PH 102: Interactive Lecture 2 Topics

- Unbound states
- Particle in a 1-D infinite potential well
- Particle in a 3-D infinite potential well
  - Schrodinger Equation
  - Separation of Variables
  - Energy quantization
  - Wave functions
  - Energy degeneracy
  - Energy split
- 3D Schrodinger Equation for Hydrogen atom
  - Separation of variables
  - Three equations

Schrodinger Equation

Time-Dependent Schrodinger Equation

$$\frac{-\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + U(x)\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

Separation of Variables $\Psi(x,t) = \psi(x)\,\phi(t)$

Spatial part of $\Psi(x,t)$: $\frac{-\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + U(x) = \mathrm{C}$

Temporal part of $\Psi(x,t)$: $i\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t} = \mathrm{C}$

$$\phi(t) = Ae^{(C/i\hbar)t} = Ae^{-i(C/\hbar)t}$$

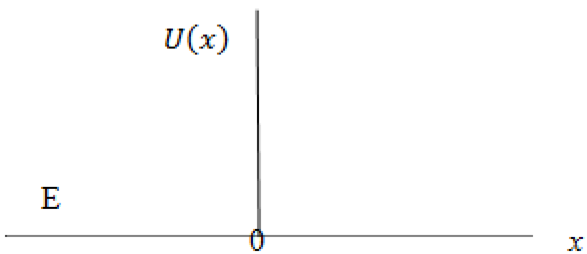
time-independent Schrodinger Equation:

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + U(x)\,\psi(x) = \mathrm{E}\,\psi(x)$$

Unbound states

time-independent Schrodinger Equation:

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + U(x)\,\psi(x) = \mathrm{E}\,\psi(x)$$



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

$$\frac{\partial^2\psi(x)}{\partial x^2} = \frac{-2mE}{\hbar^2}\psi(x) = -k^2\,\psi(x) \quad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

Solutions:

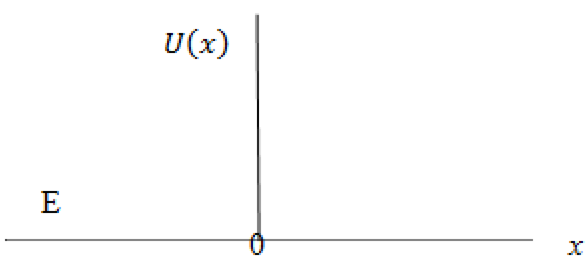
$e^{+ikx} = \cos kx + i \sin kx$ *for a particle* moving in the positive direction (→) on the x axis.

$e^{-ikx} = \cos kx - i \sin kx$ *for a particle* moving in the opposite direction (←) on the x axis.

Unbound states

time-independent Schrodinger Equation:

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



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

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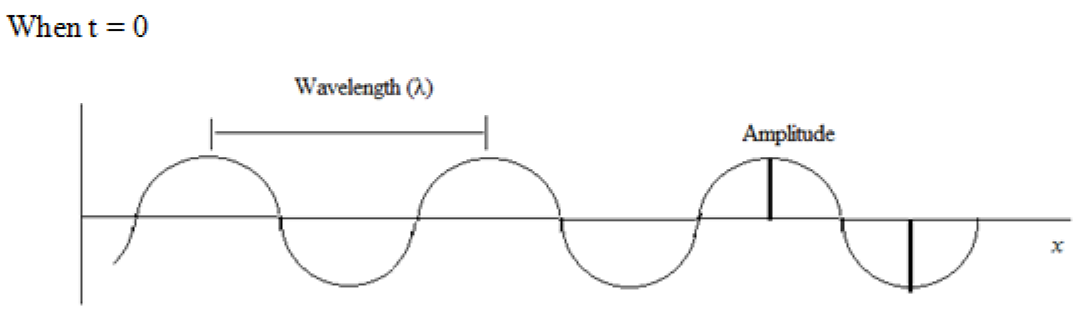
For Free Particle

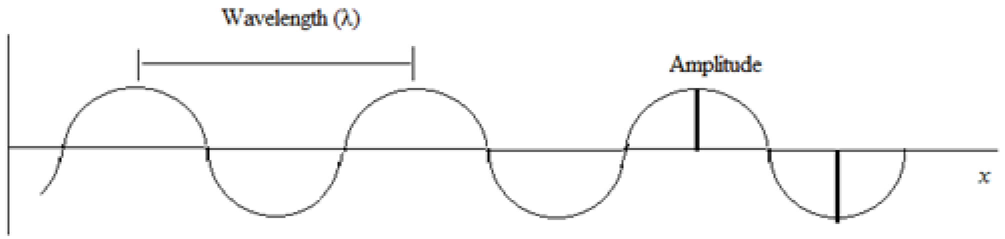


1.4 Momentum (p) =

1.5 Energy quanta (E) =

For Free Particle

When t = 0



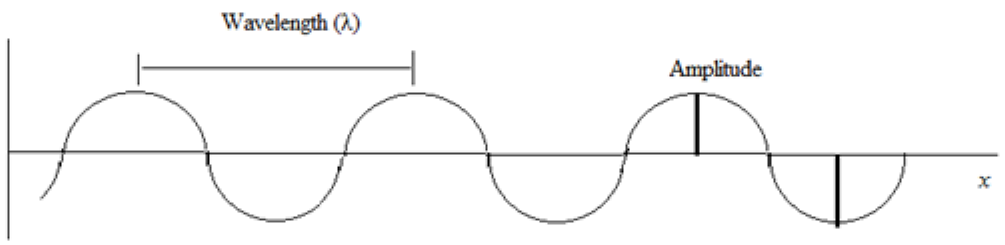
$$\Psi(x,t) = \psi(x)\ \phi(t) = \psi(x)\ e^{-i(C/\hbar)t}$$

1.4 Momentum (p) =

1.5 Energy quanta (E) =

For Free Particle

When t = 0



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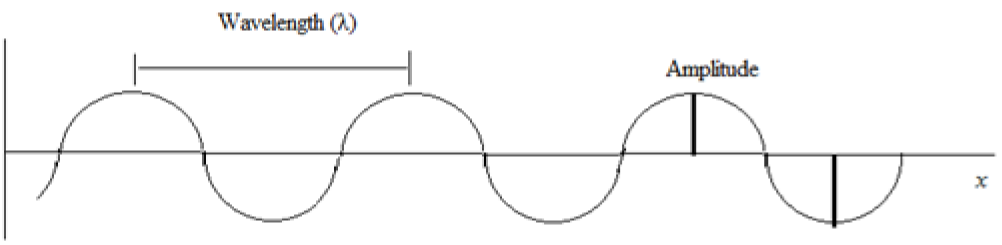


