Some topics in research Atomic Physics

at the Inter-University Accelerator Center

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During April 2013
Beginning – 10 April – 10 am

I am also available almost any time
To discuss questions about the course (and life in the USA)

See http://www3.nd.edu/~hgberry/berry1.html for course files

Checking the IUAC storage tanks

What are you expecting from this course……?

It is helpful to know how much we know…..

It is helpful to know what we want to know…..

It is helpful to know that we are learning something new….

What are you expecting from this course?

Answer these three questions…

1. **What do you want to know about atomic physics?**

2. **What do you already know about atomic physics?**

3. **If you were the only physicist in the world, what would you tell all the non-physicists?**

A mini-quiz – 5 minutes

1. Write down the ground state wavefunction of the hydrogen atom?

2. What is the radius of the ground state of the hydrogen atom?

3. What is the radius of the n=120 state (L=119) of the hydrogen atom?

4. What is the radius of the n=120 state (L=119) of the 91-times ionized uranium atom? (ignore relativity in this and the next question)

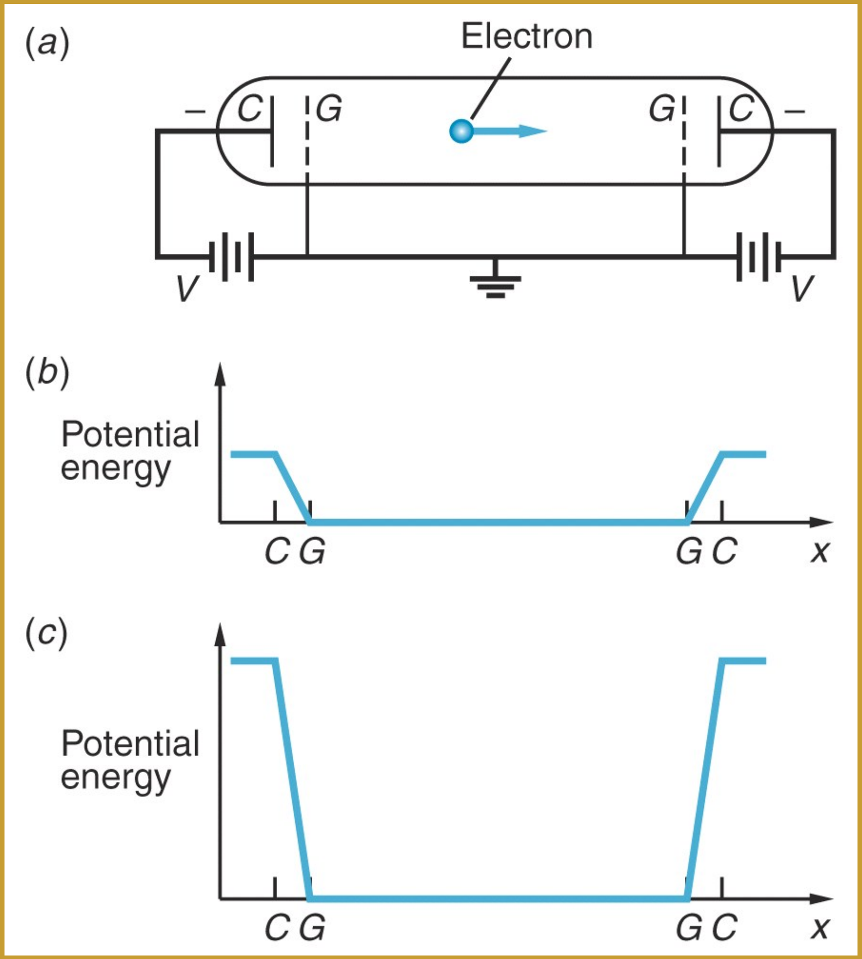
5. What is the radius of the ground state of neutral uranium ?

6. How does relativity change the answers to Q4 and Q5?

7. Draw an energy level diagram indicating binding energies of the lowest 10 states in neutral helium – as close to scale as possible (giving their approximate binding energies)

