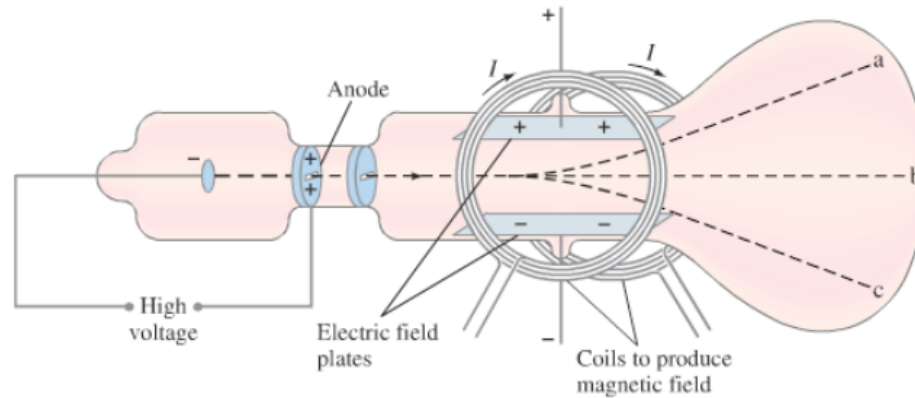


Theoretical Catastrophe, Unwanted Solutions, and the Quantum Revolution

Early Hints

- **1897:** J. J. Thomson experiments with cathode ray tubes—glass tubes filled with certain rarefied gases that has a cathode (negative plate) on one end and an anode (positive plate) connected to the other end.



- When a high enough voltage was used, beams of glowing gasses could be seen. The path of these beams could be manipulated with electric or magnetic fields which indicated that they were charged particles.
- When only the electric field plate is charged, the particles deflected upwards; when only the magnetic field was in place, they deflected downwards, indicated that the charges involved were negative.
- Without electric field, only magnetic, the curve path is described by

$$evB = m\frac{v^2}{r} \rightarrow \frac{e}{m} = \frac{v}{Br}$$

We can measure the radius of curvature as well as the magnetic field applied, but what about v ? Let's dump it.

- We can eliminate v by turning the electric field back on so that the force from the electric field is $F = eE$. We adjust this field so that the beam is no longer deflected. *Remember a problem like this from last trimester? Now you see why it is so useful.* Then we have the magnetic force and electric force equal: $eE = evB$ such that $v = E/B$ and

$$\frac{e}{m} = \frac{E}{B^2r}$$

- This ratio of charge to mass is 1.76×10^{11} c/kg. This marks the discovery of electrons and suggesting that charge is carried on individual particles and can be found only as multiples of some elementary value. In other words, *charge is quantized*.

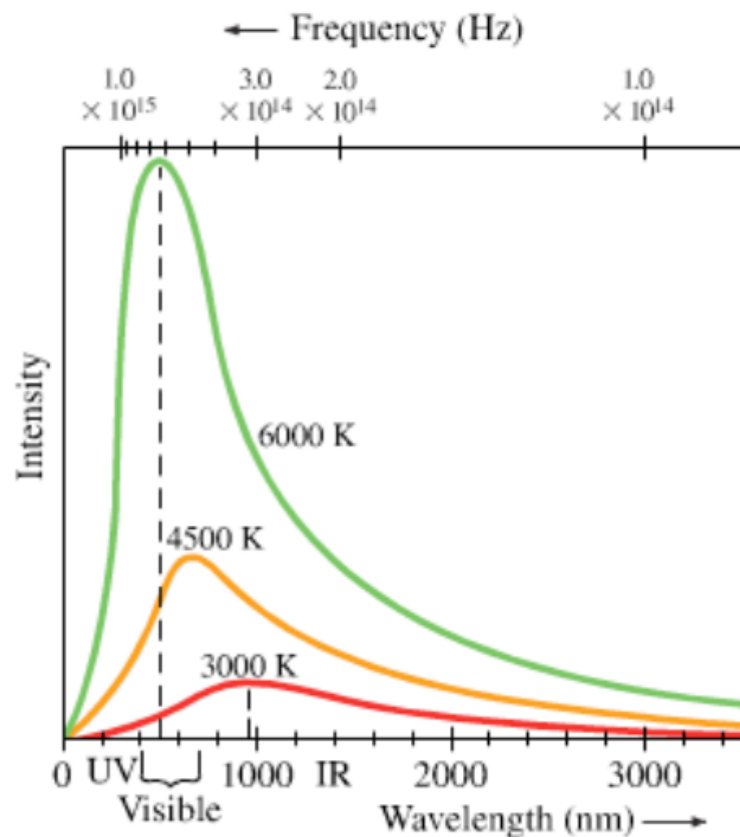
- **1913:** Millikan's oil drop experiment finds that ions are affected by an electric field in discrete multiples of e , the charge of the electron. Not only does this work prove the discrete theory of electrons, it is able to find the value of those charges. If we adjust the field that an ion is in so that it is at rest, then we have exactly balanced out the gravitational pull, i.e. $qE = m_{\text{drop}}g$. The mass can be found by finding the terminal velocity of the particle, and so the charge is found to be $q = mg/E$. This charge was found to be **integer** multiples of an elementary charge $e = 1.602 \times 10^{-19}\text{C}$.
- Proof beyond the shadow of doubt that **charge is quantized**.