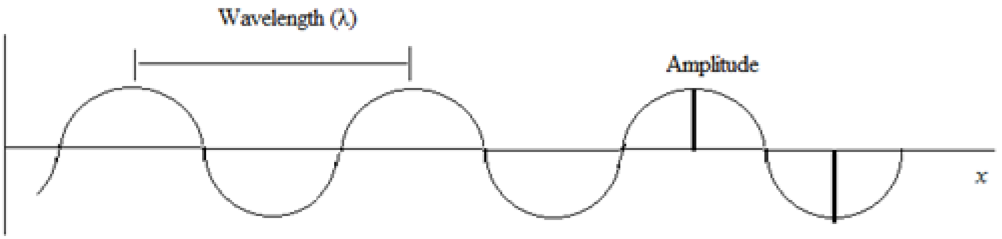
$$\Psi(x,t) = \psi(x)\,\phi(t) = \psi(x)\,e^{-i(C/\hbar)t} = e^{ikx}e^{-iwt}$$

1.4 Momentum (p) =

1.5 Energy quanta (E) =

For Free Particle

When t = 0



$$p = \frac{\hbar}{i}\frac{\partial}{\partial x} \quad \text{and} \quad E = i\hbar\,\frac{\partial}{\partial t}$$

$$\Psi(x,t) = \psi(x)\,\phi(t) = \psi(x)\,e^{-i(C/\hbar)t} \quad = e^{ikx}e^{-iwt}$$

1.4 Momentum (p) =

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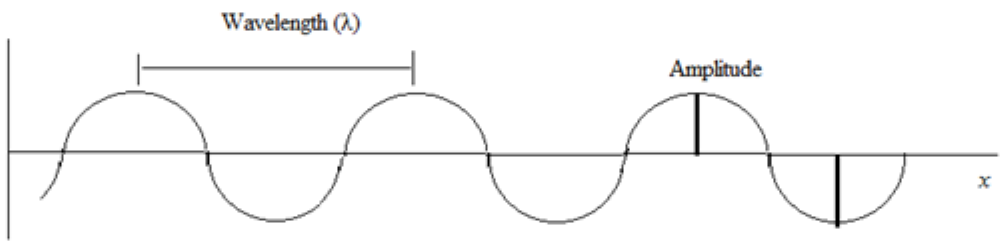
When t = 0



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$$\Psi(x,t) = \psi(x)\,\phi(t) = \psi(x)\,e^{-i(C/\hbar)t}$$

$$e^{ikx}e^{-iwt}$$

1.4 Momentum (p) = $\hbar k = \hbar\left(\frac{2\pi}{\lambda}\right) = \frac{h}{\lambda}$ (de Broglie relation)

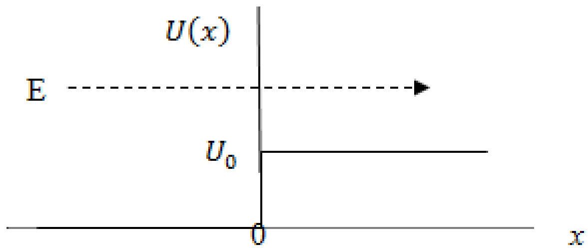
1.5 Energy quanta (E) = $\hbar\omega$

Unbound states

time-independent Schrodinger Equation:

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

$$U(x) = \begin{cases} 0 & x < 0 \\ U_0 & x \geq 0 \end{cases}$$



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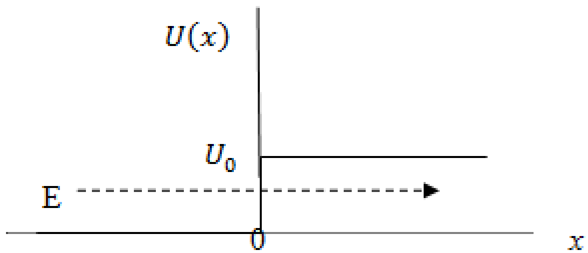

Bound vs. unbound states

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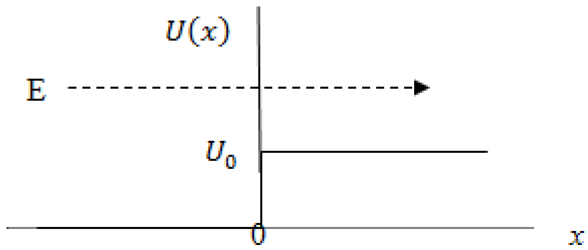

Where $x < 0$,

Where $x \geq 0$

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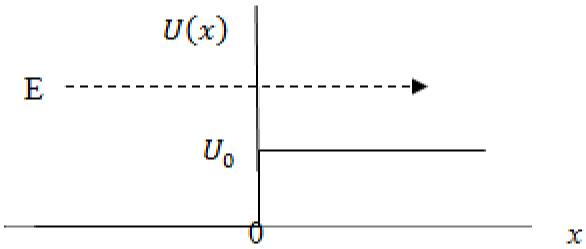

Where $x < 0$,

$$\frac{\partial^2\psi(x)}{\partial x^2} = \frac{-2m\,E}{\hbar^2}\psi(x) = -\,k^2\,\psi(x) \quad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

Where $x \geq 0$

$$\frac{\partial^2\psi(x)}{\partial x^2} = \frac{-2m(E-U_0)}{\hbar^2}\psi(x) = -\,k'^2\,\psi(x) \quad \text{where } k' = \sqrt{\frac{2m(E-U_0)}{\hbar^2}}$$

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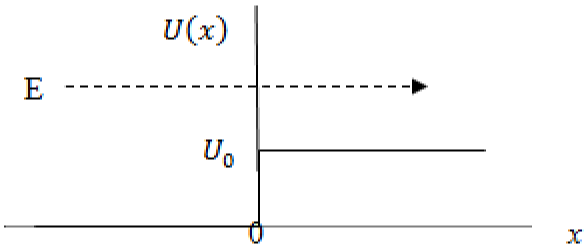

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$\psi_{x<0}$ = Incoming wave function + Reflected wave function

$= A\,e^{+ikx} + B\,e^{-ikx}$

Where $x \geq 0$

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$\psi_{x\geq 0}$ = the transmitted wave function,

$= Ce^{ik'x}$

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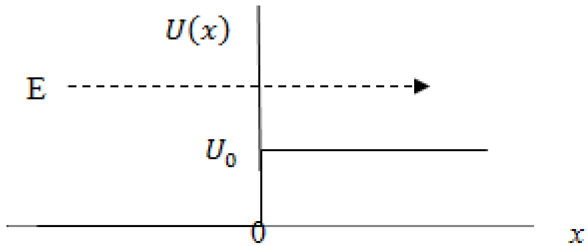

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$\psi_{x\geq 0}$ = the transmitted wave function,

