# QM-3: Quantum Mechanics

Everything that we covered up to this point (especially the Bohr atom) falls into the category of "*Old Quantum Mechanics*." **We're now ready to start to use what the old quantum mechanics reveals to develop what is known today as Quantum Mechanics.**

**We start with de Broglie's discovery that particles have wave properties, and ask:**

**If a particle has wave properties, What is doing the waving?**

**An Assertion** (*formally it's a postulate of quantum mechanics*):

For every particle, there exists a wave, $\Psi(x,t)$, called the **Wave Function**, where $|\Psi(x,t)|^2$ *is related to the probability of finding the particle at position* $x$ *at time* $t$.
*(Note for now, we're just considering the particle in one dimension.)*

**Where did such an idea come from?**

$$\text{For a light wave: Intensity, } I \propto |\text{wave amplitude, } E|^2$$

$$\text{Or, in terms of photons: Intensity, } I \propto \text{number of photons}$$

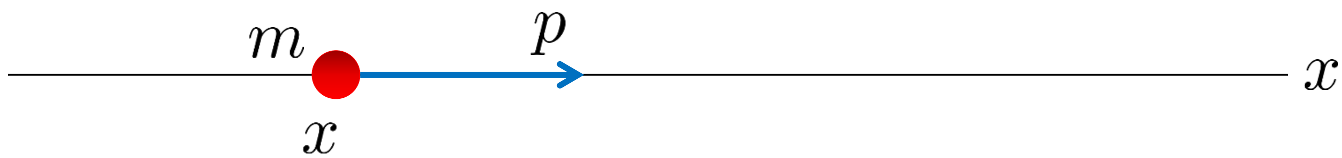
$$\propto \text{probability of finding a photon}$$

So, $|\Psi(x,t)|^2 \propto$ probablility of finding the particle.
And the wave function, $\Psi(x,t)$, is a *probability amplitude*

# Quantum Mechanics

## What should a wave function for a free particle in 1D look like?

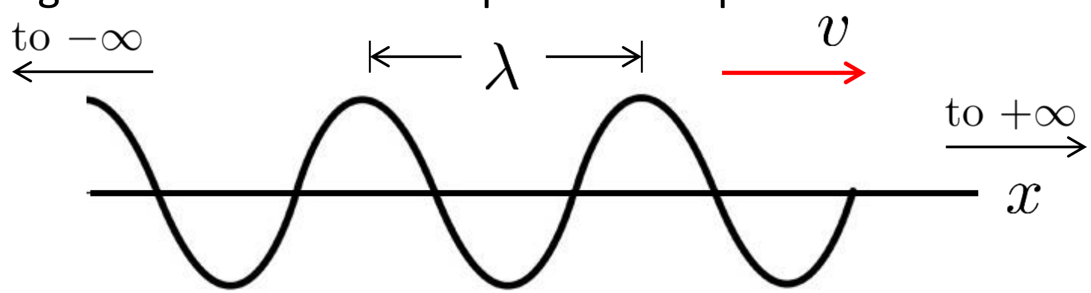
**Classically**, a particle of mass m has a position, x, and momentum, p:




**In QM**, **what if** we use a travelling sinusoidal wave to represent the particle in 1D?

$$\Psi(x,t) = A\sin(kx - \omega t)$$

$$k = \frac{2\pi}{\lambda} \qquad \omega = 2\pi f$$




**Now for the particle:** $p = \frac{h}{\lambda} = \frac{h}{2\pi/k} = \hbar k$ **(a well-defined momentum)**

**But, where is the particle located?** probability that particle is at $x \propto |\Psi(x,t)|^2$

***The particle is equally likely to be anywhere on the x-axis!***

**For a sinusoidal wave: our knowledge of p is perfect:** Uncertainty, $\Delta p = 0$

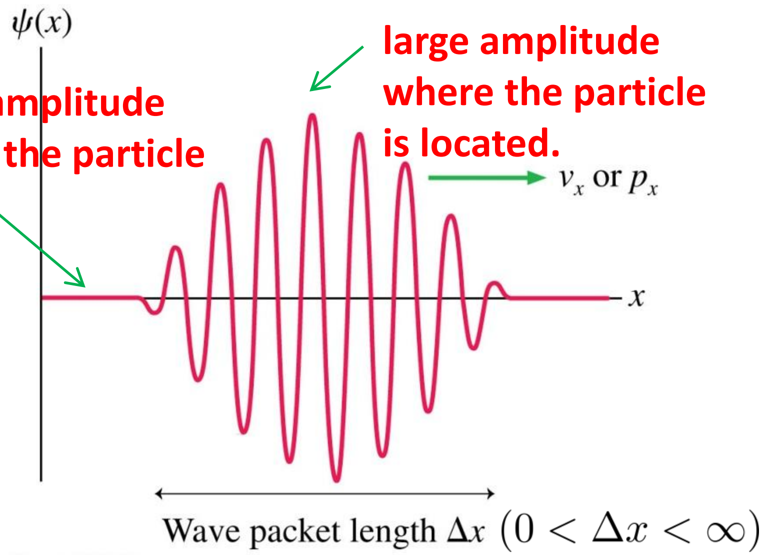
**But, our knowledge of x is totally imperfect:** Uncertainty, $\Delta x = \infty$

# Quantum Mechanics - HUP

**To represent a free particle**, we would like a **wave packet** that looks like this:

**small amplitude where the particle isn't.**

**large amplitude where the particle is located.**




**(position of particle is somewhere in here)**

To get a **wave packet** like this, you have to add together many many waves of different wavelengths, and

$$\lambda \leftrightarrow p \Rightarrow 0 < \Delta p < \infty$$

*So, to get more knowledge of the particle's position, we must lose knowledge of it's momentum.*

## Heisenberg Uncertainty Principle (HUP):

In 1927, Werner Heisenberg quantified this relation between how well you can simultaneously know the position and momentum of a particle:

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

**Important point**: ***HUP is not a statement about instrument imperfection and how well we can measure things in the lab. It is an inherent property of the particle due to its wave characteristics.***

Cass_qm_heis

# Whiteboard QM-9: HUP

**a) Can a particle confined in a 1D box of width L have zero energy?**


**Use the HUP to find an expression for the minimum kinetic energy of the particle. (LC)**

We know its position to an uncertainty $\Delta x = L$

and, $\Delta x \Delta p \geq \frac{h}{2} \;\; \Rightarrow \Delta p \geq \frac{h}{2\Delta x} = \frac{h}{2L}$

So, the minimum momentum is, $p_{\text{min}} = 0 \pm \Delta p = \pm \frac{h}{2L}$

Thus, the minimum kinetic energy is, $K_{\text{min}} = \frac{p_{\text{min}}^2}{2m} = \frac{h^2}{8mL^2}$

**Does this look familiar?**

***It's the same ground state energy (n=1) that we got in WB QM-8 (or in HW) by fitting standing deBroglie waves in the box.***

**More:**

*Think of the Hydrogen atom; the electron is confined in a region of space, can it have zero energy?*

# More on WB QM-9

In the part a, we found that HUP shows that if a particle of mass m is confined (in 1D) to a region of space L that the particle's minimum kinetic energy is

$$K_{\text{min}} = \frac{h^2}{8mL^2}$$

**b) Calculate the minimum speed of an electron that is confined to a 1D region L = 1nm. (LC)**

$$K_{\text{min}} = \frac{h^2}{8m_eL^2} = \frac{1}{2}m_e v_{\text{min}}^2 \quad \Rightarrow v_{\text{min}} = \frac{h}{2m_eL} = 3.6 \times 10^5 \ m/s$$

Of course, none of us have ever experienced anything like this, e.g.

