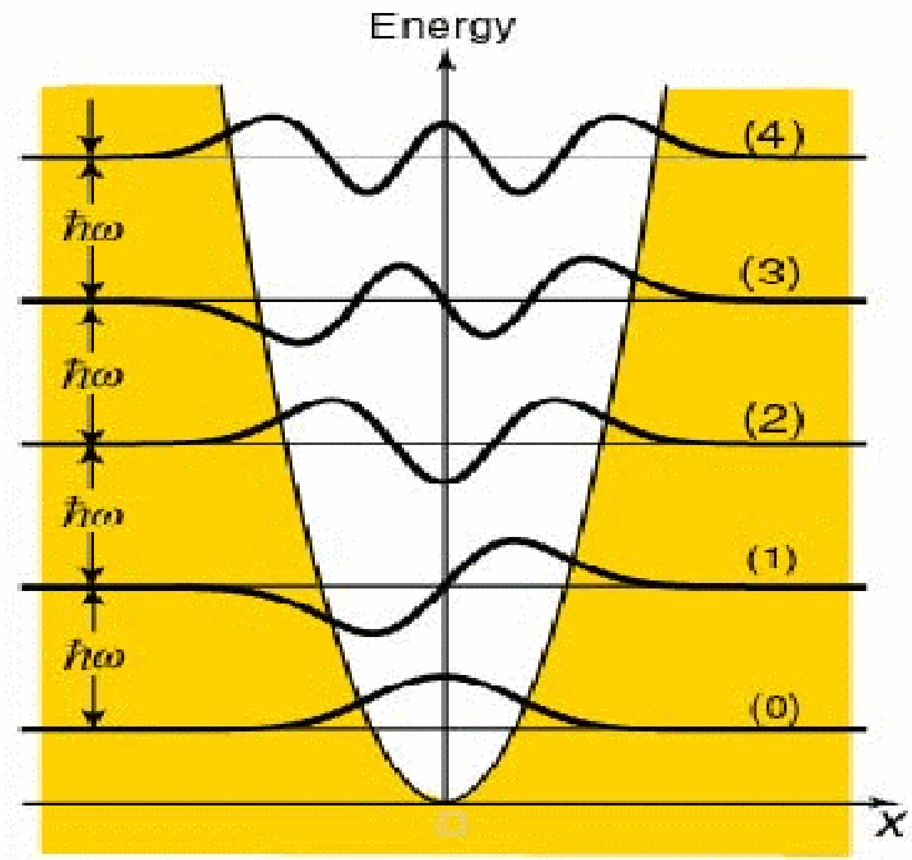
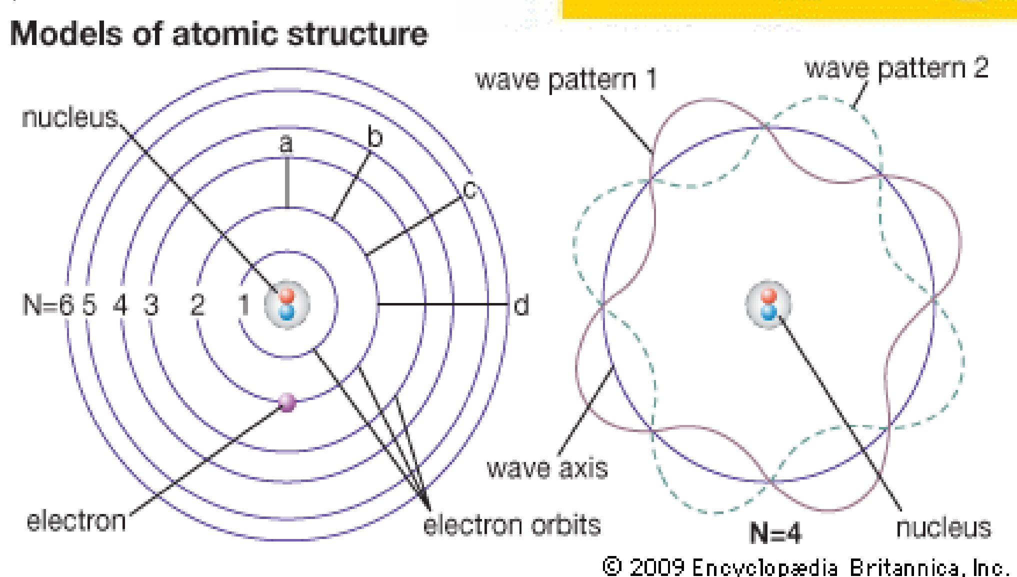
Few Problems of bound state in quantum mechanics