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- $\psi_{x<0}(x=0) = \psi_{x\geq 0}(x=0)$ → $A + B = C$
- $\frac{d\psi_{x<0}}{dx}\Big|_{x=0}\ \frac{d\psi_{x\geq 0}}{dx}\Big|_{x=0}$ → $k(A - B) = k'C$

Bound vs. unbound states

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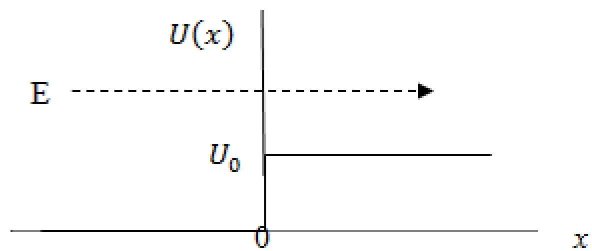

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$$\text{Reflection probability} = \frac{\text{reflected particle flux}}{\text{incoming particle flux}} = \frac{|\psi_{reflected}|^2\,k}{|\psi_{incoming}|^2\,k} = \frac{B^*B}{A^*A}$$

$$\text{Transmission probability} = \frac{\text{transmitted particle flux}}{\text{incoming particle flux}} = \frac{|\psi_{trans}|^2\,k'}{|\psi_{incoming}|^2\,k} = \frac{C^*C\,k'}{A^*A\,k}$$

Bound vs. unbound states

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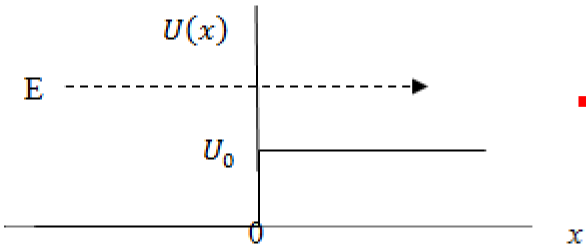

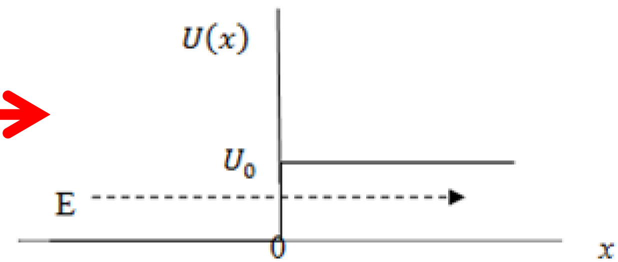

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$\psi_{x\geq 0}$ = the transmitted wave function,

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- $\psi_{x<0}(x=0) = \psi_{x\geq 0}(x=0)$ → $A + B = C$
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Bound vs. unbound states

time-independent Schrodinger Equation:

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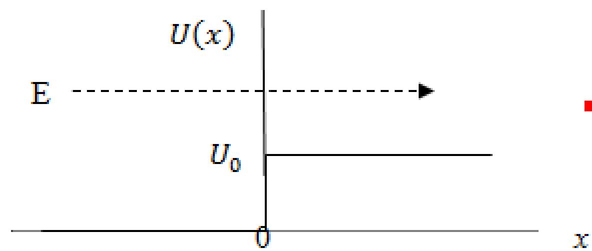

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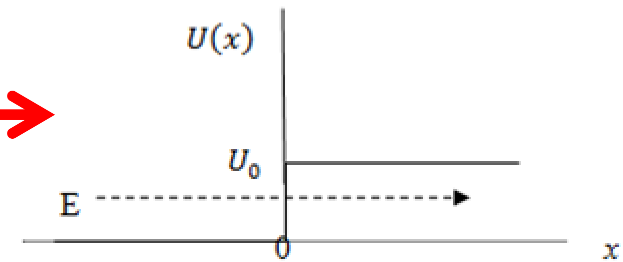

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$\psi_{x<0}$ = Incoming wave function + Reflected wave function

$= \quad A\,e^{+ikx} \quad + \quad B\,e^{-ikx}$

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$\psi_{x\geq 0}$ = the transmitted wave function,

$= Ce^{ik'x}$ → $Ce^{-\alpha x}$

$$\alpha = \sqrt{\frac{2m(U_0-E)}{\hbar^2}}$$

- $\psi_{x<0}(x=0) = \psi_{x\geq 0}(x=0)$ → $A + B = C$
- $\frac{d\psi_{x<0}}{dx}\Big|_{x=0} = \frac{d\psi_{x\geq 0}}{dx}\Big|_{x=0}$ → $k(A-B) = -\alpha\, C$

Reflection probability $= \frac{\text{reflected particle flux}}{\text{incoming particle flux}} = \frac{|\psi_{reflected}|^2\,k}{|\psi_{incoming}|^2\,k} = \frac{B^*B}{A^*A}$

Transmission probability = 0

→ 0

Bound vs. unbound states

time-independent Schrodinger Equation:

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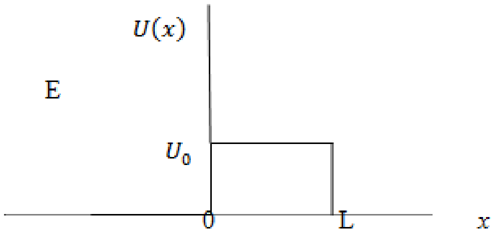
$$U(x) = \begin{cases} 0 & x < 0 \\ U_0 & 0 \le x \le L \\ 0 & x > L \end{cases}$$

E



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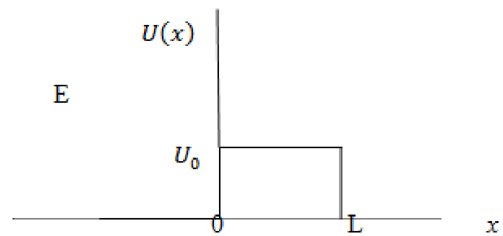