That isn't too radical, and in fact it probably seems like common sense to most of us today. The revolution truly began in 1900.

Planck the reluctant revolutionary

0.1 Blackbody Radiation

- Hot objects emit a regular spectrum of light:



- That is an idealized version, in real life these curves wouldn't be so smooth. These curves describe the light emitted by something called an **idealized blackbody**—a body

that would absorb all the radiation falling on it. The radiation in the graph above is called **blackbody radiation**. It only approximates what real-world objects would emit, but it is a good approximation.

- Experimentally it has been found that the peak value of wavelength is

$$\lambda_p = \frac{2.90 \times 10^{-3} \text{m} \cdot \text{K}}{T}$$

where K stands for Kelvin (degrees Celsius + 273.15 = degrees K) and T temperature. For reference, this is referred to as **Wien's Law**.

- **Example:**

1. What color would a star that has a surface temperature of 22500 K appear?
2. What color would a star that has a surface temperature of 3500 K appear?

Red stars are cool stars; Blue stars are hot stars.

3. The sun's peak wavelength occurs somewhere near the yellow-green part of the visible spectrum at $\lambda_p = 500 \text{ nm}$. Estimate how hot the sun is.

The Ultraviolet Catastrophe

- It was also found with a mix of theory and experiment that the power of the radiation emitted by a blackbody was approximately

$$P = \sigma A e T^4$$

which is known as **Stefan's Law** where P is power in watts, $\sigma = 5.670 \times 10^{-8} \text{W/m}^2 \cdot \text{K}^4$ is called the Stefan-Boltzmann constant, A is the surface area of the object, T is temperature of course, and e is emissivity of the surface (times 100 = percentage of radiation that gets emitted rather than reabsorbed and is equal to one for blackbodies).

- Compare this to Wien's displacement law. The power emitted by the peak wavelength is proportional to the inverse of the wavelength to the fourth power.
- What's the big deal? Think about what happens at lower and lower wavelength. As $\lambda \rightarrow 0$, $P \rightarrow \infty$. But this is *not* at all what we see (see graph above), where the power goes to zero as the wavelength goes to zero (the ultraviolet side of the spectrum). Theory makes a catastrophically wrong prediction, the "ultraviolet catastrophe".
- The classical prediction is called the Rayleigh-Jeans law; here it is for comparison with the quantum answer (nevermind the constants for now):

$$I(\lambda, T) = \frac{2\pi ck_B T}{\lambda^4}$$

- Max Planck found a way out, but it was a deal with the devil of **quantization**. Planck wasn't a fan of his solution and thought that it would prove to be a mathematical artifact that could be explained away somehow.
- Planck assumed that blackbody radiation came from atomic oscillators in the cavity walls which could only have certain **discrete** energy values $E_n = nhf$ where n is a positive integer (we write this as $n \in \mathbf{N}$). We call n the **quantum number**, f is the oscillator frequency, and h is a new universal constant called **Planck's constant**. Each energy level corresponds to a separate **quantum state**.
- Planck postulated that the oscillators emit or absorb energy when making different transitions from one quantum state to another. The difference between the starting and ending state corresponds to the energy absorbed or emitted and will be equal to some integer multiple of hf .
- The probability of a state being occupied is given as $e^{-E/k_B T}$ where $k_B = 1.38 \times 10^{-23} \text{m}^2 \text{kg} \text{s}^{-2} \text{K}^{-1}$ is the Boltzmann constant.
- Consult active figure 40.7 for a conceptual perspective.
- Planck found:

$$I(\lambda, T) = \frac{2\pi hc^2}{\lambda^5 \left(e^{\frac{hc}{\lambda k_B T}} - 1 \right)}$$