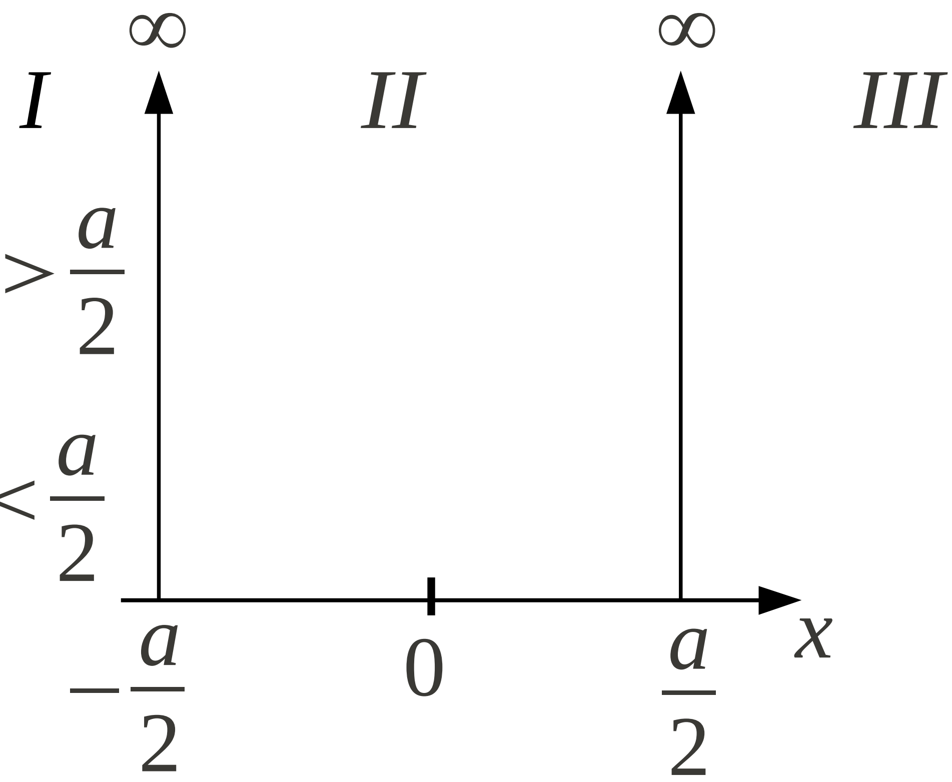




Particle in a infinite potential well

$$V(x) = \infty \qquad x < -\frac{a}{2} \qquad x > \frac{a}{2}$$

$$V(x) = 0 \qquad x > -\frac{a}{2} \qquad x < \frac{a}{2}$$



There are infinite energy states are possible for classical particle but only finite energy levels are possible for particle in a box – We solve the time independent Schroedinger equation

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

Inside the potential well and in one dimension

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

$$\frac{\partial^2}{\partial x^2}\phi(x)=-\frac{2mE}{\hbar^2}\phi(x)$$

This is the standard form of the harmonic oscillator problem with

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

$$k=-\frac{\sqrt{2mE}}{\hbar}$$

The general solution of this equation has the form inside the potential well

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

outside the potential well and in one dimension in region I III

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

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

This is also the standard form of the harmonic oscillator problem with

$$k_1=-\frac{\sqrt{2m(E-V)}}{\hbar}=\pm i\alpha$$

we assume $E<V$

The general solution of this equation has the form outside the potential well in region I

$$\phi(x)=Ce^{\alpha x}+De^{-\alpha x}$$

In this region I as $x\rightarrow-\infty$ the wave function become infinite this is prevented by setting the constant $D=0$

In the region I the form of the wave function is

$$\phi_I(x) = C e^{\alpha x}$$

In the similar manner the general wave function in the region III is given by

$$\phi(x) = E e^{\alpha x} + F e^{-\alpha x}$$

In this region III as $x \rightarrow \infty$ the wave function become infinite this is prevented by setting the constant $E = 0$