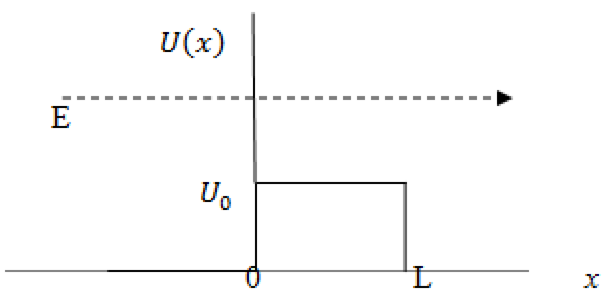

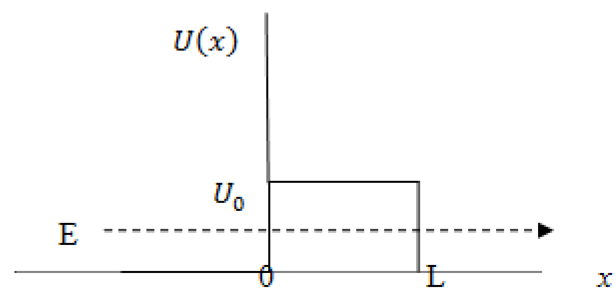

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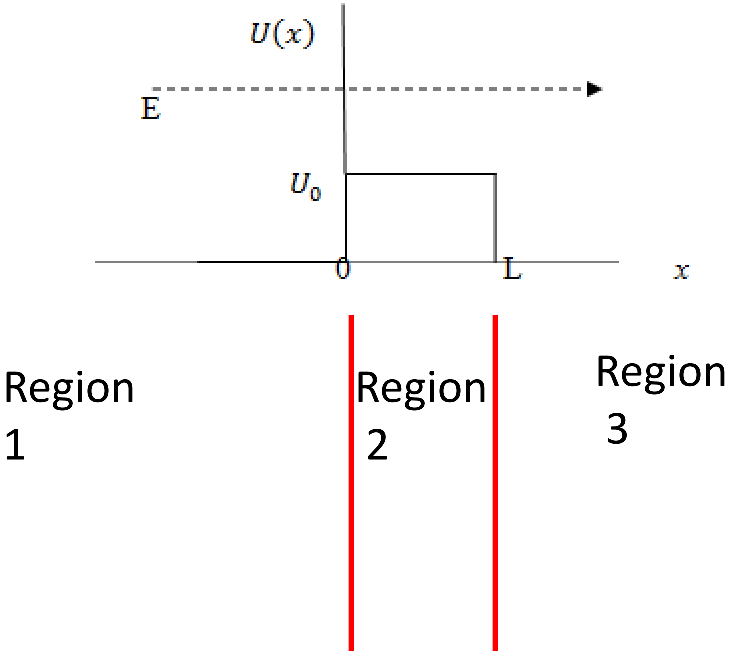

Bound vs. unbound states

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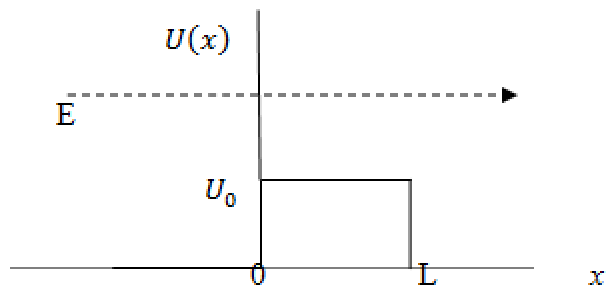

Region 1

$\mathrm{A}\,e^{+ikx} \quad + \quad \mathrm{B}\,e^{-ikx}$

Region 2

$\mathrm{C}\,e^{+ik'x} \quad + \quad \mathrm{D}\,e^{-ik'x}$

Region 3

$\mathrm{F}e^{ikx}$

Bound vs. unbound states

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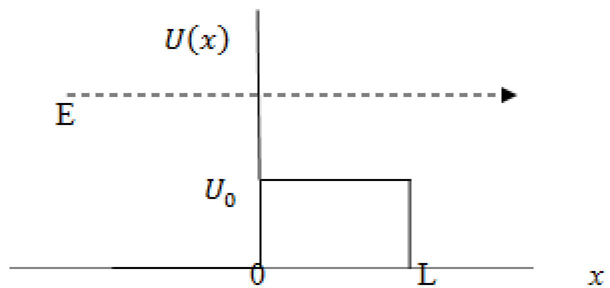

Transmission probability $= \frac{F*F}{A^*A}$

Reflection probability $= \frac{B^*B}{A^*A}$

Region 1

Region 2

Region 3

$\mathrm{A}\,e^{+ikx} \quad + \quad \mathrm{B}\,e^{-ikx}$

$\mathrm{C}\,e^{+ik'x} \; + \mathrm{D}\,e^{-ik'x}$

: $\mathrm{F}e^{ikx}$

- $\psi_{x<0}(x=0) = \psi_{0\le x\le L}\,(x=0)$ → $\mathrm{A} + \mathrm{B} = \mathrm{C} + \mathrm{D}$
- $\frac{d\psi_{x<0}}{dx}\big|_{x=0} = \frac{d\psi_{0\le x\le L}}{dx}\big|_{x=0}$ → $k\,(\mathrm{A}-\mathrm{B}) = k'(\mathrm{C}-\mathrm{D})$
- $\psi_{\psi_{0\le x\le L}}(x=L) = \psi_{0x>L}\,(x=\mathrm{L})$ → $\mathrm{C}e^{+ik'L} + \mathrm{D}e^{-ik'L} = \mathrm{F}e^{+ikL}$
- $\frac{d\psi_{0\le x\le L}}{dx}\big|_{x=\mathrm{L}} = \frac{d\psi_{x>L}}{dx}\big|_{x=\mathrm{L}}$ → $ik'\,(\mathrm{C}e^{+ik'L} - \mathrm{D}e^{-ik'L} = ik\;\mathrm{F}e^{+ikL}$

Bound vs. unbound states

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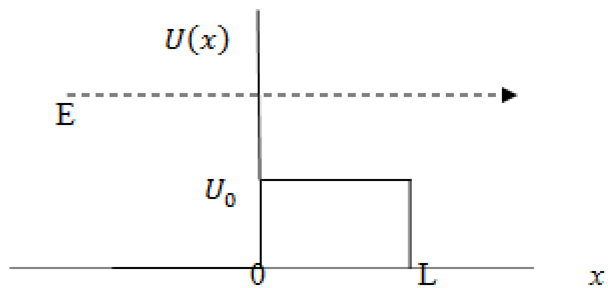
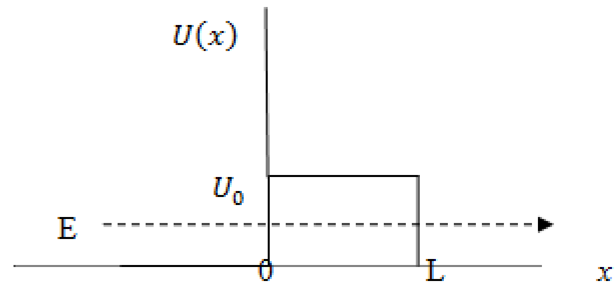




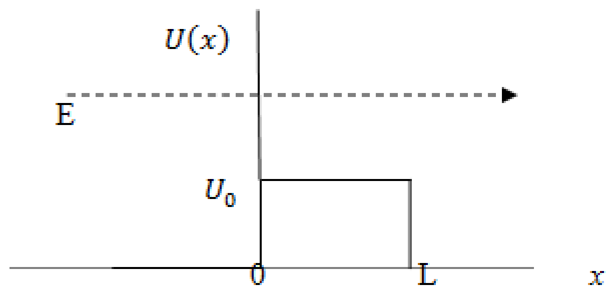
Region 1	Region 2	Region 3
$A\,e^{+ikx} + B\,e^{-ikx}$	$C\,e^{+ik'x} + D\,e^{-ik'x}$	Fe^{ikx}