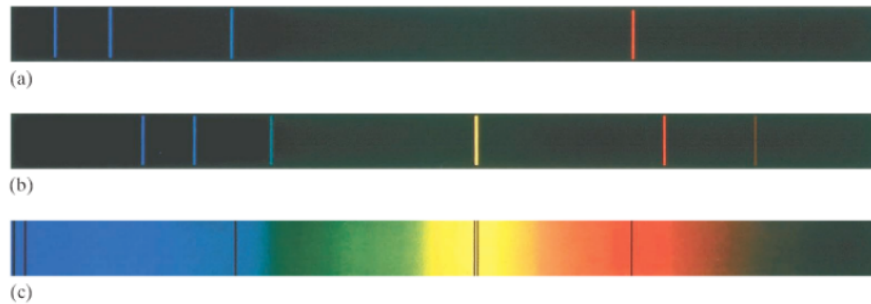
where $h = 6.626 \times 10^{-34} \text{ J} \cdot \text{s}$ was set by Planck to match experimental data. The match was superb. This was the right equation.

- Planck was not happy with this because it expanded the quantization regime to energy. He searched for ways to reconcile this with the classical picture. Other established physicists also searched for a classical escape hatch. None was to be found.
1. A 234.0 kg block is attached to an ideal classical spring with a force constant $k = 125 \text{ N/m}$ and is stretched 1.4 m from its equilibrium position.

- (a) Find the energy and frequency of oscillation.
- (b) Assume now that this is a quantum system. Find the quantum number n .
- (c) Finally suppose this system were to make a quantum leap into the next highest energy state. What is the energy change?

Atomic mystery

- Quantization of energy solved the Blackbody Radiation problem and the Photoelectric Effect. It solved the scattering problem (Compton effect) and although nobody could quite make sense of it,
- Another mystery dominated atomic physics—nobody could explain the spectra of gasses.
- We might expect a continuous distribution of wavelengths, but instead we find discrete line spectrum called the *emission spectrum*.
- Passing white light through gasses result in discrete missing wave-lengths, this is called the absorption spectrum.
- Example emission (hydrogen, mercury, and neon) and absorption spectrum for hydrogen:



- 19th century physicists can't explain these spectra.
- Balmer found an empirical equation that correctly predicted the wavelengths of four of the visible emission lines; Rydberg expanded this equation to find all emission lines:

$$\frac{1}{\lambda} = R_H \left(\frac{1}{2^2} - \frac{1}{n^2} \right), \quad n = 3, 4, 5, \dots$$

- R_H is a constant called the Rydberg constant and is equal to $1.0973732 \times 10^7 m^{-1}$.
- The shortest wavelength is found when $n \rightarrow \infty$ is called the series limit with wavelength 364.6 nm (ultraviolet).
- Other physicists started experimenting with these numbers and found similar equations that described other lines in the spectrum:

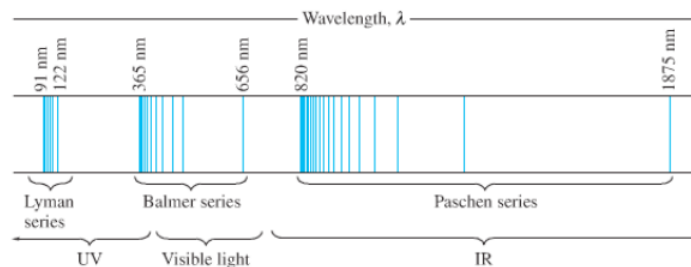
$$\text{Lyman series: } \frac{1}{\lambda} = R_H \left(1 - \frac{1}{n^2} \right), \quad n = 2, 3, 4, \dots$$

$$\text{Paschen series: } \frac{1}{\lambda} = R_H \left(\frac{1}{3^2} - \frac{1}{n^2} \right), \quad n = 4, 5, 6, \dots$$

$$\text{Bracket series: } \frac{1}{\lambda} = R_H \left(\frac{1}{4^2} - \frac{1}{n^2} \right), \quad n = 5, 6, 7, \dots$$

- It all works very well, but nobody knows why.

FIGURE 27–23 Line spectrum of atomic hydrogen. Each series fits the formula $\frac{1}{\lambda} = R \left(\frac{1}{n'^2} - \frac{1}{n^2} \right)$ where $n' = 1$ for the Lyman series, $n' = 2$ for the Balmer series, $n' = 3$ for the Paschen series, and so on; n can take on all integer values from $n = n' + 1$ up to infinity. The only lines in the visible region of the electromagnetic spectrum are part of the Balmer series.



Quantum solution: A fix that nobody was happy with

A physicist named Niels Bohr saw that energy quantization had solved the blackbody and photoelectric problem, and he wondered if it could solve the mystery of the atomic spectrum lines as well. Here is a basic outline of his reasoning.