Count off….
– answer your numbered question – try to be quantitative

Example of a potential well



The grids G are at ground potential

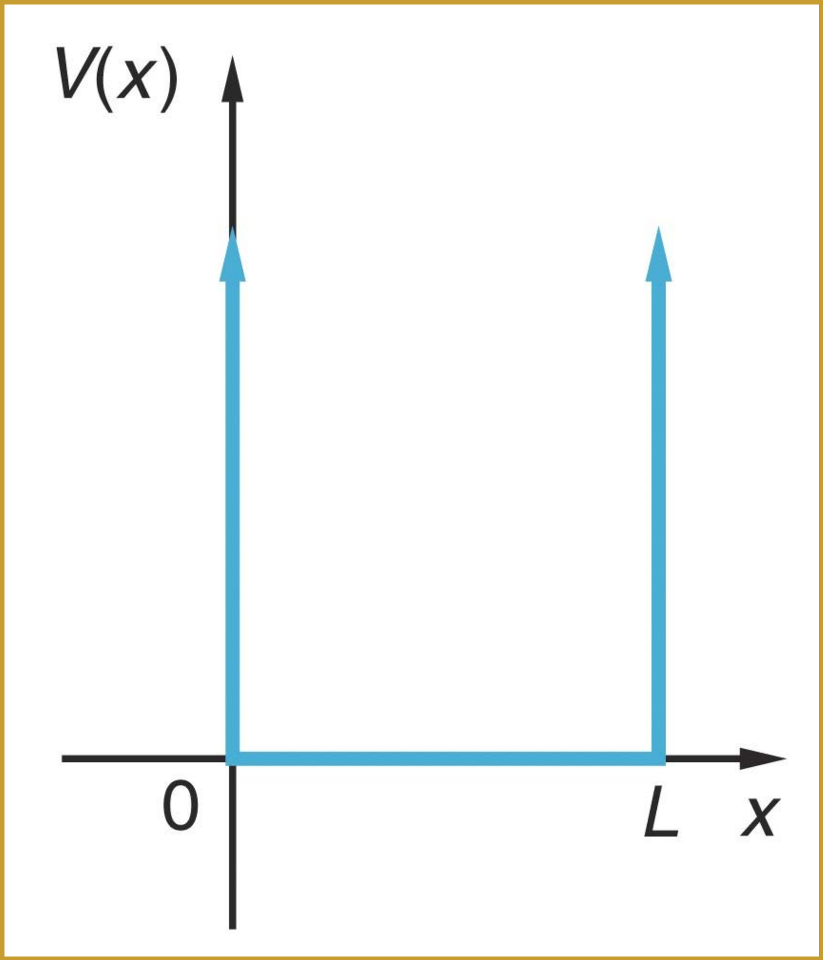
And produce an "almost"-square well.

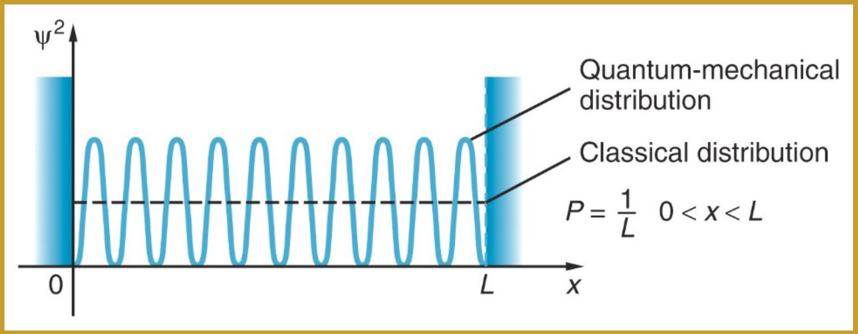
Classically, an electron starting with zero velocity at one electrode will just reach the other electrode (with zero velocity).

Between G and G, the electrons will have a constant velocity, and between G and C they speed up or slow down.

In the wave form – this corresponds to a pure sine-wave between G and G.

A "perfect" square-well





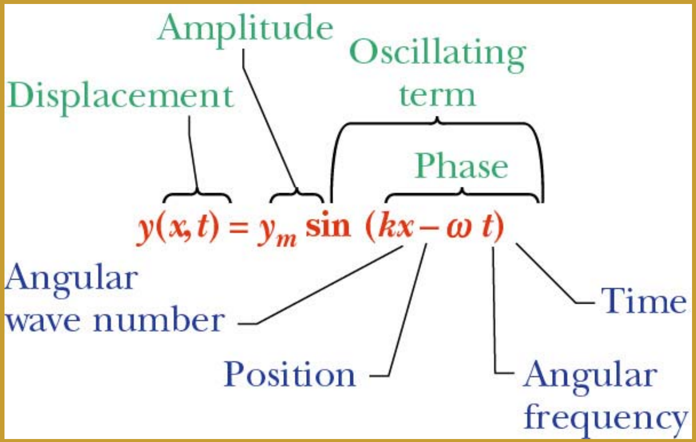
Picture above shows
the PROBABILITY
of finding the electron at a certain place
Classically this is constant (the same everywhere)
As a wave it can vary between zero and the maximum "amplitude" of the wave.