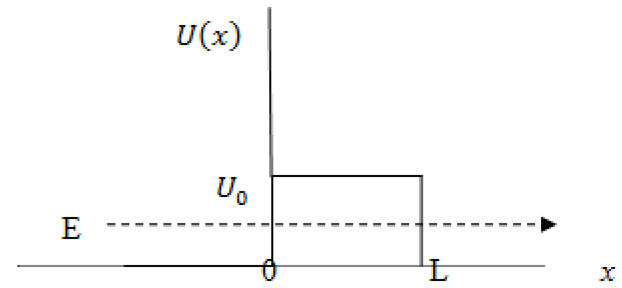
- $\psi_{x<0}(x=0) = \psi_{0\le x\le L}(x=0)$ → $A + B = C + D$
- $\frac{d\psi_{x<0}}{dx}\Big|_{x=0} = \frac{d\psi_{0\le x\le L}}{dx}\Big|_{x=0}$ → $k(A - B) = k'(C - D)$
- $\psi_{\psi_{0\le x\le L}}(x=L) = \psi_{0x>L}(x=L)$ → $Ce^{+ik'L} + De^{-ik'L} = Fe^{+ikL}$
- $\frac{d\psi_{0\le x\le L}}{dx}\Big|_{x=L} = \frac{d\psi_{x>L}}{dx}\Big|_{x=L}$ → $ik'(Ce^{+ik'L} - De^{-ik'L} = ik\,Fe^{+ikL}$

Bound vs. unbound states

time-independent Schrodinger Equation:

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + U(x)\,\psi(x) = \mathrm{E}\,\psi(x)$$





Region 1

Region 2

Region 3

$\mathrm{A}\,e^{+ikx} \quad + \quad \mathrm{B}\,e^{-ikx}$

$\mathrm{C}\,e^{+\alpha x} \quad + \quad \mathrm{D}\,e^{-\alpha x}$

$\mathrm{F}e^{ikx}$

Schrodinger Equation

Hamiltonian operator (H)

$$H\Psi(x,t) = E\Psi(x,t)$$

Since H = Total Energy = Kinetic energy (T) + Potential energy (U)

$$\left(\frac{p^2}{2m} + U\right)\Psi(x,t) = E\Psi(x,t)$$

$$p = \frac{\hbar}{i}\frac{\partial}{\partial x} \quad \text{and} \quad \mathrm{E} = i\hbar\,\frac{\partial}{\partial t}$$

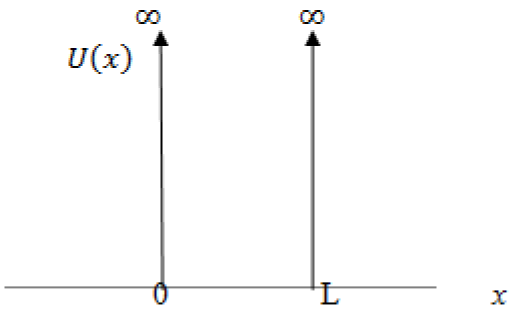
Time-Dependent Schrodinger Equation

$$\frac{-\hbar^2}{2m}\,\frac{\partial^2\Psi\,(x,t)}{\partial x^2} + U(x)\Psi(x,t) = i\hbar\,\frac{\partial\,\Psi(x,t)}{\partial t}$$

1-D infinite potential well

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + U(x)\,\psi(x) = \mathrm{E}\,\psi(x)$$

$$U(x) = \begin{cases} \infty & x \le 0 \\ 0 & 0 < x < L \\ \infty & x \ge L \end{cases}$$



1-D infinite potential well

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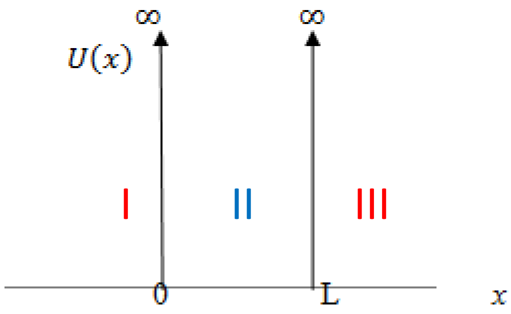
$x \le 0$ → Region I

$0 < x < L$ → Region II

$x \ge L$ → Region III



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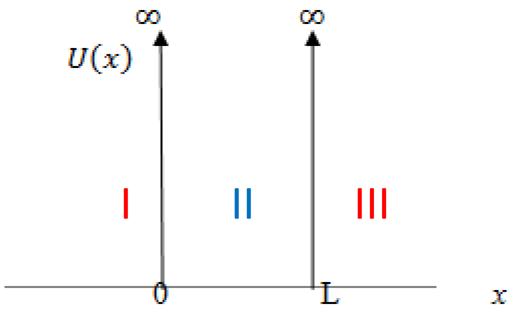


Regions I and III, no wave function can exist →

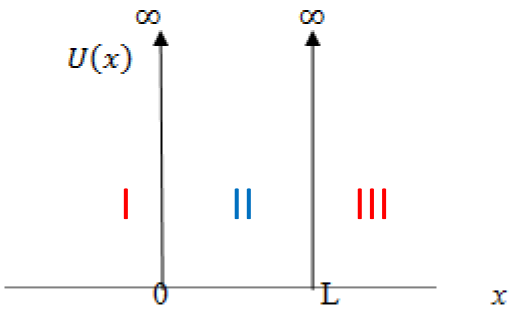
$$\psi_{x\le 0}(x) = 0$$
$$\psi_{x\ge L}(x) = 0$$

1-D infinite potential well

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + U(x)\,\psi(x) = \mathrm{E}\,\psi(x)$$

$$U(x) = \begin{cases} \infty & x \le 0 \\ 0 & 0 < x < L \\ \infty & x \ge L \end{cases}$$

→ Region I
→ Region II
→ Region III



Regions I and III, no wave function can exist → $\psi_{x\le 0}(x) = 0$, $\psi_{x\ge L}(x) = 0$

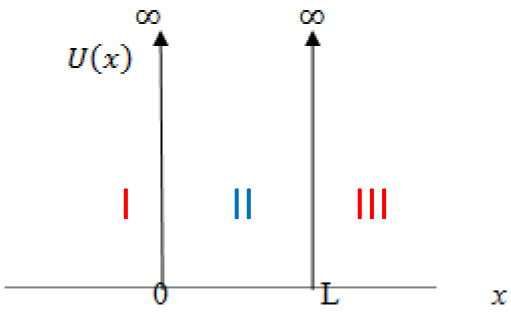
Region II, $\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} = \mathrm{E}\,\psi(x)$ →