- Assume the classical model of the electron orbiting the nucleus of the hydrogen atom under electrical forces. In this case the total energy is

$$E = K + U = \frac{1}{2}m_e v^2 - k_e \frac{e^2}{r}$$

and since we assume the electron is going in a circle, the electric force must act as a centripetal force:

$$\frac{k_e e^2}{r^2} = \frac{m_e v^2}{r} \implies v^2 = \frac{k_e e^2}{m_e r}$$

Using this value for velocity, we have kinetic energy:

$$K = \frac{1}{2}m_e v^2 = \frac{k_e e^2}{2r} \quad \text{and} \quad E = -\frac{k_e e^2}{2r}$$

- So far, so classical.
- Next comes the quantum step. Assume that only certain orbits are stable (called *stationary states*, which validates our previous assumption of using classical physics). The atom emits radiation when it makes a *quantum leap* from one state to another. The change in its energy after making this leap is *quantized*:

$$E_f - E_i = hf, \quad \text{positive value means absorbed, negative value means emitted}$$

- Bohr next a new leap: quantizing the electron's orbital angular momentum:

$$m_e v r = n \frac{h}{2\pi} = n\hbar$$

where $\hbar = h/2\pi$. The energy quantization was enough to fluster some, but this latter assumption was a radically new expansion of the concept of quantization.

- Now let's apply this radical concept:

$$v^2 = \frac{n^2 \hbar^2}{m_e^2 r^2} = \frac{k_e e^2}{m_e r} \implies r_n = \frac{n^2 \hbar^2}{m_e k_e e^2}, \quad n = 1, 2, 3$$

- Call the orbit with the smallest radius the Bohr radius (when $n = 1$):

$$a_0 = \frac{\hbar^2}{m_e k_e e^2} = 0.0529 \text{ nm}$$

Plug this all back into the energy equation to find:

$$E_n = -\frac{k_e e^2}{2a_0} \left(\frac{1}{n^2} \right), \quad n = 1, 2, 3, \dots$$

or numerically:

$$E_n = -\frac{13.606 \text{ eV}}{n^2}, \quad n = 1, 2, 3, \dots$$

Now let's find out the frequency of light emitted from a quantum leap:

$$f = \frac{E_i - E_f}{h} = \frac{k_e e^2}{2a_0 h} \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

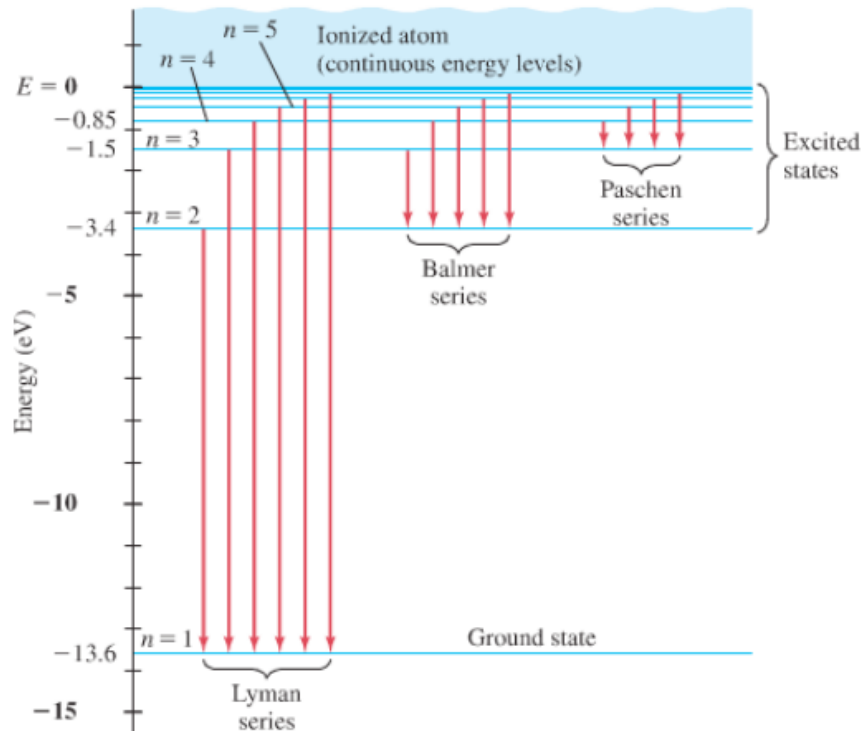
That looks familiar...

$$\frac{1}{\lambda} = \frac{f}{c} = \frac{k_e e^2}{2a_0 h c} \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

Plugging in all of our numbers:

$$\frac{k_e e^2}{2a_0 h c} = 1.0973732 \times 10^7 \text{ m}^{-1} = R_H$$

- Quantum mechanics had **theoretically** predicted the value of R_H . At this point, attempts to rescue classical physics were beginning to look hopeless.
- We see it again: integers describing physical reality—one of the key signatures of quantum mechanics. This made most physicists uncomfortable, but also energized by the revolutionary spirit in the air.



