Phyx 320
Modern Physics

March 22, 2021

Reading: 39.5 - 39.6, 40.1 - 40.4

Homework #8 and Reading Reflection Thursday 11:59 pm

Heisenberg Uncertainty Principle

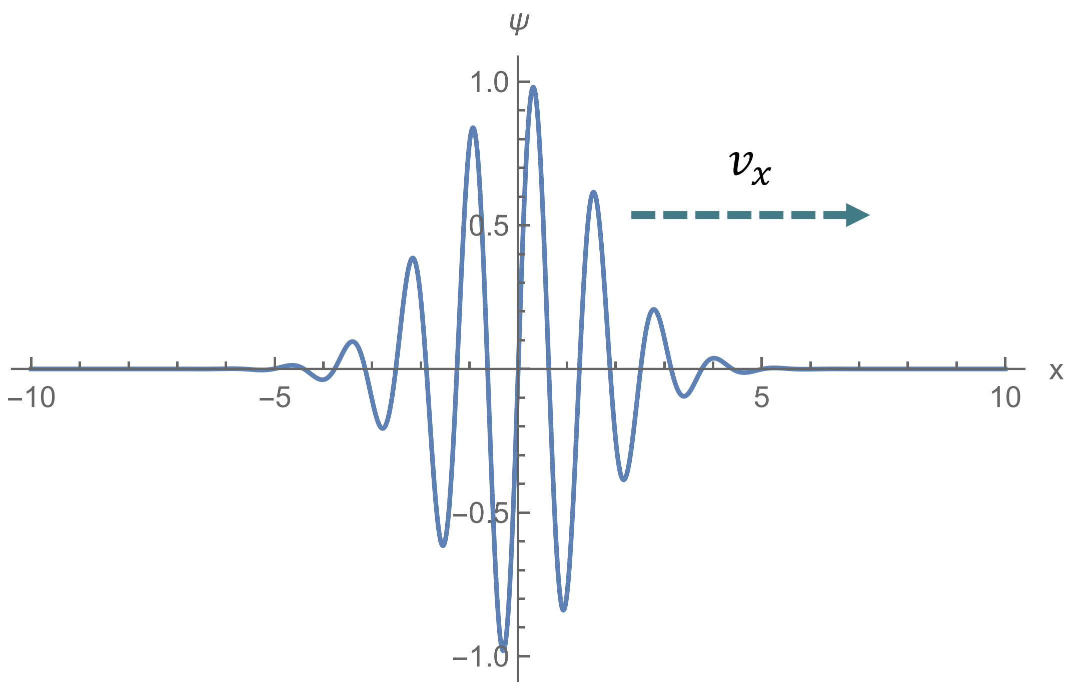
Heisenberg's Uncertainty Principle:

$$\Delta p_x \Delta x \geq \frac{h}{2}$$

We can't know both the momentum and the position of a particle at the same time

The uncertainties in measurements of position and momentum are anticorrelated
(more precise position = less precise momentum)

Because of the wave nature of matter, the properties of a particle are inherently uncertain



Schrödinger Equation

In 1925, Erwin Schrödinger discovered the fundamental equation of quantum mechanics:

mass

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}[E - U(x)]\,\psi(x)$$

total Energy

Potential

wavefunction

Tells us how wavefunctions and energy are related

Quantum mechanical equivalent of Newton's laws

Schrödinger Equation

The Schrödinger Equation can not be derived but we can justify it

Schrödinger aimed to find a wave equation like those in electromagnetism

Let's look at a sinusoidal wavefunction:

$$\psi(x) = \psi_0 \sin\left(\frac{2\pi}{\lambda}x\right)$$

$$\frac{d^2\psi}{dx^2} = \frac{d}{dx}\left[\frac{2\pi}{\lambda}\psi_0 \cos\left(\frac{2\pi}{\lambda}x\right)\right]$$

$$= -\left(\frac{2\pi}{\lambda}\right)^2 \underbrace{\psi_0 \sin\left(\frac{2\pi}{\lambda}x\right)}_{\psi(x)}$$