1-D infinite potential well

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + U(x)\,\psi(x) = \mathrm{E}\,\psi(x)$$

$$U(x) = \begin{cases} \infty & x \le 0 \\ 0 & 0 < x < L \\ \infty & x \ge L \end{cases}$$

$x \le 0$ → Region I
$0 < x < L$ → Region II
$x \ge L$ → Region III



Regions I and III, no wave function can exist → $\psi_{x\le 0}(x) = 0$, $\psi_{x \ge L}(x) = 0$

Region II, $\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} = \mathrm{E}\,\psi(x)$ → $\psi_{0<x<L}(x) = A\sin(kx)$; $k = \sqrt{\frac{2mE}{\hbar^2}}$

1-D infinite potential well

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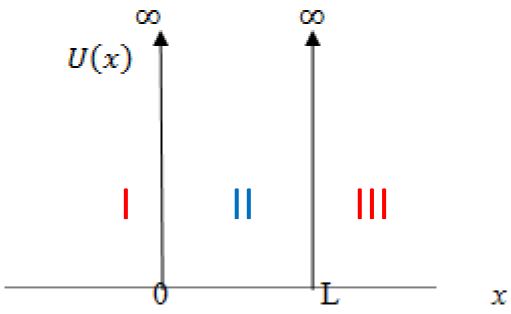
→ Region I
→ Region II
→ Region III



Regions I and III, no wave function can exist → $\psi_{x\le 0}(x) = 0$
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Region II, $\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} = \mathrm{E}\,\psi(x)$ → $\psi_{0<x<L}(x) = A\sin(kx)$: $k = \sqrt{\frac{2mE}{\hbar^2}}$

$\psi_{x\ge L}(x=0) = 0$ → $\psi_{0<x<L}(x=L) = \sin(kL) = 0$

1-D infinite potential well

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + U(x)\,\psi(x) = \mathrm{E}\,\psi(x)$$

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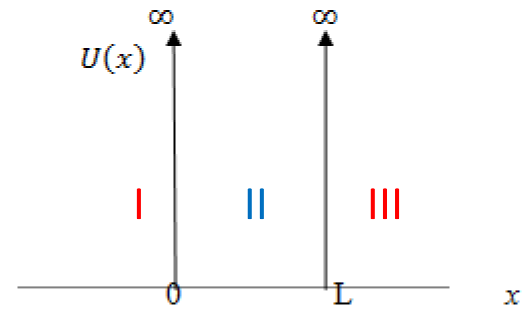
→ Region I
→ Region II
→ Region III



Regions I and III, no wave function can exist → $\psi_{x\leq 0}(x) = 0$, $\psi_{x\geq L}(x) = 0$

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$\psi_{x\geq L}(x=0) = 0$ → $\psi_{0<x<L}(x=L) = \sin(kL) = 0$

$$kL = \sqrt{\frac{2mE}{\hbar^2}}L = n\pi$$ where n =1, 2, 3, etc.

$$E = \frac{n^2\pi^2\hbar^2}{2mL^2}$$ Energy quantization

1-D infinite potential well

Normalization:

$$\psi_{0<x<L}(x) = A\sin(kx) = \text{A}\sin(\frac{n\pi x}{L})$$

$$\int_0^L |\psi_{0<x<L}(x)|^2 = 1 = \text{A}^2 \int_0^L \sin\left(\frac{n\pi x}{L}\right)^2 dx =$$

$$sin^2 x = \frac{1 - cos2x}{2}$$

$$cos^2 x = \frac{1 + cos2x}{2}$$

1-D infinite potential well

Normalization:

$$\psi_{0<x<L}(x) = A\sin(kx) = \mathrm{A}\sin(\frac{n\pi x}{L})$$

$$\int_0^L |\psi_{0<x<L}(x)|^2 = 1 = \mathrm{A}^2 \int_0^L \sin\left(\frac{n\pi x}{L}\right)^2 dx = \mathrm{A}^2 \frac{\mathrm{L}}{2} \rightarrow \mathrm{A} = \sqrt{\frac{2}{L}}$$

$$sin^2 x = \frac{1 - cos2x}{2}$$

$$cos^2 x = \frac{1 + cos2x}{2}$$

1-D infinite potential well

Normalization:

$$\psi_{0<x<L}(x) = A\sin(kx) = \mathrm{A}\sin(\frac{n\pi x}{L})$$

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Wave function: $\psi_{0<x<L}(x) = \sqrt{\frac{2}{L}}\,\sin(\frac{n\pi x}{L})$

Energy $E = \frac{n^2\,\pi^2\,\hbar^2}{2mL^2}$

1-D infinite potential well

Normalization:

$$\psi_{0<x<L}(x) = A\sin(kx) = \text{A}\sin(\frac{n\pi x}{L})$$

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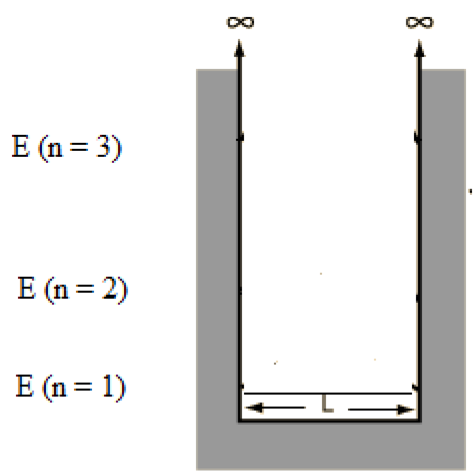
Wave function: $\psi_{0<x<L}(x) = \sqrt{\frac{2}{L}}\ \sin(\frac{n\pi x}{L})$

Energy $E = \dfrac{n^2\pi^2\hbar^2}{2mL^2}$

Obtain the first three energy levels ($\dfrac{\pi^2\hbar^2}{2mL^2}$) and draw their associated wave functions



1-D infinite potential well

Normalization:

$$\psi_{0<x<L}(x) = A\sin(kx) = \text{A}\sin(\frac{n\pi x}{L})$$

$$\int_0^L |\psi_{0<x<L}(x)|^2 = 1 = \text{A}^2 \int_0^L \sin\left(\frac{n\pi x}{L}\right)^2 dx = \text{A}^2 \frac{\text{L}}{2} \rightarrow \text{A} = \sqrt{\frac{2}{L}}$$

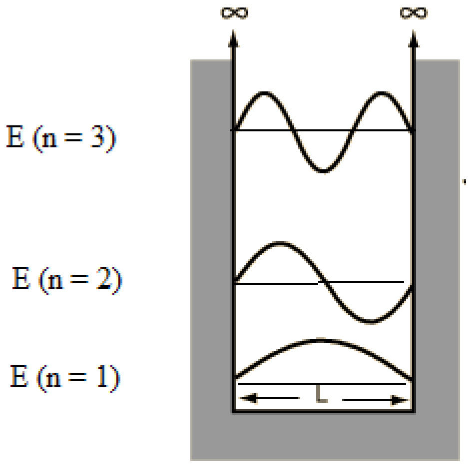
Wave function: $\psi_{0<x<L}(x) = \sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L})$