A pivot towards formalization

- Classical physics had major holes in its attempt to describe our universe.
- Physicists resorted to a technique called quantization to try to patch these holes.
- Quantization worked so well that it started dominating physics.
- This patchwork isn't professional, Bohr's model had a major flaw—an electron traveling in a circle is undergoing centripetal acceleration and thus should be radiating energy and collapse into the nucleus. Bohr had to posit that it could only reach certain states and not get any closer. Very sloppy if effective.
- Bohr's model turns out to be just that, a model that gets correct results but doesn't exactly describe the true story.
- Also, classical physics still worked—mostly. Bohr posited that where quantum predictions and classical predictions overlap, they should agree. This is called the **correspondence principal**.
- Bohr's work was further supported (10 years later) by de Broglie's wave-particle duality theory for matter. He proposed that the wavelength of matter is given by $\lambda = \frac{h}{mv}$. If we see each electron orbiting an atom as a standing wave with such a wavelength, then

$$2\pi r_n = n\lambda$$

and

$$2\pi r_n = \frac{nh}{mv} \rightarrow mvr_n = \frac{nh}{2\pi}$$

This was Bohr's prediction. Thus Bohr's radical quantization of angular momentum went hand in hand with de Broglie's radical proposal that matter is a wave and a particle all at once.

- The search was on for a more formal way to describe the theory.

Quantum Mechanics is born

At this point, we are settling down from our riotous state and learning to live with the reality that our brains have deceived us about the true nature of reality. So let's accept that the world is quantized at the very fundamental levels, and see what this implies.

- If particles are waves, how do we discuss their amplitudes and displacements like we do for classical waves? We need some sort of **wave function** to do so, which we write as Ψ .
- For light, the intensity of the wave is proportional to the square of the electric field. The more intense the light, the more photons we can find, and so the number of photons is proportional to the intensity is proportional to the square of the electric field (the EM wave amplitude).
- Put another way, the square of the electric field amplitude is proportional to the probability that we will find a photon at a certain region.
- We seek a matter wave such that Ψ^2 is proportional the probability of finding an electron at a certain place and time.
- Schrödinger found the equation that properly describes how these matter waves behave:

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

- This is called the Schrödinger equation.
- For most particles, we can separate the time-dependence so that

$$\Psi(r, t) = \psi(r)e^{-i\omega t}$$

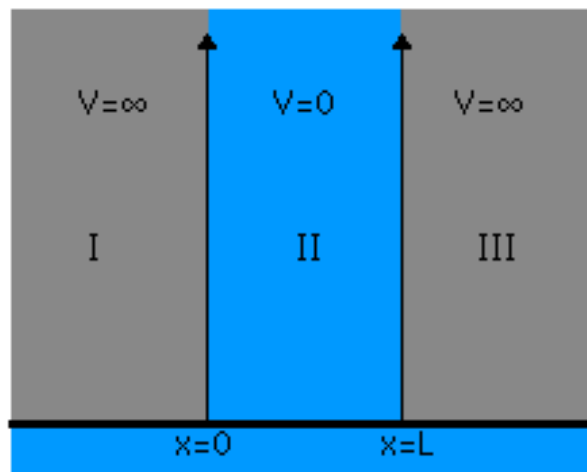
- This is a **probabilistic equation**, where the probability of finding a particle whose wave is ψ within any given region of space is $P(x, y, z)dV = |\psi|^2 dV$.
- What is matter then? A particle? A wave? Is ψ the true manifestation of matter?
- ψ is the true manifestation of matter.

Heisenberg's Uncertainty Principal

A statistical side effect of quantum mechanics is **Heisenberg's Uncertainty Principle**: Call the uncertainty of the measurement of a particles position as Δx and Δp_x , then quantum mechanics requires that $\Delta x \Delta p_x \geq \frac{\hbar}{2}$. In that momentum is related to energy, this result restricts the accuracy of the Energy levels we can measure. For small groups of atoms this isn't a problem, but very large groupings of atoms clustered together result in very closely spaced energy levels, getting so close that we would be better off of speaking of bands of energy states rather than discrete spectrum.

A particle in an infinite well

Let's find out how a single subatomic particle inside an infinite well behaves.