$$\frac{d^2\psi}{dx^2} = -\left(\frac{2\pi}{\lambda}\right)^2 \psi(x)$$

Schrödinger Equation

Let's plug in de Broglie wavelength:

$$\frac{(mv)^2}{2m} = \frac{1}{2}mv^2$$

$$\lambda = \frac{h}{p} \qquad K = \frac{p^2}{2m}$$

$$p = \sqrt{2mK}$$

$$\lambda = \frac{h}{\sqrt{2mK}}$$

$$\frac{d^2\psi}{dx^2} = -\left(\frac{2\pi}{\lambda}\right)^2 \psi(x)$$

$$\frac{1}{\hbar}$$

$$\frac{d^2\psi}{dx^2} = -\left(\frac{2\pi}{h}\sqrt{2mK}\right)^2 \psi(x)$$

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

Schrödinger Equation

So far, we've assumed that the kinetic energy is constant

Only true if potential energy is constant

Let's say we have a position dependent potential energy (spring, gravity, …)

$$E = K + U(x)$$

$$K = E - U(x)$$

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

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2} \left(E - U(x)\right) \psi(x)$$

Schrödinger Equation

Schrödinger Equation is a second-order differential equation:

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}\left[E - U(x)\right]\psi(x)$$

Once the potential, $U(x)$, is defined then we can solve of the wavefunction, $\psi(x)$

Not all mathematical solutions of the Schrödinger Equation are physical

Must obey the following:

- $\psi(x)$ must be continuous
- $\psi(x) = 0$ in regions where it is physically impossible for the particle to be
- $\psi(x) \rightarrow 0$ as $x \rightarrow \pm\infty$
- $\psi(x)$ must be normalizable ($\int_{-\infty}^{\infty} |\psi(x)|^2 dx$ must converge)

Schrödinger Equation

If we find multiple independent equations that solve the Schrödinger Equation for a given potential, then the general solution is the linear combination of them

Independent solution = can not be made from linear combinations of the other solutions