Energy $E = \frac{n^2\pi^2\hbar^2}{2mL^2}$

$$E\ (n=3) = 9\frac{\pi^2\hbar^2}{2mL^2}$$

$$E\ (n=2) = 4\frac{\pi^2\hbar^2}{2mL^2}$$

$$E\ (n=1) = 1\frac{\pi^2\hbar^2}{2mL^2}$$

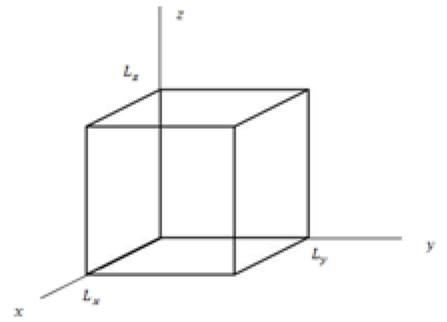


Particle in a 3-d infinite well

$$\frac{-\hbar^2}{2m}\nabla^2\psi(\vec{x}) + U(\vec{x})\psi(\vec{x}) = E\,\psi(\vec{x})$$

In (x, y, z) coordinates, $\vec{x} = (x, y, z)$, $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi(x, y, z) = -\frac{2m}{\hbar^2}(E - U(x, y, z))\psi(x, y, z)$$



$$U(\vec{x}) = \begin{cases} 0 & 0 < x < L_x, 0 < y < L_y . 0 < z < L_z \\ \infty & otherwise \end{cases}$$

Wave functions exist only inside the 3-d infinite well.

Particle in a 3-d infinite well

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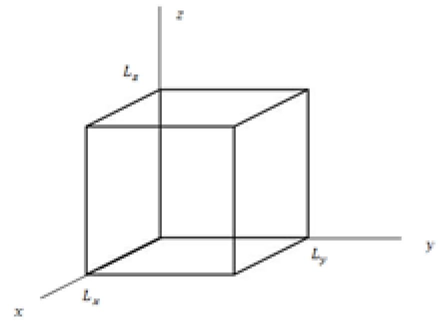


$$U(\vec{x}) = \begin{cases} 0 & 0 < x < L_x, 0 < y < L_y, 0 < z < L_z \\ \infty & otherwise \end{cases}$$

Wave functions exist only inside the 3-d infinite well.

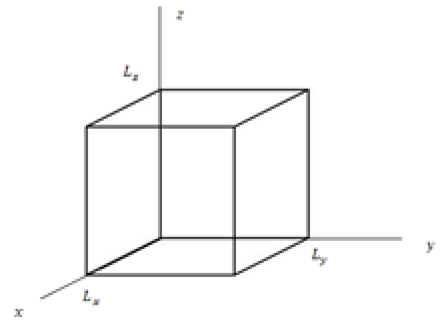
Separation of variables: $\psi(\vec{x}) = \psi(x, y, z) = F(x)G(y)H(z)$

Particle in a 3-d infinite well

$$\frac{-\hbar^2}{2m}\nabla^2\psi(\vec{x}) + U(\vec{x})\psi(\vec{x}) = E\,\psi(\vec{x})$$

In (x, y, z) coordinates, $\vec{x} = (x, y, z)$, $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi(x, y, z) = -\frac{2m}{\hbar^2}(E - U(x, y, z))\psi(x, y, z)$$



$$U(\vec{x}) = \begin{cases} 0 & 0 < x < L_x, 0 < y < L_y, 0 < z < L_z \\ \infty & otherwise \end{cases}$$

Wave functions exist only inside the 3-d infinite well.

Separation of variables: $\psi(\vec{x}) = \psi(x, y, z) = F(x)G(y)H(z)$

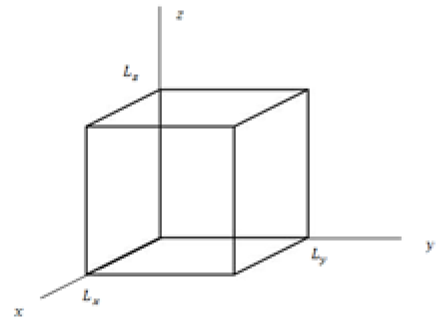
$$\frac{1}{F(x)}\frac{\partial^2 F(x)}{\partial x^2} + \frac{1}{G(y)}\frac{\partial^2 G(y))}{\partial y^2} + \frac{1}{H(z)}\frac{\partial^2 H(z)}{\partial z^2} = -\frac{2mE}{\hbar^2}$$

Particle in a 3-d infinite well

$$\frac{-\hbar^2}{2m}\nabla^2\psi(\vec{x}) + U(\vec{x})\psi(\vec{x}) = E\,\psi(\vec{x})$$

In (x, y, z) coordinates, $\vec{x} = (x, y, z)$, $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi(x,y,z) = -\frac{2m}{\hbar^2}(E - U(x,y,z))\psi(x,y,z)$$



$$U(\vec{x}) = \begin{cases} 0 & 0 < x < L_x, 0 < y < L_y, 0 < z < L_z \\ \infty & otherwise \end{cases}$$

Wave functions exist only inside the 3-d infinite well.

Separation of variables: $\psi(\vec{x}) = \psi(x,y,z) = F(x)G(y)H(z)$

$$\frac{1}{F(x)}\frac{\partial^2 F(x)}{\partial x^2} + \frac{1}{G(y)}\frac{\partial^2 G(y))}{\partial y^2} + \frac{1}{H(z)}\frac{\partial^2 H(z)}{\partial z^2} = -\frac{2mE}{\hbar^2}$$

=constant

constant=Cx Constant=Cy Constant=Cz

$$Cx + Cy + Cz = -\frac{2mE}{\hbar^2}$$

Particle in a 3-d infinite well

1-D solutions:

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

Wave function: $\psi_{0<x<L}(x) = \sqrt{\frac{2}{L}}\,\sin(\frac{n\pi x}{L})$

Energy $E = \frac{n^2\,\pi^2\,\hbar^2}{2mL^2}$

$$\begin{cases} \frac{d\,F(x)}{dx^2} = C_x F(x) \\ \frac{d\,G(y)}{dy^2} = C_y G(y) \\ \frac{d\,H(z)}{dz^2} = C_z H(z) \end{cases}$$

Particle in a 3-d infinite well

1-D solutions:

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

Wave function: $\psi_{0<x<L}(x) = \sqrt{\frac{2}{L}}\,\sin(\frac{n\pi x}{L})$

Energy $E = \frac{n^2\,\pi^2\,\hbar^2}{2mL^2}$

3-D solutions: wave functions

$$\begin{cases} \frac{d\,F(x)}{dx^2} = C_x F(x) & \rightarrow F(x) = A_x \sin\frac{n_x \pi x}{L_x} \\ \frac{d\,G(y)}{dy^2} = C_y G(y) & \rightarrow G(y) = A_y \sin\frac{n_y \pi y}{L_y} \\ \frac{d\,H(z)}{dz^2} = C_z H(z) & \rightarrow H(z) = A_z \sin\frac{n_z \pi z}{L_z} \end{cases}$$

Particle in a 3-d infinite well

1-D solutions:

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

Wave function: $\psi_{0<x<L}(x) = \sqrt{\frac{2}{L}}\,\sin(\frac{n\pi x}{L})$

Energy $E = \frac{n^2\,\pi^2\,\hbar^2}{2mL^2}$

3-D solutions: wave functions

$$\begin{cases} \frac{d\,F(x)}{dx^2} = C_x F(x) & \rightarrow F(x) = A_x \sin\frac{n_x \pi x}{L_x} \\ \frac{d\,G(y)}{dy^2} = C_y G(y) & \rightarrow G(y) = A_y \sin\frac{n_y \pi y}{L_y} \\ \frac{d\,H(z)}{dz^2} = C_z H(z) & \rightarrow H(z) = A_z \sin\frac{n_z \pi z}{L_z} \end{cases}$$

Cx = $-\frac{n_x^2 \pi^2}{L_x{}^2}$ Cy = $-\frac{n_y^2 \pi^2}{L_y{}^2}$ Cz= $-\frac{n_z^2 \pi^2}{L_z{}^2}$

Cx + Cy + Cz = $-\frac{2mE}{\hbar^2}$ = $-\frac{n_x^2 \pi^2}{L_x{}^2} - \frac{n_y^2 \pi^2}{L_y{}^2} - \frac{n_z^2 \pi^2}{L_z{}^2}$

Particle in a 3-D infinite well

$$E_{(n_x,n_y,n_z)} = \left(\frac{n_x^2}{L_x{}^2} + \frac{n_y^2}{L_y{}^2} + \frac{n_z^2}{L_z{}^2}\right)\frac{\pi^2\hbar^2}{2m}$$

$$\psi\,(x,y,z) = F(x)G(y)H(z) = A\,\sin\frac{n_x\pi x}{L_x}\sin\frac{n_y\pi y}{L_y}\sin\frac{n_z\pi z}{L_z}$$

Lowest energy state =

Wave function for the lowest energy state =

Particle in a 3-D infinite well

$$E_{(n_x,n_y,n_z)} = \left(\frac{n_x^2}{{L_x}^2} + \frac{n_y^2}{{L_y}^2} + \frac{n_z^2}{{L_z}^2}\right)\frac{\pi^2\hbar^2}{2m}$$

$$\psi\,(x,y,z) = F(x)G(y)H(z) = A\ \sin\frac{n_x\pi x}{L_x}\sin\frac{n_y\pi y}{L_y}\sin\frac{n_z\pi z}{L_z}$$

Lowest energy state = $E_{(1,1,1)} = \left(\frac{1^2}{{L_x}^2} + \frac{1^2}{{L_y}^2} + \frac{1^2}{{L_z}^2}\right)\frac{\pi^2\hbar^2}{2m}$

Wave function for the lowest energy state = $\psi_{(1,1,1)} = A\ \sin\frac{\pi x}{L_x}\sin\frac{\pi y}{L_y}\sin\frac{\pi z}{L_z}$

Particle in a 3-D infinite well

$$E_{(n_x,n_y,n_z)} = \left(\frac{n_x^2}{L_x{}^2} + \frac{n_y^2}{L_y{}^2} + \frac{n_z^2}{L_z{}^2}\right)\frac{\pi^2\hbar^2}{2m}$$

$$\psi\,(x,y,z) = F(x)G(y)H(z) = A\,\sin\frac{n_x\pi x}{L_x}\sin\frac{n_y\pi y}{L_y}\sin\frac{n_z\pi z}{L_z}$$

When $L_x = L_y = L_z = L$

Lowest energy state =

Wave function for the lowest energy state =

Second lowest energy state(s) =

Wave functions for the second lowest energy state(s) =

Particle in a 3-D infinite well

$$E_{(n_x,n_y,n_z)} = \left(\frac{n_x^2}{L_x{}^2} + \frac{n_y^2}{L_y{}^2} + \frac{n_z^2}{L_z{}^2}\right)\frac{\pi^2\hbar^2}{2m}$$

$$\psi\,(x,y,z) = F(x)G(y)H(z) = A\ \sin\frac{n_x\pi x}{L_x}\sin\frac{n_y\pi y}{L_y}\sin\frac{n_z\pi z}{L_z}$$

When $L_x = L_y = L_z = L$

Lowest energy state = $\mathrm{E} = 3\ (\frac{\pi^2\hbar^2}{2mL^2})$

Wave function for the lowest energy state = $\psi_{(1,1,1)} = A\ \sin\frac{\pi x}{L}\sin\frac{\pi y}{L}\sin\frac{\pi z}{L}$

Second lowest energy state(s) = $E_{(2,1,1)} = E_{(1,2,1)} = E_{(1,1,2)} = (2^2 + 1^2 + 1^2)\left(\frac{\pi^2\hbar^2}{2mL^2}\right) = 6\ \left(\frac{\pi^2\hbar^2}{2mL^2}\right)$

Wave functions for the second lowest energy state(s) = $\begin{cases} \psi_{(2,1,1)} = A\ \sin\frac{2\pi x}{L}\sin\frac{\pi y}{L}\sin\frac{\pi z}{L} \\ \psi_{(1,2,1)} = A\ \sin\frac{\pi x}{L}\sin\frac{2\pi y}{L}\sin\frac{\pi z}{L} \\ \psi_{(1,1,2)} = A\ \sin\frac{\pi x}{L}\sin\frac{\pi y}{L}\sin\frac{2\pi z}{L} \end{cases}$

Some problems

An electron in a cubit 3d infinite well of 1 nm at the E(2,1,1) state

$$\text{Where}\begin{cases}\text{electron mass} = 9.11 \text{ x } 10^{-31}\text{kg} \\ h = 1.055 \text{ x } 10^{-34} \text{ J sec} \\ L = 10^{-9} \text{ m}\end{cases} \quad \text{and } 1 \text{ eV} = 1.602 \text{ x } 10^{-19} \text{ J}$$

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$$= 3.62 \times 10^{-19}\ \text{J} = 2.26\ \text{eV}\ \ (\text{the same as } E_{(1,2,1)} = E_{(1,1,2)})$$

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Since the value of $(sin\theta)^2$ *is highest when* $\theta = \frac{1}{2}\pi, \frac{3}{2}\pi, etc.$, the probability