$$\phi_{III}(x) = F e^{-\alpha x}$$

As the potential outside the region becomes infinite the

$$k_1 = -\frac{\sqrt{2m(E-V)}}{\hbar} = \pm i\alpha = \pm i\infty$$

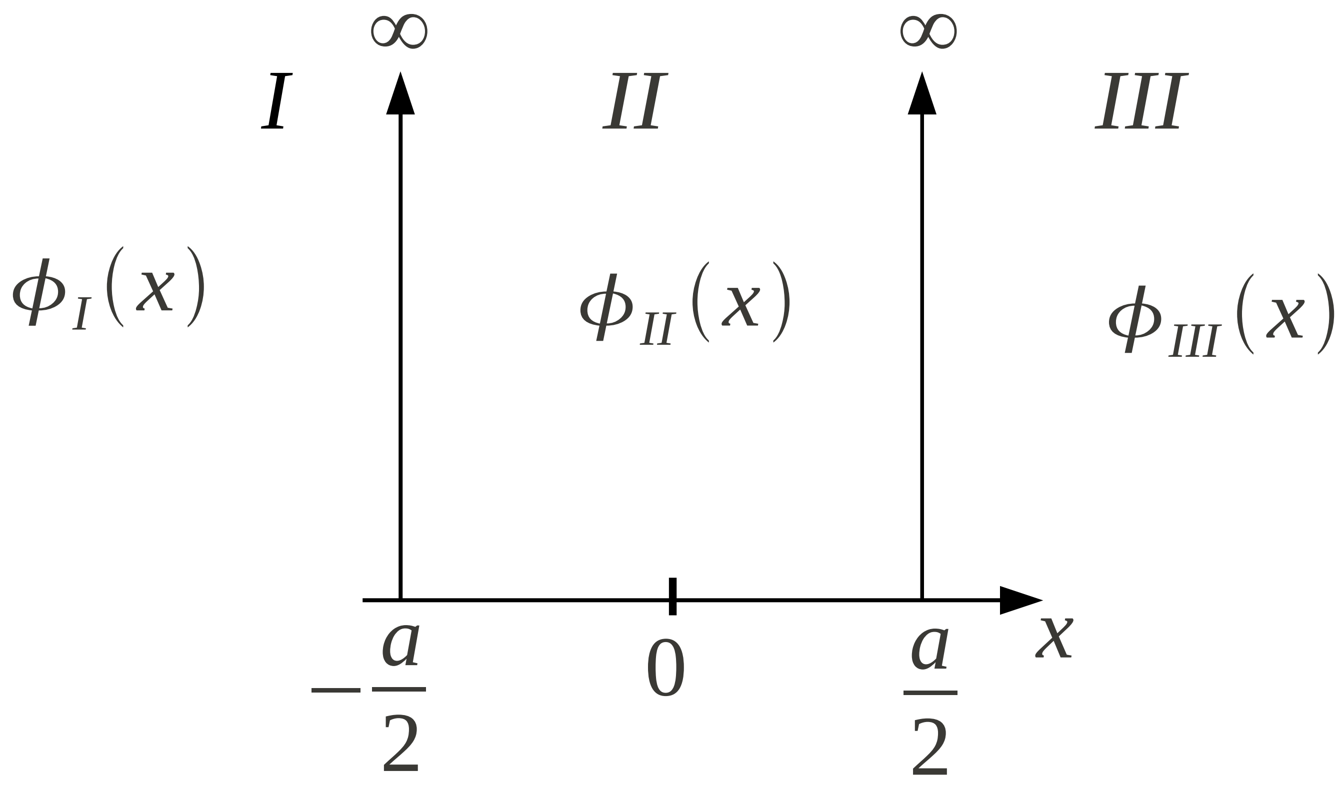
This means wavefunction does not exist outside an infinite potential well

$$\phi_I(x) = \phi_{III}(x) = 0$$

For any region of finite potential barrier the wavefunction exist inside the barrier region

In order the define the constants of the general solution we have to solve the equation inside well with required boundary condition

$$\phi_I(x) = \phi_{III}(x) = 0$$



The wavefunction in the box has to satisfy the boundary condition

$$\phi_{II}(x) = 0$$

at the end points

The value of the wave function at the boundary $x=\frac{a}{2}$ is given by

$$\phi\left(\frac{a}{2}\right)=A\sin\frac{ka}{2}+B\cos\frac{ka}{2}=0$$

The value of the wave function at the boundary $x=-\frac{a}{2}$ is given by

$$\phi\left(\frac{a}{2}\right)=A\sin\left(-\frac{ka}{2}\right)+B\cos\left(-\frac{ka}{2}\right)=0$$

$$-A\sin\left(\frac{ka}{2}\right)+B\cos\left(\frac{ka}{2}\right)=0$$

by addition

$$2B\cos\left(\frac{ka}{2}\right)=0$$

by subtraction

$$2A\sin\left(\frac{ka}{2}\right)=0$$

These are the two type of wavefunctions that satisfy the boundary conditions as well as other criteria for wavefunction must satisfy

$$\psi(x)$$ finite

$$\frac{d\psi(x)}{dx}$$ single valued

continuous

Since both wavefunctions satisfy the criteria

$$\phi(x) = A\cos\left(\frac{kx}{2}\right) \qquad \phi(x) = B\sin\left(\frac{kx}{2}\right)$$

Both are proper wavefunction representing the problem, however, both cannot simultaneously satisfy the boundary condition, therefore we may choose one them by either choosing $A=0$ and $\sin\left(\frac{ka}{2}\right)=0$