- Start with the Shrödinger equation:

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

- Think about the potential. The particle would have to have infinite energy to overcome the infinite potential (this isn't very realistic but can be a conceptual approximation to a particle being trapped in a low electrical potential regions between two very high electric potential regions in optoelectronics). Since the particle can't have infinite energy, we assume that it can't exist in the region of infinite potential, and so its wave function must go to zero on the borders.
- This simplifies the wave equation—we only have to look at the zero-potential region and assume that the function goes to zero on the edges.

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

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

- This looks familiar from previous discussions we had on springs. Let's assume that the solution takes the form:

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

- If the length of the zero-potential region starts from zero and goes to $x = L$, then we require that $\sin(kL) = 0$. Thus we require that $kL = n\pi$. Quantization comes out of the boundary conditions.
- Putting it all together, we find that:

$$\sqrt{\frac{2mE}{\hbar^2}}L = n\pi$$

$$\frac{2mE}{\hbar^2}L^2 = n^2\pi^2$$

$$E = \frac{n^2\pi^2\hbar^2}{2mL^2} = \frac{n^2h^2}{8mL^2} \quad \text{since} \quad \hbar = \frac{h}{2\pi}$$

Overall, the wave function can be written most simply as

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

The total probability over all space must be:

$$\int_0^L |\psi^2(x)| = \int_0^L A^2 \sin^2\left(\frac{n\pi x}{L}\right) = 1$$

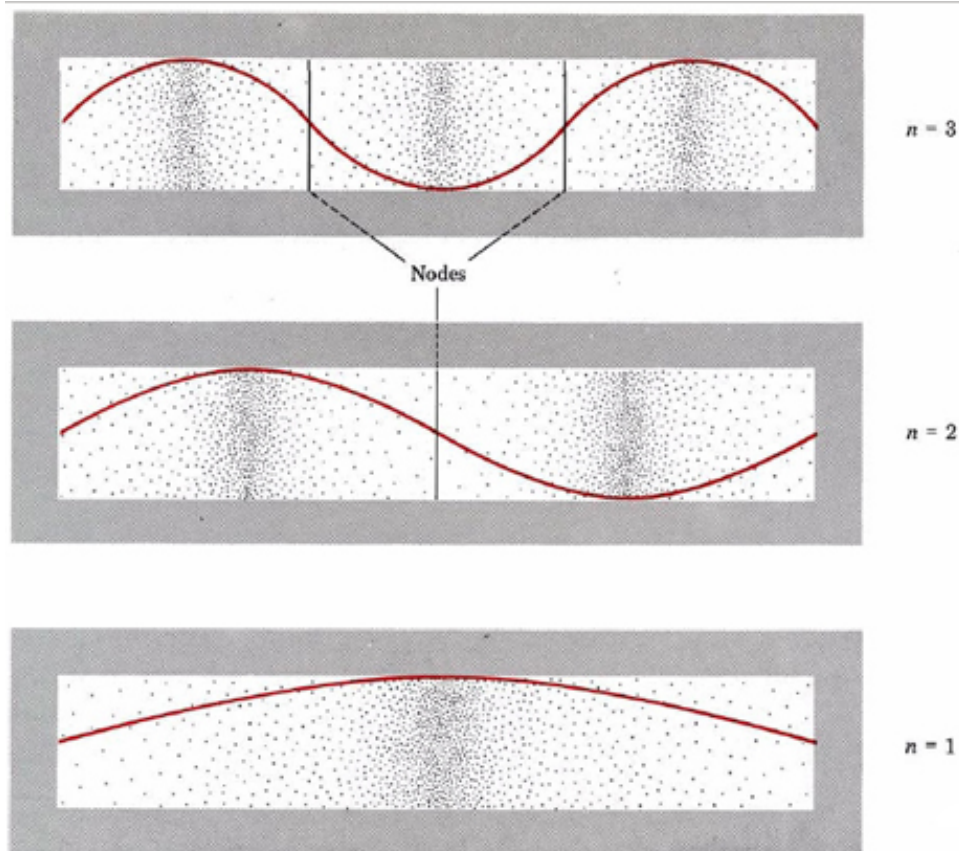
That is, the particle must have 100% probability to exist *somewhere* in the box.

$$1 = A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) = A^2 \frac{x}{2} - A^2 \frac{L}{4n\pi} \sin\left(\frac{n\pi x}{L}\right) \Big|_0^L = \frac{L}{2}$$

so that

$$A = \sqrt{\frac{2}{L}}$$

- The probability of finding the particle at certain places inside the box depends on the energy of the particle:



- The $n = 1$ value corresponds to what is called **ground state** and anything with $n > 1$ is **excited states**.
- The **expectation value** of the position x is given by