$\psi_1(x)$ and $\psi_2(x)$

$$\psi(x) = A\psi_1(x) + B\psi_2(x)$$

Let's say

$$\psi_1(x) = 2$$

$$\psi_2(x) = 3x$$

Then

$$\psi_3(x) = 5x+4$$

not independent

$$= \frac{5}{3}(\psi_2) + 2\psi_1$$

But

$$\psi_3(x) = 3x^2$$

is independent

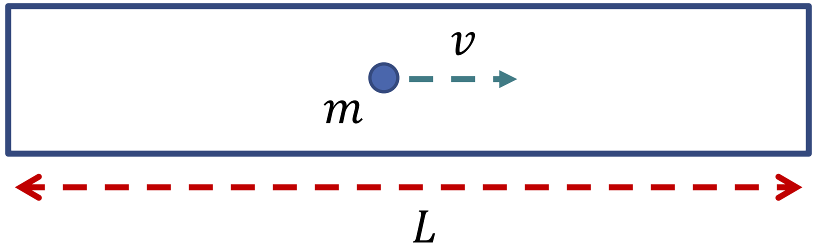
Particle in a Box

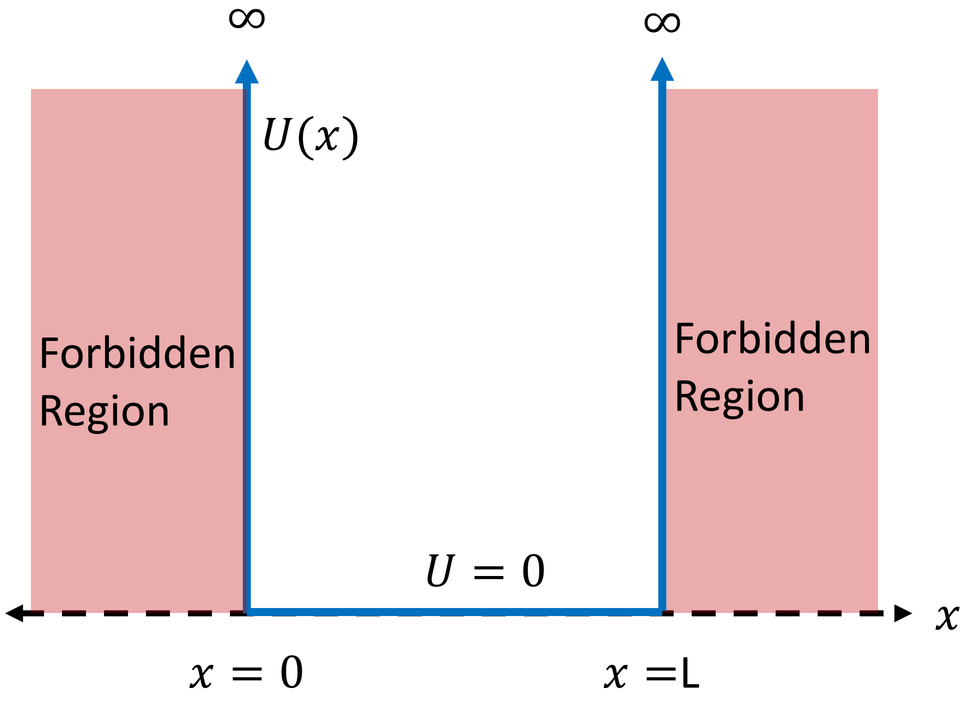
Let's return to our particle in a box

Particle is free to move between $x = 0$ and $x = L$

Particle can not leave box, $x < 0$ and $x > L$ are forbidden

$$U(x) = \begin{cases} 0 ; & 0 \leq x \leq L \\ \infty ; & x < 0 \text{ or } x > L \end{cases}$$





Particle in a Box

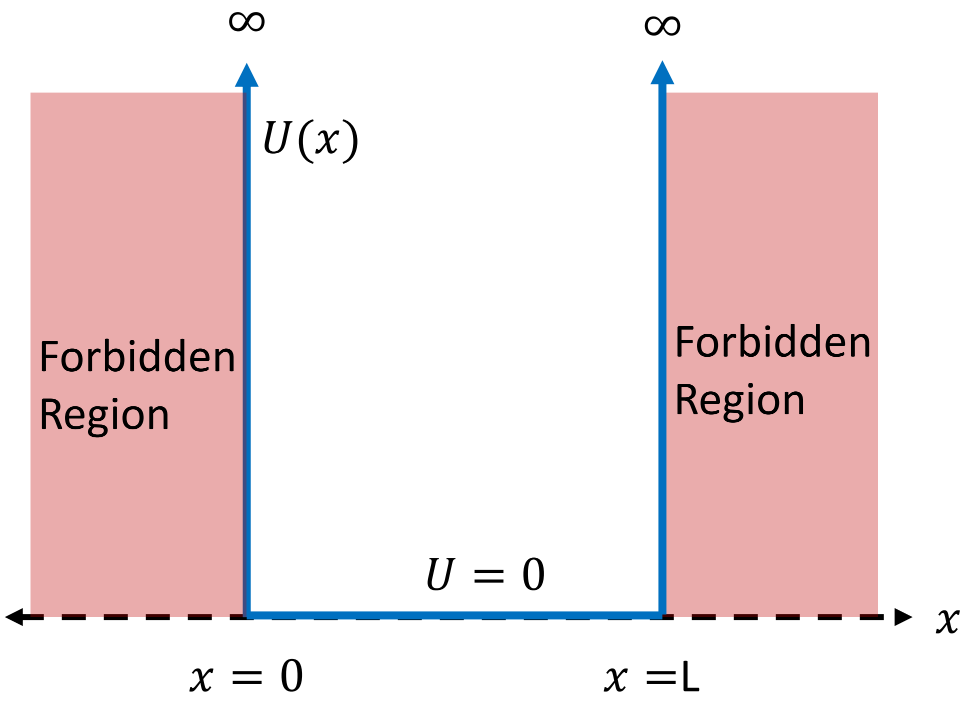
In forbidden region: $x<0$

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

Only solution:

$$\psi(x)=0$$

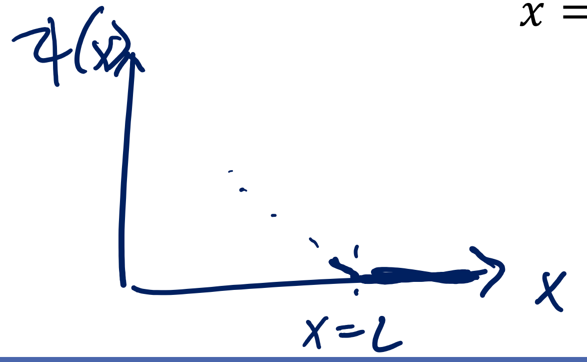
$$\frac{d^2\psi}{dx^2}=0=-\frac{2m}{\hbar^2}(E-\infty)(0)$$



Must be continuous:

$$\psi(x=0)=0$$

$$\psi(x=L)=0$$



Particle in a Box

Let's find a function that works with this:

$$\frac{d^2\psi}{dx^2} = -\beta^2 \psi(x) \qquad \beta = \sqrt{\frac{2mE}{\hbar^2}}$$

Guess:

$$\psi_1(x) = \sin \beta x$$

$$\psi_2(x) = \cos \beta x$$

$$\frac{d^2\psi_1}{dx^2} = -\beta^2 \sin \beta x = -\beta^2 \psi_1(x) \checkmark$$

$$\frac{d^2\psi_2}{dx^2} = -\beta^2 \cos \beta x = -\beta^2 \psi_2(x) \checkmark$$

Particle in a Box

General solution is any linear combination of these

Need to find A and B based on potential

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

$$x = 0, \quad \psi(0) = 0$$

$$\psi(0) = A\cancel{\sin}(0)^{0} + B\cancel{\cos}(0)^{1}$$

$$0 = B$$

$$\psi(x) = A\sin\beta x$$

$$x = L, \quad \psi(L) = 0$$

$$\psi(L) = A\sin\beta L$$

$$0 = A\sin\beta L$$

$$\cancel{A = 0} \qquad \sin\beta L = 0$$

$$\beta L = n\pi \qquad n = 1, 2, 3 \ldots$$

$$\beta = \frac{n\pi}{L}$$

Particle in a Box

General solution is any linear combination of these

Need to find A and B based on potential

$$\psi(x) = A \sin\left(\frac{n\pi}{L} x\right)$$

normalization constant

Particle in a Box

What about energies?

$$\beta = \sqrt{\frac{2mE}{\hbar^2}} = \frac{n\pi}{L} \qquad n = 1, 2, 3 \ldots$$

$$E = \frac{n^2\pi^2}{L^2}\frac{\hbar^2}{2m} = n^2 \frac{h^2}{8L^2m}$$

previous result

quantized

$$E = n^2 E_1$$

ground state

$$E_1 = \frac{h^2}{8L^2m}$$

Particle in a Box

Final step, normalize the wavefunction:

$$\psi(x) = A\sin\left(\frac{n\pi}{L}x\right)$$

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

$$\int_{-\infty}^{0} \cancel{|\psi(x)|^2} dx + \int_{0}^{L} |\psi(x)|^2 dx + \int_{L}^{\infty} \cancel{|\psi(x)|^2} dx = 1$$

$$\int_{0}^{L} |\psi(x)|^2 dx = 1$$

$$\int_{0}^{L} A^2 \sin^2\left(\frac{n\pi}{L}x\right) dx = 1 \Rightarrow A = \sqrt{\frac{2}{L}}$$

