Solving the Schrödinger equation

In order to solve the Schrödinger equation

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

we assume $\Psi(x,t) = \psi(x)\, f(t).$

$$\frac{\partial \Psi}{\partial t} = \psi \frac{df}{dt}, \quad \frac{\partial^2 \Psi}{\partial x^2} = \frac{d^2\psi}{dx^2} f$$

$$i\hbar\psi \frac{df}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} f + V\psi f.$$

Dividing through by ψf:

$$i\hbar \frac{1}{f}\frac{df}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V.$$

This can be true only if both sides are constant (say, Then

$$i\hbar \frac{1}{f}\frac{df}{dt} = E, \text{ or } \frac{df}{dt} = -\frac{iE}{\hbar} f, \Rightarrow f(t) = e^{-iEt/\hbar}.$$

and

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

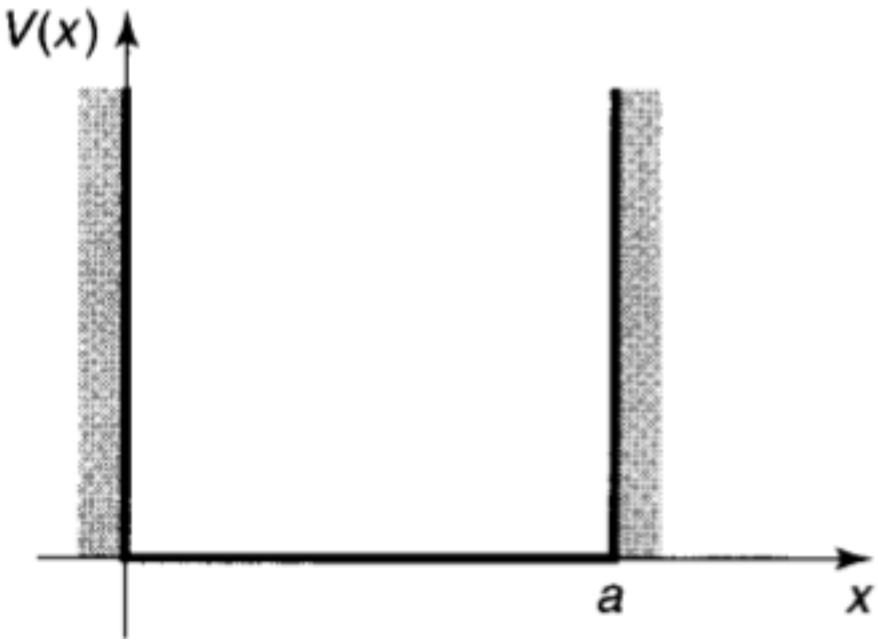
or

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi.}$$

This is the time-independent Schrödinger equation

This can be solved when the potential *V(x)* is specified

The infinite square well potential (or particle in a box)



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

Outside the well $\psi(x)=0$

(The probability of finding the particle there is zero).

Inside the well, where $V = 0$, the Schrödinger equation become

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

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

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

This is like the (classical) simple harmonic oscillator equatior
The general solution is:

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

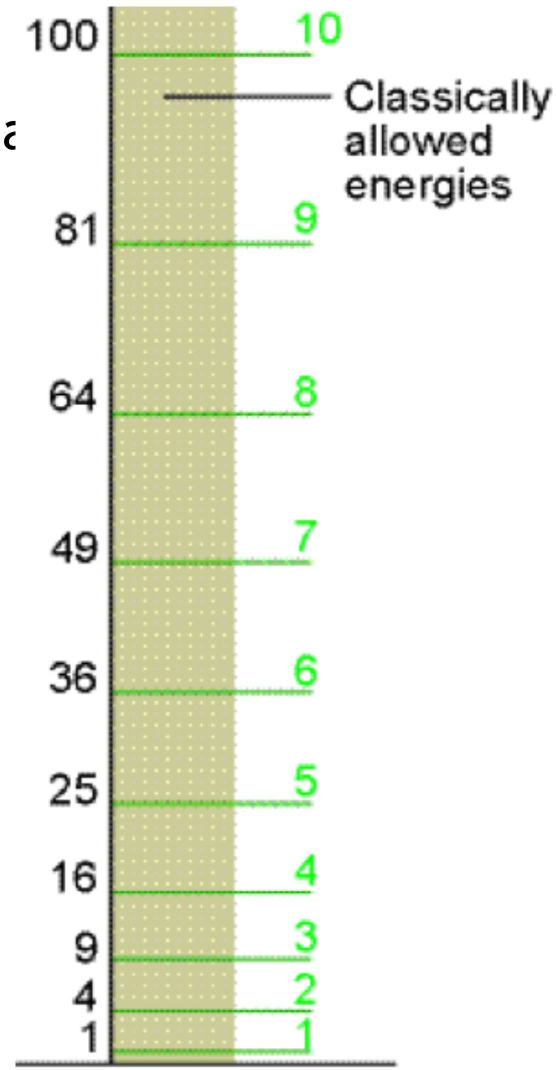
Boundary conditions: $\psi(0) = \psi(a) = 0,$