**c) Calculate the minimum speed of a 50 kg person confined to a width of 1.0m – e.g. a closet. (LC)**

$$v_{\text{min}} = \frac{h}{2mL} = 6.6 \times 10^{-36} \ m/s$$

Why don't we ever observe anything like this in our everyday lives?

Because Planck's constant, h, is so small.

**d) Repeat the calculation from part c in a Universe where h = 1000 Js. (LC)**

$$v_{\text{min}} = \frac{h}{2mL} = 10 \ m/s$$

*So, if h was this big, we would want to avoid narrow areas!*

# The Schrodinger Equation

In 1925, Erwin Schrodinger realized that a particle's wave function had to obey a wave equation that would govern how the function evolves in space and time.

He *isolated* himself in the Alps for a few months, and arrived at his famous equation. The wave function for a mass m in 1D subject to a potential energy U(x,t) obeys the following equation:

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

**The 1D Time Dependent Schrodinger Equation (TDSE)**

**Notes:**

1.) $i = \sqrt{-1} \Rightarrow \Psi$ isn't necessarily a real quantity.
(Observable physics depends on $|\Psi(x,t)|^2 = \Psi^*\Psi$ which is real.)

2.) somewhat different than the standard wave equation.

3.) Can the Schrodinger Equation be derived?

Can Newton's Second Law? The Shrodinger equation is postulated, and its validity is established by how well it agrees with experiment.

# The 1D Time Independent Schrodinger Equation (TISE)

For many important problems (*including the Infinite Square Well, the Simple Harmonic Oscillator, and the Hydrogen Atom*), the potential energy depends only on the position and not on the time. Then the wavefunction can be written as:

$$\Psi(x,t) = \psi(x)\phi(t)$$

And the time part of the wave function can be solved for:

$$\phi(t) = e^{i\omega t} = \cos\omega t + i\sin\omega t$$

$$\text{where: } \omega = \frac{E}{\hbar} \qquad (E = \text{total energy} = K + U)$$

Then the spatial part of the wavefunction obeys this equation:

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

**The 1D Time Independent Schrodinger Equation (TISE)**

Cass_qm_schrod

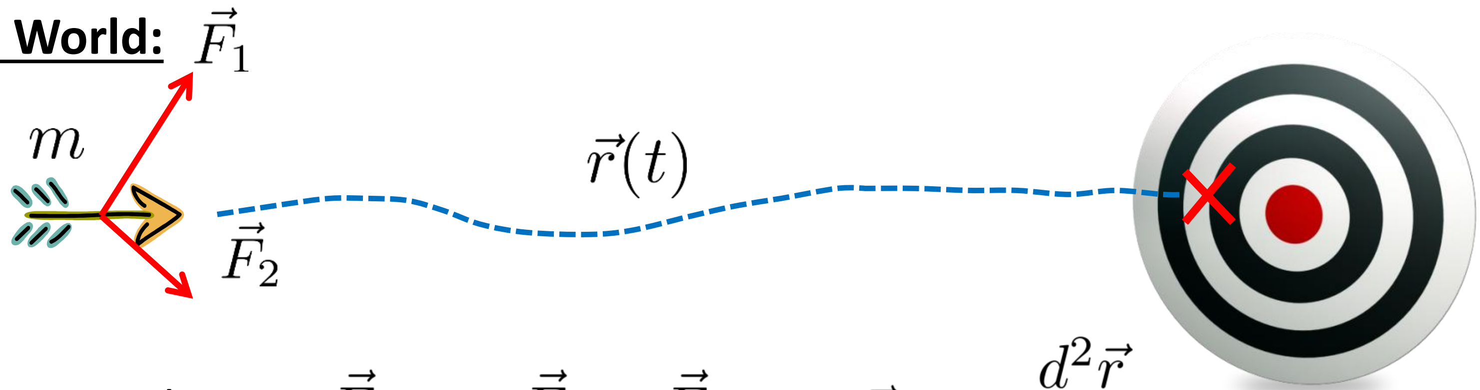
# The Essence of Quantum Mechanics

**What do we do with the Schrodinger Equation and the Wavefunction?**

The same thing that we do with Newton's Laws – ***we try to predict the future***!
In other words, we try to predict the results of experiments. Consider shooting arrows at a target and predicting where they will hit:

**Newton's World:**

know $\vec{r}(t=0)$
and
$\vec{v}(t=0)$




**Use Newton's 2nd Law:** $\vec{F}_{\text{net}} = \vec{F}_1 + \vec{F}_2 = m\vec{a} = m\dfrac{d^2\vec{r}}{dt^2}$

$$\text{Solve for the Trajectory, } \vec{r}(t)$$

If we know the arrow's trajectory, we know exactly where it hits the target.

If we do the experiment over and over with identical forces and initial conditions, the arrow hits the same spot every time.

We call this a **"deterministic"** prediction since we can (in principle) determine the precise outcome of a single experiment.

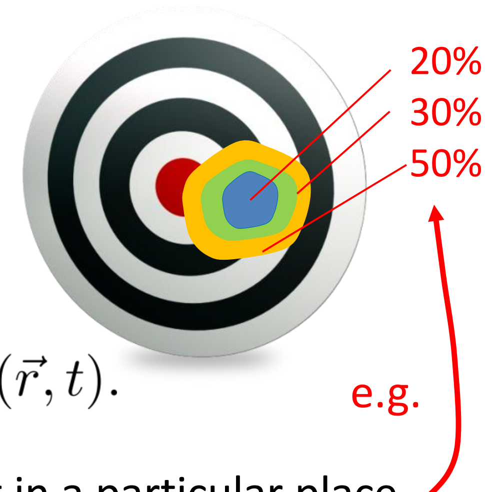
# The Essence of Quantum Mechanics

**How does Schrodinger and Quantum Mechanics predict the outcome of this experiment?**

## Schrodinger's World:

$m$

know the potential energy: $U(\vec{r}, t)$




know: $\Psi(\vec{r} = 0, t = 0)$

Put $U(\vec{r}, t)$ into the Schrodinger equation, solve for $\Psi(\vec{r}, t)$.

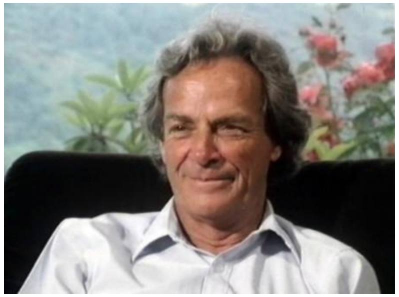
The **Wave Function predicts the Probability** that the arrow will hit in a particular place.

We can't predict the outcome of any single shot. All we can say is where the arrow is likely to hit or we can calculate the average over many identical shots.

We call this an "**indeterministic**" prediction since we can't (in principle) determine the precise outcome of a single experiment.

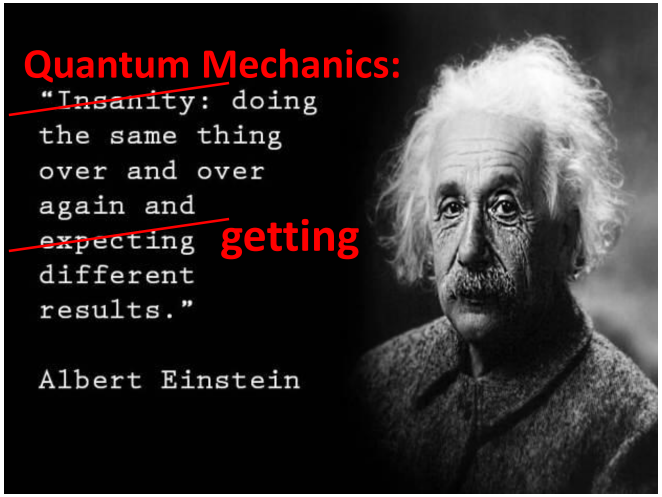
**Is this really the way Nature works on a fundamental level?**