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^* x \psi dx$$

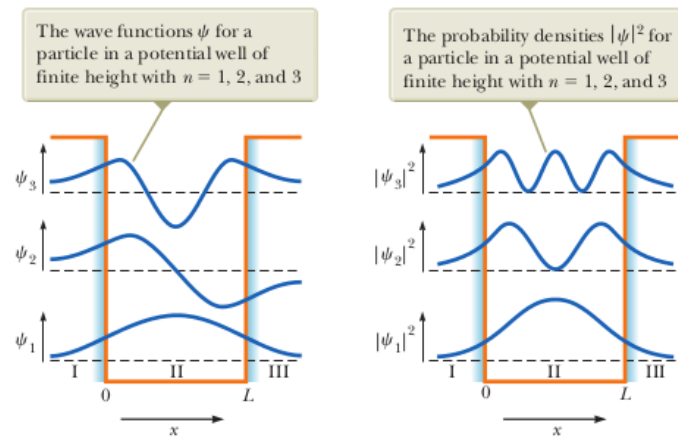
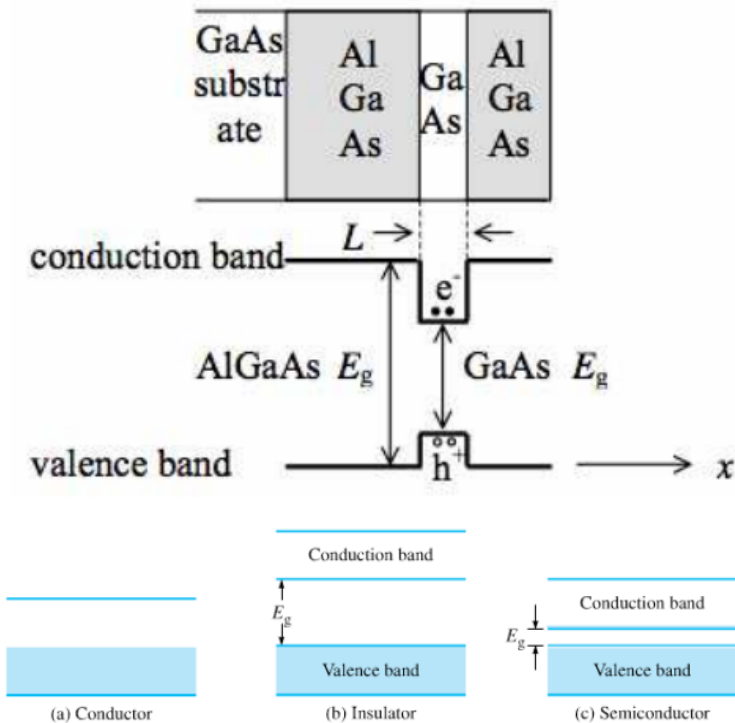
where ψ^* is the *complex conjugate* of ψ , that is, if $\psi = \alpha + i\beta$ then $\psi^* = \alpha - i\beta$. See Example 41.3 for a full derivation, but the result is that the expectation value for the position is $L/2$. This makes classical sense (why?) but we need to remember that this expectation value is a **statistical result** which can only be obtained by measuring thousands of equivalent systems.

- Review examples in textbook on page 1227.

Particle in a finite well

A more realistic example involves a finite potential well. Solid state transistors, for example, involves a mixing of substrates of materials with different compositions, such as Aluminum-Gallium-Arsenic layered with Gallium-Arsenic. The former has a smaller band-gap (difference

in energy between the valence band and the conduction band) than the latter. The valence band represents the highest range of energies for a material in which electrons are typically present. Electrons in this band are bound to atoms and don't typically allow them to "transfer" and so don't conduct current. The next higher band of accessible energy states is called the conduction band. If this band is very close to or intersects the valence band, then the material is a good conductor. If the band-gap between them is very large, then the material is an insulator.



- The Schrödinger equation for this system is:

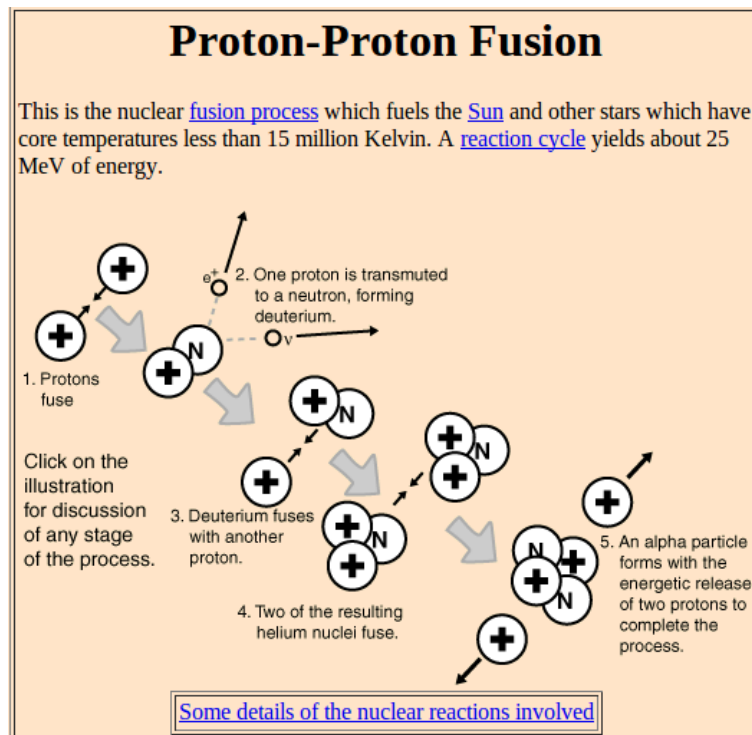
$$\frac{d^2\psi}{dx^2} = \frac{2m(U - E)\psi}{\hbar^2}$$

for the particle outside of the well.

- Let's assume that $U > E$ so that the particle should be classically bound, then write $C^2 = 2m(U - E)/\hbar^2$ where the general solution might be

$$\psi = Ae^{Cx} + Be^{-Cx}$$

- This can't work because it would explode infinitely. For $x < 0$, we have $\psi = Ae^{Cx}$ and for $x > L$ we have $\psi = Be^{-Cx}$
- In between, for $0 < x < L$, we have a general solution $\psi(x) = F \sin(kx) + G \cos(kx)$
- By matching boundary conditions, we can find the full probability wave.
- But note that there is a small but real chance that the particle will be found **inside the well**. This is a new, and very strange concept called **quantum tunneling**.
- Examples of tunneling:
 - Alpha decay: Unstable heavy nuclei sometimes release a helium nucleus (called an alpha-particle—two neutrons and two protons). The unstable nucleus is the equivalent of a finite potential well that the alpha particle can sometimes tunnel through.
 - Nuclear Fusion: How can free protons be brought so close together to form deuterium? The protons must tunnel through their repulsive barriers.



- Scanning Tunneling Microscopes: Voltage difference is applied across tip of microscope and material. The electron can tunnel through the “barrier” that is the

space between the material and the probe—the closer they are, the more tunneling will occur and so the resulting current indicates how far away that object is.

– Other examples will follow next week.

Harmonic Oscillator

The potential energy of a HO is

$$U = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2$$

where $\omega = \sqrt{k/m}$. What will a quantized version of such a system look like?

Schrödinger's equation for this system will be:

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

The solution is $\psi = Be^{-Cx^2}$ where $C = \frac{m\omega}{2\hbar}$ and $E = \frac{1}{2}\hbar\omega$. This corresponds to the ground state of the HO. It can be shown that the energy levels for excited states are given by,

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega$$

Quantization of ElectroMagnetic Fields

When the EM field is quantized, it predicts an energy that looks as:

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega$$

This is currently giving physics some problems...

1. Lightning produces a maximum air temperature on the order of 10^4 K whereas a nuclear explosion produces a temperature on the order of 10^7 K. Use Wien's displacement law to find the order of magnitude maximum intensity wavelength and name the part of the EM spectrum this belongs to.

2. Chapter 40–7: What is the surface temperature of Betelgeuse, a red giant star in the constellation Orion which radiates at a peak wavelength of about 970 nm? Rigel radiates with a peak wavelength of 145 nm. What is the surface temperature of each star?

3. A simple pendulum has a length of 1.00 m and a mass of 1.00 kg. The maximum horizontal displacement of the pendulum bob from equilibrium is 3.00 cm. Calculate the quantum number n for the pendulum.

4. Two light sources are used in a photoelectric experiment to determine the work function for a particular metal surface. When green light from a mercury lamp $\lambda = 546.1$ nm is used, a stopping potential of 0.376 V reduced the photocurrent to zero. Based on this measurement, what is the work function for this metal? What stopping potential would be observed when using the yellow light from a helium discharge tube $\lambda = 587.5$ nm?

5. Calculate the de Broglie wavelength for a proton moving with a speed of 1.00×10^6 m/s.

6. Calculate the momentum of a photon whose wavelength is 4.00×10^{-7} m. Find the speed of an electron having the same momentum as the photon.

7. Use the uncertainty principle to show that if an electron were confined inside an atomic nucleus of diameter on the order of 10^{-14} m, it would have to be moving relativistically whereas a proton would not.