$$\Rightarrow \quad \psi(x) = A\sin kx.$$

Then $\psi(a) = A\sin ka, = 0$

$A \sin ka = 0$

- Either $A = 0$ (trivial solution) or sin ka $f(t) = e^{-iEt/\hbar}$.
- $ka = 0,\ \pm\pi,\ \pm 2\pi,\ \pm 3\pi, \ldots.$



We exclude $n = 0$ as this would make $\psi(x)=0$, and a negative values as this can be absorbed in A, as sin $(-ka)$ = -sin ka . Thus,

$$k_n = \frac{n\pi}{a}, \quad \text{with } n = 1,\ 2,\ 3, \ldots.$$

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

In sharp contrast to the classical case, a quantum particle in the infinite square well potential cannot have any possible energy – but only these special allowed values (bound states).

We normalize the wave function Ψ

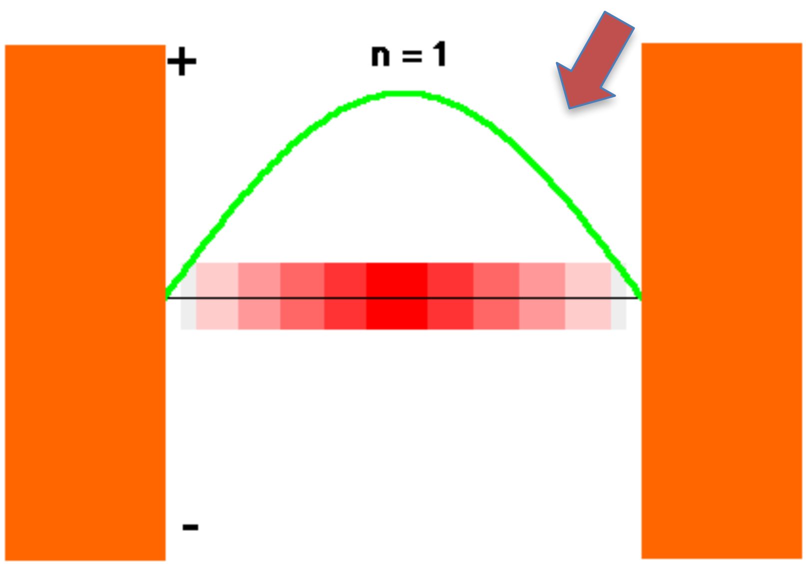
$$\int_0^a |A|^2 \sin^2(kx)\, dx = |A|^2 \frac{a}{2} = 1, \quad \text{so} \quad |A|^2 = \frac{2}{a}.$$

Inside the well, then the solutions are

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

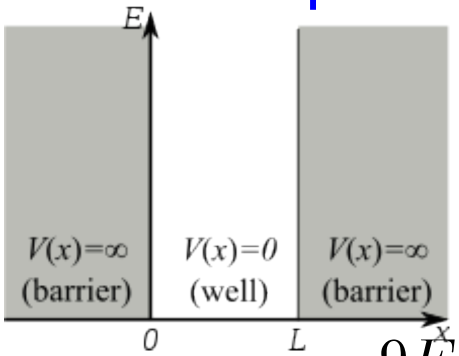
$\psi_n(x)$:

for n = 1 - 9

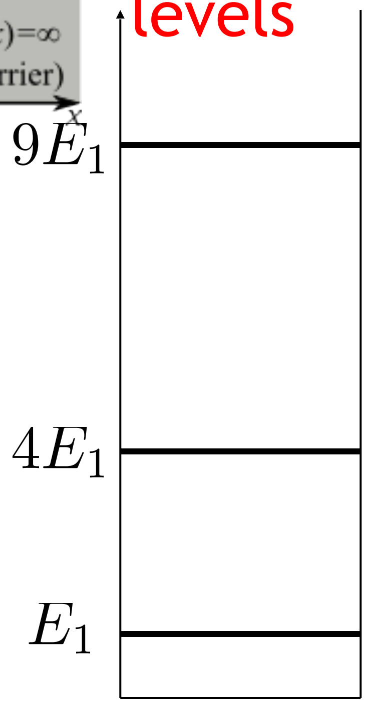


Summary

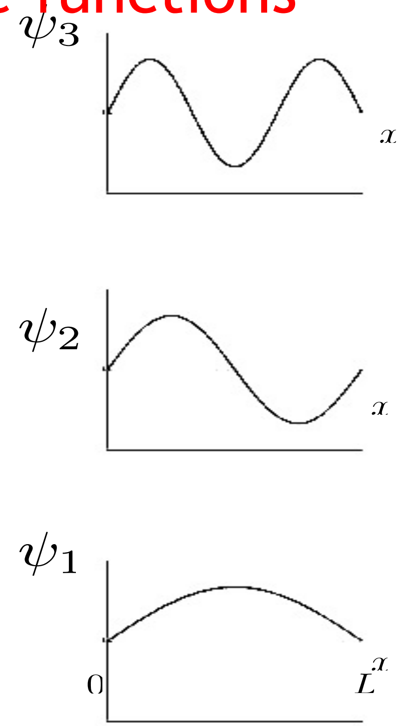
For a particle confined in a one-dimensional infinite potential well of dimension *L*



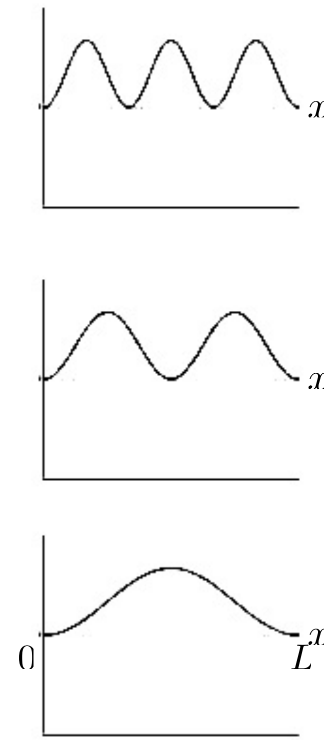
Energy levels



Wave functions



Probability [*P(x)*]



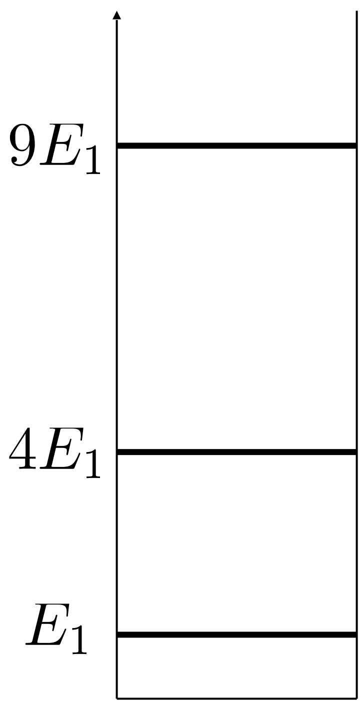
$$\boxed{E = \frac{n^2h^2}{8mL^2},}$$

$$\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

$$P(x) = |\psi(x)|^2\, dx = \frac{2}{L} \sin^2 \frac{n\pi x}{L} dx$$

This is an example of bound states

Energy levels



$$\boxed{E = \frac{n^2h^2}{8mL^2},}$$

Bound states are produced when
$E < V(+/-\ \infty)$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi.$$

$$H_{op}\psi_i = E_i\psi_i$$

For a general operator Q

eigenfunction

$$Q_{op}\psi_i = q_i\psi_i$$

operator

eigenvalue

$$\Psi(x,t) = \psi(x)\, f(t).$$

$$f(t) = e^{-iEt/\hbar}. \qquad E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}.$$

So, the solution of the Schrodinger equation is:

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

This one-dimensional box model can be easily extended to two- and three-dimensions.

Although particle-in-a-box is a simple model, it is a very useful model.