"Quantum mechanics" is going to help us in predicting this wave form…

Find Schrődinger's wave equation!

The classical wave equation for a traveling electric field (wave in the x-direction) is:

$\partial^2 E/\partial x^2 = (1/c^2)\cdot(\partial^2 E/\partial t^2)$



Has the solution $E = E_0 \cos(kx-\omega t)$

verify by differentiating this twice…

To find that $k^2 = \omega^2/c^2$ **or** $\omega = kc$

N.B. - Substitute $\omega=E/\hbar$ **and** $k=p/\hbar$ **to give E=pc just as we knew for a *massless* particle (a photon)**

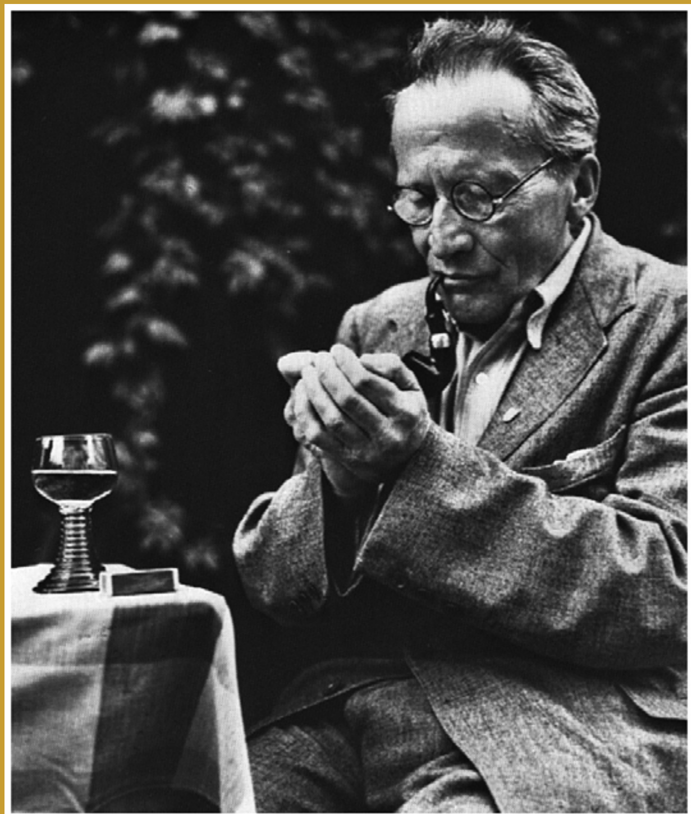
For a particle with charge q, mass m – e.g. an electron in the voltage trap, we can write the energy as $E= p^2/(2m) + V$ **where V is the "potential energy" = qV in this case**

Applying De Broglie's hypothesis, this becomes

$\hbar\omega = \hbar^2 k^2/(2m) + V$ **Now find a NEW wave equation…**

Notes: ω and k are NOT linearly related; so introduce a first order derivative in time to balance the spatial derivatives…i.e. d/dt instead of the 2nd derivative, and try to include the potential V

Schrődinger's equation



Work backwards…

1. **Generalize the classical wave equation by adding an imaginary part –**

i.e. assume we want a solution of the form

$\Psi \sim \exp[i(kx-\omega t)] = \cos(kx-\omega t) + i\sin(kx-\omega t)$

^^^

2. **Since the probability of finding a particle is always real (it might be zero) but can have only positive values between 0 and 1, therefore**

Assume that the absolute value squared will represent the probability $|\Psi|^2$

3. **Do a test:**

   differentiate once with respect to time t

   differentiate twice with respect to length x

We need to find that $[\hbar^2k^2/(2m) + V]\,\Psi = \hbar\omega\,\Psi$ (everywhere in space and time)

This works if we can write $[-\hbar^2/(2m)]\bullet\partial^2\Psi/\partial x^2 + V\,\Psi = i\hbar\partial\Psi/\partial t$

Conditions for solving Schrodinger's equation

Conditions:

Most of these are just to make the mathematics fit into reality or to make the wavefunction sufficiently localized…

(0) A wavefunction $\Psi(x,t)$ must exist and satisfy the equation

For the spatial part of the wavefunction…
(see below how to separate the spatial and timelike parts)

(1) assume the solution (probability) and any spatial derivatives are continuous – they have no discontinuities.
(2) they both go to zero at large –x and large +x.
(3) they are both always finite
(4) they are both single-valued.
(5) the probability is normalizable – i.e. can be equal to ONE.