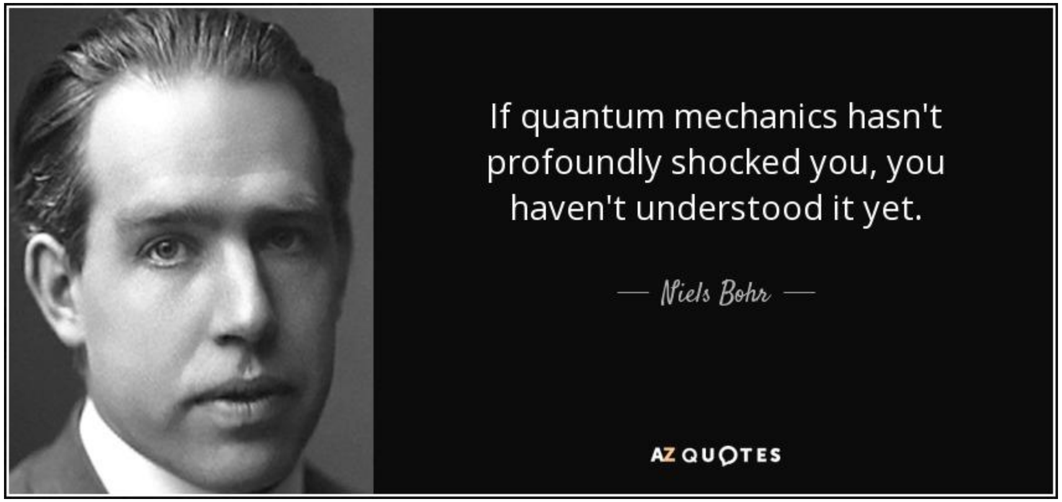
*"I think its safe to say that no one understands quantum mechanics. Do not keep saying to yourself, if you can possibly avoid it, "But how can it be like that?" because you will get "down the drain" into a blind alley from which nobody has yet escaped. Nobody knows how it can be like that."*