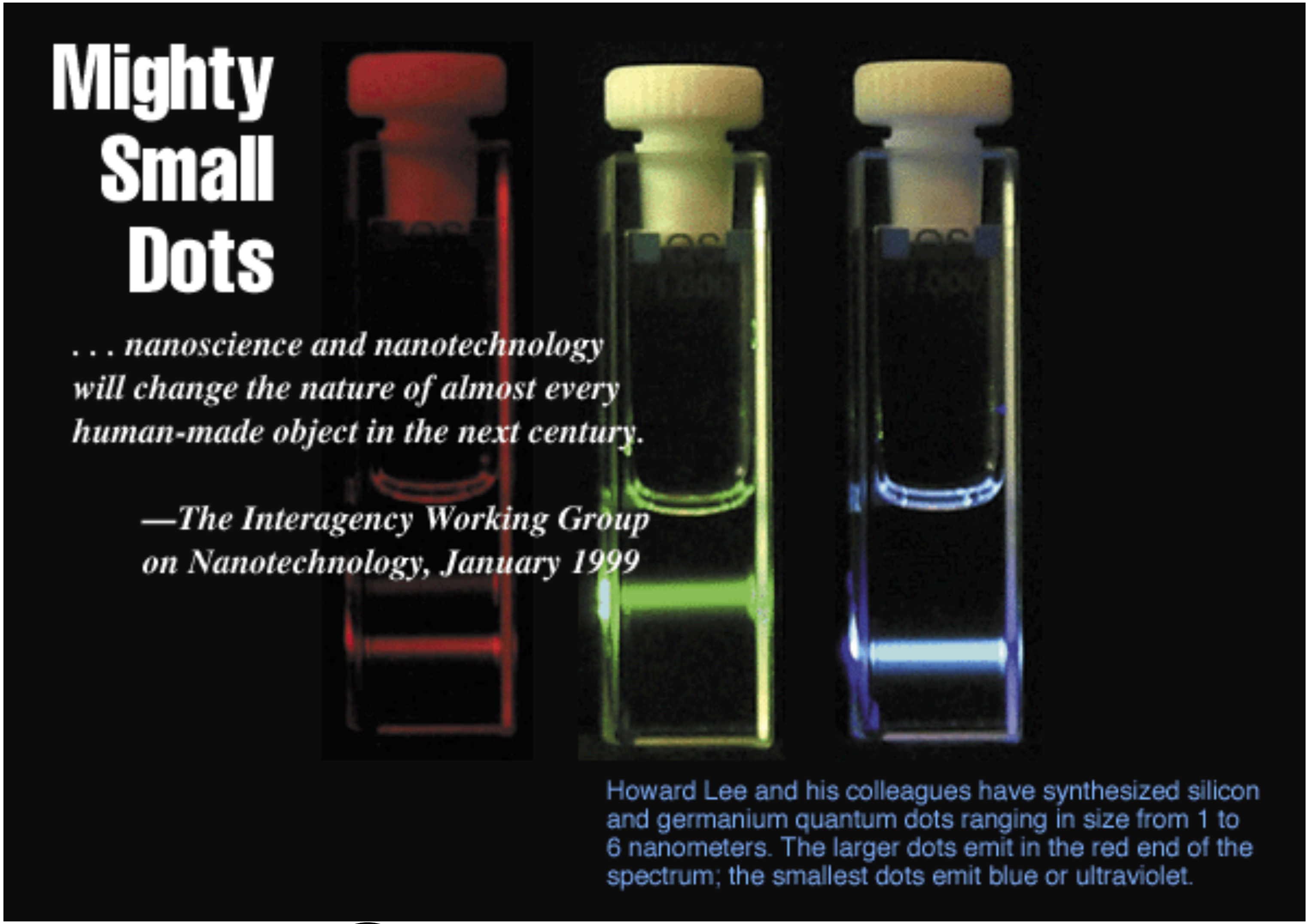
The particle in a box model can be applied to quantum well lasers.

The quantization of the energy levels of the electrons allows a quantum well laser to emit light more efficiently than conventional semiconductor lasers.

Particle-in-a-box approximation is applied to quantum dots, which are extremely small semiconductors (usually in the scale of nanometers).

A model of Samsung Quantum Dot TV

In a quantum dot, electrons are confined within the size of the material. For different sizes of the quantum dots, the energy level separation changes. So, the transition between these levels produce radiation of different colours.


Mighty Small Dots
. . . nanoscience and nanotechnology will change the nature of almost every human-made object in the next century.
—The Interagency Working Group on Nanotechnology, January 1999
Howard Lee and his colleagues have synthesized silicon and germanium quantum dots ranging in size from 1 to 6 nanometers. The larger dots emit in the red end of the spectrum; the smallest dots emit blue or ultraviolet.