Preliminary ideas about solving Schrődinger's equation – part 1

1. **Expansion from the classical realm:**

The wavefunction can be complex (i.e. have real and imaginary parts).
Hence, since measurements, particles, events are always REAL quantities,
we need to define a real part….

Define the PROBABILITY at time t, and position x as

$$\mathbf{P(x,t) = \Psi^{*}(x,t) \bullet \Psi\,(x,t) \quad = \quad |\,\Psi\,(x,t)\,|^{2}}$$

This becomes the physical quantity to represent all particles and measurements…
For example, if Ψ represents 1 electron, then the total probability of finding the 1 electron anywhere in space at a particular time MUST BE 1

Hence $\int_{-\infty}^{+\infty} \Psi^*(x,t)\,\Psi(x,t)\,dx = 1$

If Ψ represents 10 electrons, then it normalizes to 10!

Preliminary ideas about solving Schrődinger's equation – part 2

2. Try to separate the 2 variables x and t in the function Ψ (x,t)

e.g. Ψ (x,t) = ψ(x) • φ(t)

Try it….(a) substitute in the equation given on the last slide
(b) see if you can put all the terms containing t on one side and all the terms containing x on the other side of the equation
If we can do this , then both sides must be be equal to a constant
(one side is independent of x, and the other of t!)

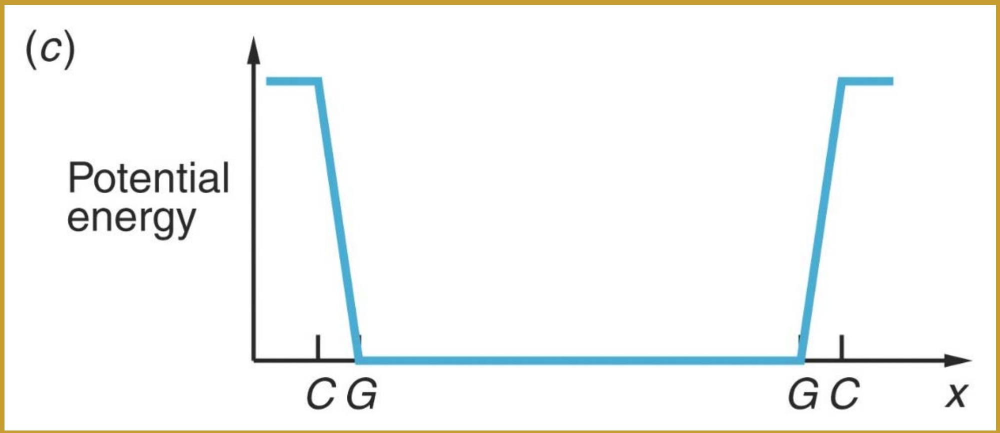
Limitation of this technique…..
The potential V cannot be a function of both x and t
(This will never happen in this course!)

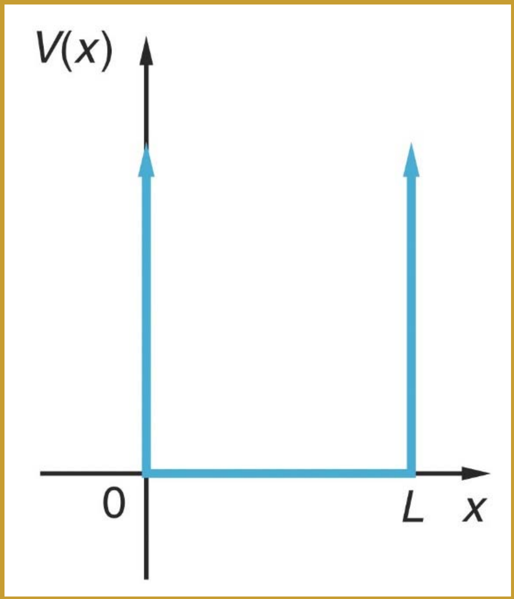
Giving us 2 equations….