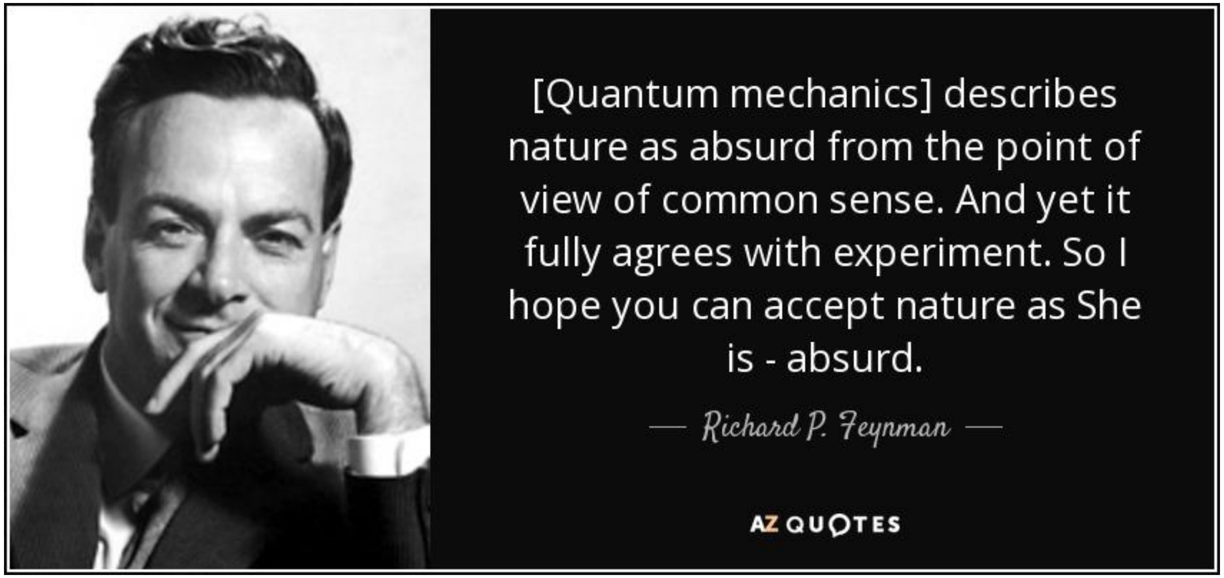


***But it really works!*** Richard Feynmann

# The Essence of Quantum Mechanics



# Quantum Recipe

**Here are the steps we use to solve a problem in Quantum Mechanics:**
(assuming a 1D time independent potential energy)

1. Specify the potential energy, $U(x)$.
2. Put $U(x)$ in the TISE:
$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + U(x)\psi(x) = E\psi(x)$$
3. Solve the TISE for the allowed energies, $E$, and wavefunctions, $\psi(x)$. These usually form a set $E_n$ and $\psi_n$. (n is a set of integers)
4. Extract physical information from the wavefunction, $\psi(x)$.

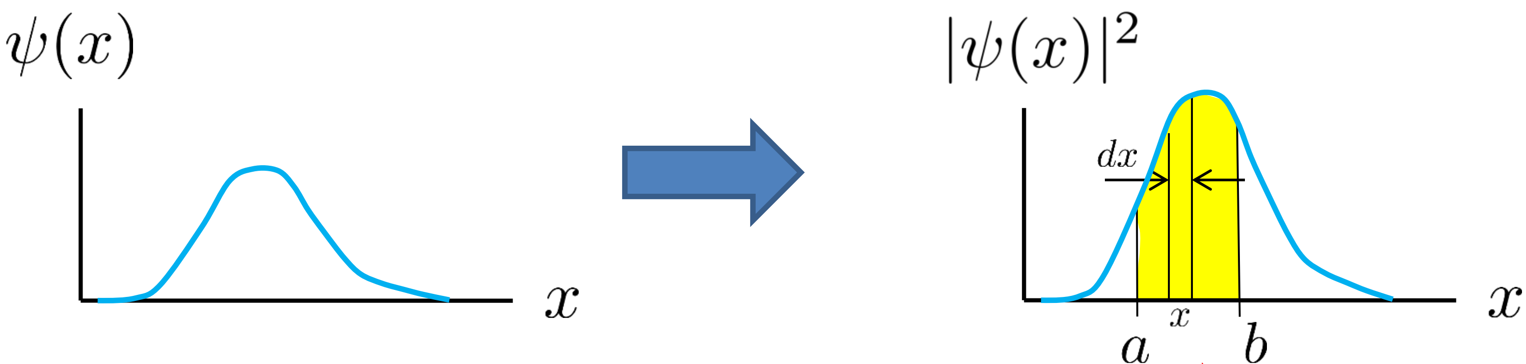
*How do we do this last part?* →

# Extracting Physical Information from the Wavefunction

First, to represent a physical system, the wavefunction must be single-valued, continuous, smooth [for finite U(x)], and **Normalizable**.

**What does Normalizable mean?** $$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = \text{ finite } \overset{\text{can set}}{=} 1$$

Suppose that we have solved the TISE for the wavefunction:




$$|\psi(x)|^2 dx =$$ Probability of finding the particle in width dx at x

**Area From a to b**

**Probability that the particle is between x = a and x = b** $$= P(a \leq x \leq b) = \int_a^b |\psi(x)|^2 dx$$

**So, normalized means that the probability of finding the particle somewhere on the x-axis is 100%**

# Extracting Physical Information from the Wavefunction

What other information can we get from the wavefunction? Since the square of the wavefunction is a probability density,
**we can apply the techniques of statistics:**

**Most probable value of x** $$x_{\mathrm{mp}} = x \text{ for } |\psi(x)|^2 \text{ maximum}$$

How do you do this? set $\frac{d}{dx}|\psi(x)|^2 = 0$ and solve for $x$

**In an experiment, the most probable value is the value that you would measure most of the time. Also, we can calculate:**