Or choosing $B=0$ and $\cos\left(\frac{ka}{2}\right)=0$

Therefore there are two class of solutions -when we choose cosine functions as solution

$$\cos\left(\frac{k\,a}{2}\right)=0$$

Allowed values of the wavectors are

$$\frac{k\,a}{2}=\frac{\pi}{2},\frac{3\pi}{2}\ldots\ldots\ldots\ldots$$

$$k=\frac{n\pi}{a} \qquad n=1,3,5.\ldots.$$

Similarly for the second class of solutions

$$\sin\left(\frac{k\,a}{2}\right)=0$$

$$\frac{k\,a}{2}=0,2\pi,4\pi\ldots\ldots\ldots\ldots$$

$$k=\frac{n\pi}{a} \qquad n=0,2,4.\ldots.$$

The wavefunctions are given by

$$\phi(x) = A_n \cos\left(\frac{k_n x}{2}\right) \qquad k = \frac{n\pi}{a} \qquad n = 1,3,5.....$$

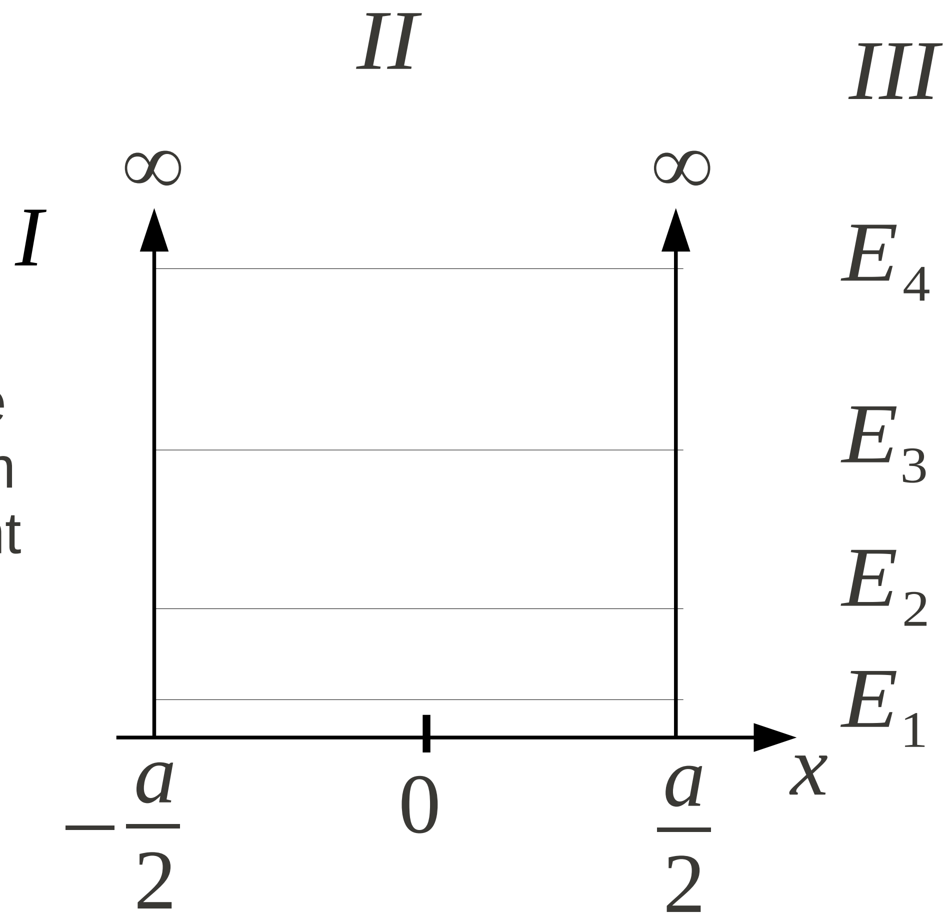
$$\phi(x) = B_n \sin\left(\frac{k_n x}{2}\right) \qquad k = \frac{n\pi}{a} \qquad n = 0,2,4.....$$

Using the expression $k = -\frac{\sqrt{2mE}}{\hbar}$

And also using the condition on the wavenumbers $k = \frac{n\pi}{a}$ energy is given by

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\pi^2 \hbar^2 n^2}{2ma^2} \qquad n = 0,1,2,3,4.....$$

Total energy of the particle in a box is quantized



In contrast to the classical case the lowest energy of the system is not zero. This is in agreement principle of uncertainty

Since the uncertainty in position of a particle is $\Delta x = a$

The associated uncertainty in the momentum $\Delta p \simeq \frac{\hbar}{2a}$