$$\phi(t) = e^{-iEt/\hbar}$$

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

Back to the electron……
in a square well potential





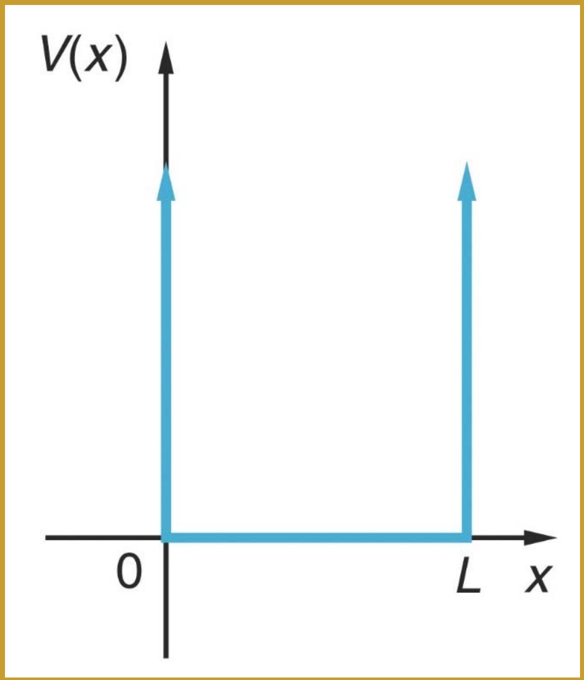
Let's assume V(x) = 0 between x=0 and x=L,
and is infinite everywhere else….

Then, independent of energy, the electron cannot get out. Classically just bounces to and fro at constant speed, and the probability of being any one position inside (along x) is the same.

Quantum mechanics: solve Schrodinger's equation for V = 0 (between 0 and L)
and V= infinity elsewhere

But with the conditions given before…….

The square-well potential solution



Within the box, the energy is constant
– hence ω and k are constant
– and also the wavelength λ, and the momentum p

Boundary conditions:

The wave-function must go to zero outside the box, at very large positive and very large negative x-values

Follow Bohr and De Broglie's ideas and fix the number of wavelengths inside the box.
e.g. sine(0) = 0 and sine(L) = 0

So we then have an integral number of half-wavelengths: **$n\,(\lambda/2) = L$** $n=1, 2, 3, 4, \ldots$

Assuming momentum $p = h/\lambda$ ➔ $\mathbf{E} = p^2/2m = h^2/(2m\lambda^2) = \mathbf{n^2 \cdot [\, h^2/(8mL^2)]}$

The square-well potential solution using the Schrodinger equation…

The time-independent equation (V=0) is ……

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

Rearranging and letting $k^2 = 2mE/\hbar^2$, we get….

$$\psi''(x) = -\frac{2mE}{\hbar^2}\psi(x) = -k^2\psi(x)$$

Square-well solution

Possible solutions are: **(verify by differentiating)**

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

$$\psi(x) = B \cos kx$$

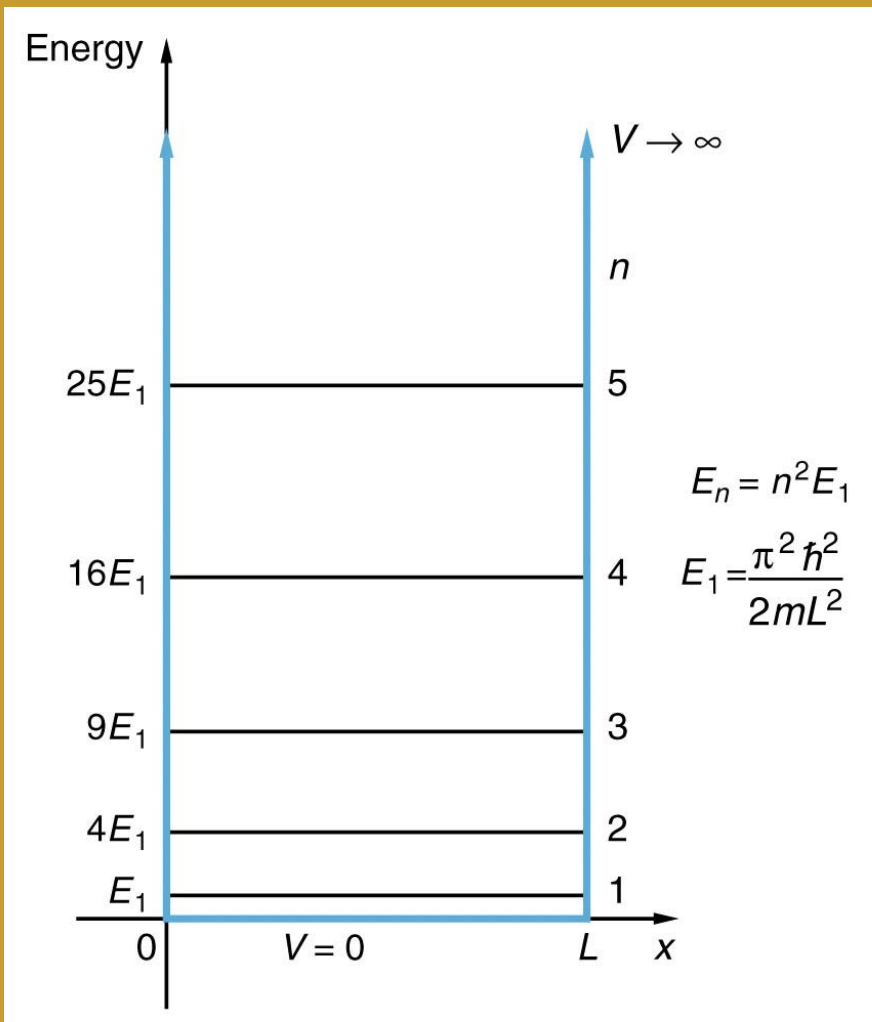
1. **Boundary condition at x=0** eliminates the 2nd solution
2. **Boundary condition at x=L** leads to the same conditions as before – a half – integral number of waves