**The expectation value of x** $$= \langle x \rangle = \int_{-\infty}^{+\infty} x|\psi(x)|^2 dx$$

**The expectation value is also called the average value since it represents the average over many measurements of identical experiments.**

# Whiteboard Problem: QM-10

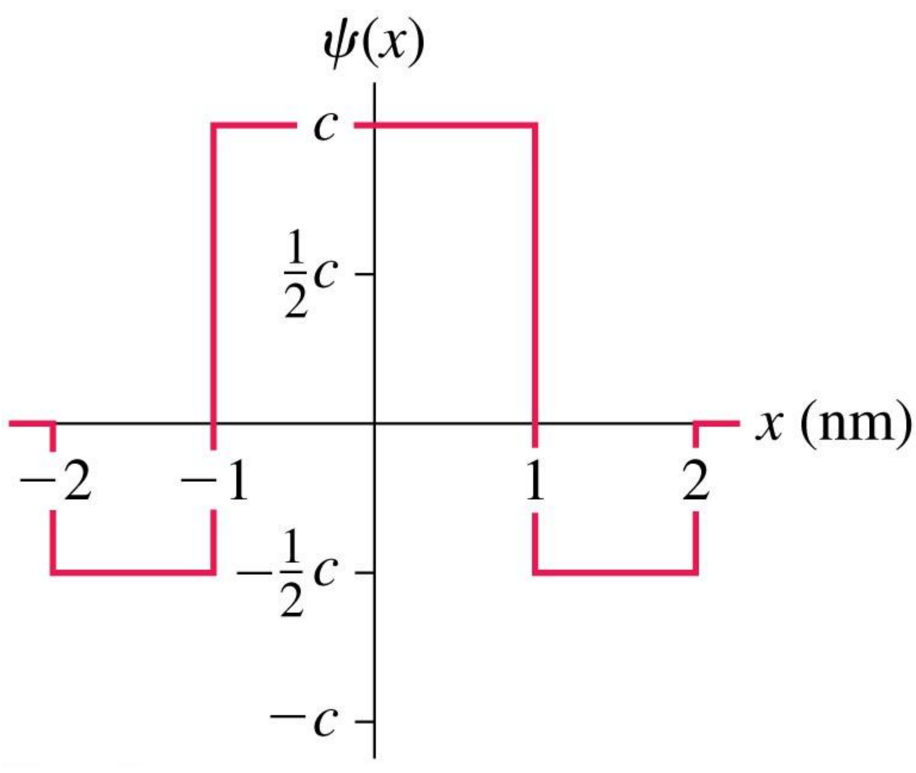
The graph below is a *fictitious* wave function for an electron.

*(c is <u>not</u> the speed of light! It is just some constant.)*

a) **Sketch a graph of** $|\psi(x)|^2$ **(LC)**

b) **What is the value of the constant c? (LC)**

c) **What is the probability that the electron is located between x = -1.0 nm and x = 1.0 nm? (LC)**



# Whiteboard Problem: QM-11

## Maybe Homework Hints

A particle that is confined to the positive x axis has the normalized wave function:

$$\psi(x) = \begin{cases} 0 & x < 0 \text{ nm} \\ (1.414 \text{ nm}^{-1/2})e^{-x/(1.0 \text{ nm})} & x \geq 0 \text{ nm} \end{cases}$$

where x is in nm.

write as: $\psi(x) = ae^{-\frac{x}{b}}$

a) **What is the probability of finding the particle in a region centered on x = 1.0 nm that is 0.010 nm wide. (LC)**
*(Think before you integrate – this one you don't have to integrate)*

b) **What is the probability of finding the particle in the interval** $0.50\ nm \leq x \leq 1.5\ nm$ **? (LC)**
*(Think before you integrate, but this one you'll have to integrate.)*