Particle in a Box

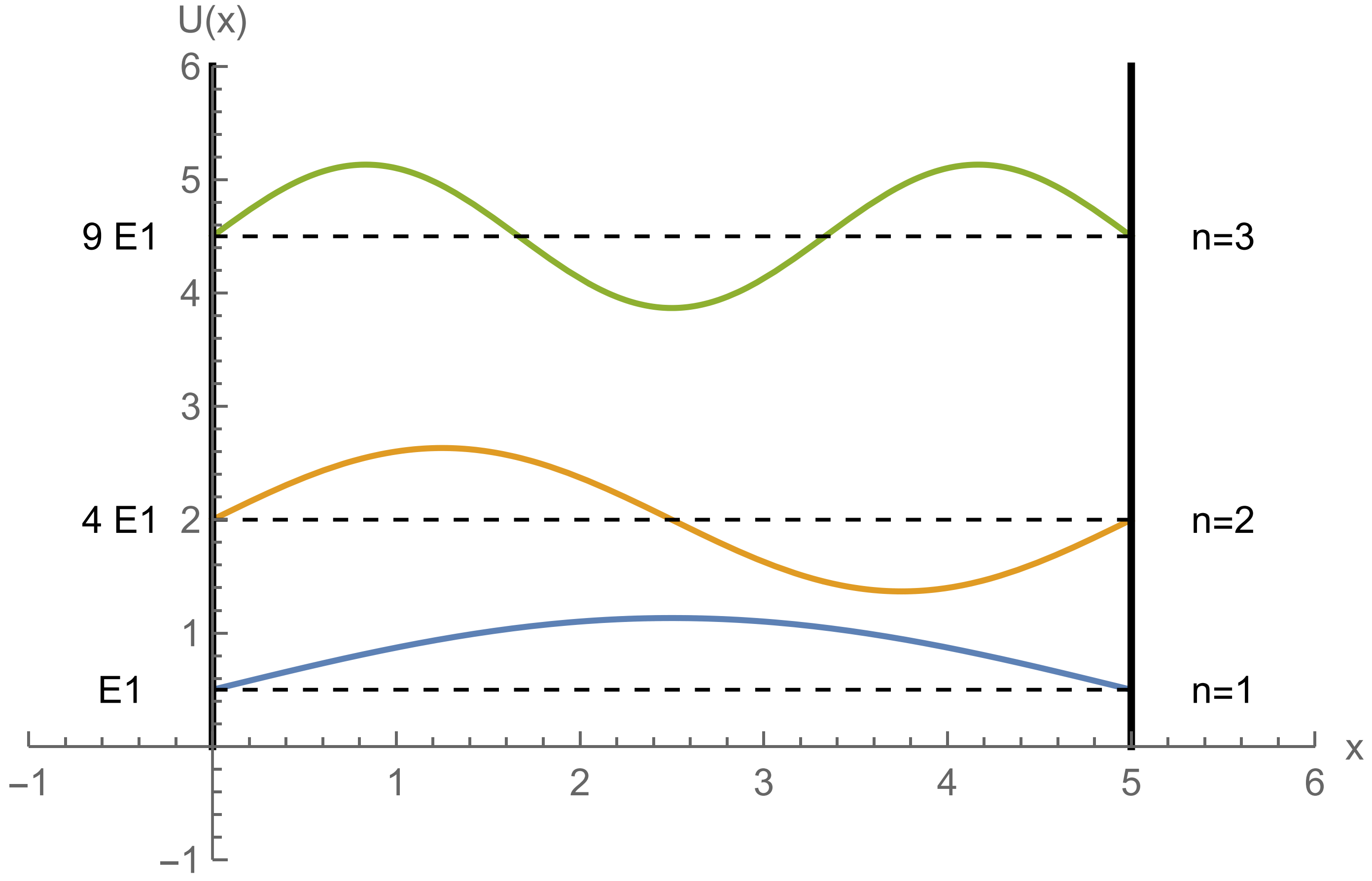
Putting all this together:

$$\psi(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right); & 0 \leq x \leq L \\ 0; & x > 0 \; and \; x < L \end{cases}$$

Energies follow:

$$E = n^2 E_1$$

$$E_1 = \frac{h^2}{8mL^2}$$



Homework Questions

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