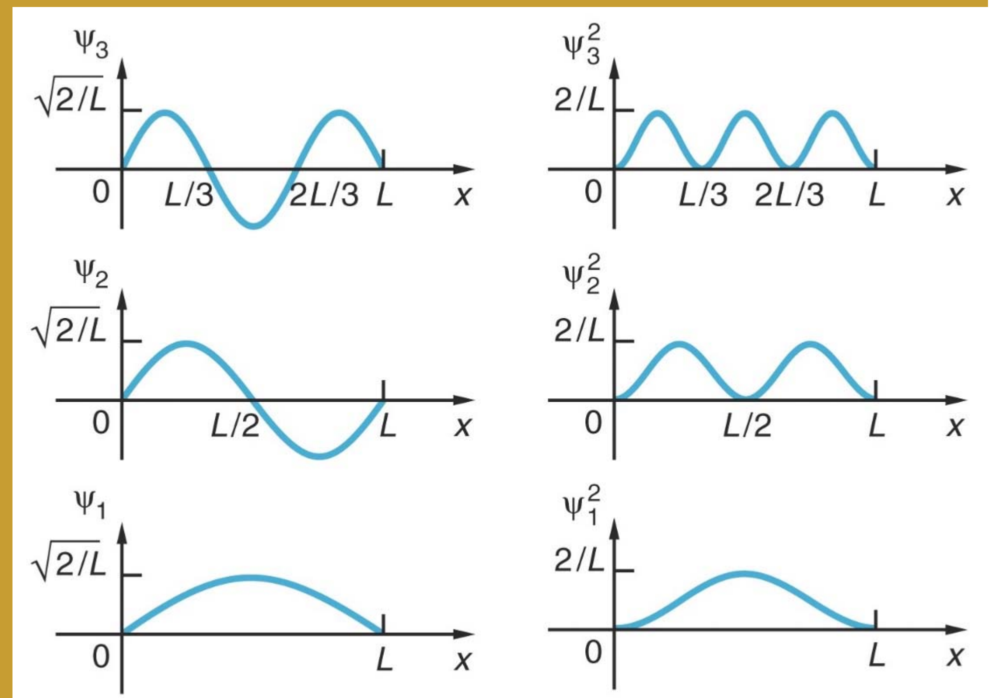
Normalization – the total probability of finding the particle is 1

$$\int_{-\infty}^{+\infty} \psi_n^* \psi_n \, dx = \int_0^L A_n^2 \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

leads to A_n = ??

The Energies and Wave-functions





$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \qquad n = 1, 2, 3, \ldots$$

Homework #1

1. Calculate the lowest 3 energy levels for an electron in a one-dimensional box, with a length dimension of
   (a) 1 mm
   (b) 1 Ångström - i.e. 0.1 nm

Give your answer in joules and/or eV.

2. For an electron in the first excited state of a 1D infinite square well, What is the probability of finding the electron in
   (a) Between 0 and L/2
   (b) Between L/3 and 2L/3
   (c) Between L/3 and L/2

3. Evaluate $<x>$, $<p>$, $<x^2>$, $<p^2>$ and $\Delta x \Delta p$ for the ground-state and first excited state of the one-dimensional harmonic oscillator