

Chapter 2

Quantum Theory

Chapter 2 - Quantum Theory

- At the end of this chapter – the class will:
 - Have basic concepts of quantum physical phenomena and a rudimentary working knowledge of quantum physics
 - Have some familiarity with quantum mechanics and its application to atomic theory
 - Quantization of energy; energy levels
 - Quantum states, quantum number
 - Implication on band theory

Chapter 2 Outline

- Basic concept of quantization
- Origin of quantum theory and key quantum phenomena
- Quantum mechanics
- Example and application to atomic theory

Concept introduction



The quantum car

Imagine you drive a car. You turn on engine and it immediately moves at 10 m/hr. You step on the gas pedal and it does nothing. You step on it harder and suddenly, the car moves at 40 m/hr. You step on the brake. It does nothing until you flatten the brake with all your might, and it suddenly drops back to 10 m/hr. What's going on?

Continuous vs. Quantization



Consider a billiard ball. It requires accuracy and precision. You have a cue stick. Assume for simplicity that there is no friction loss. How fast can you make the ball move using the cue stick? How much kinetic energy can you give to the ball?

The Newtonian mechanics answer is:

- any value, as much as energy as you can deliver. The ball can be made moving with 1.000 joule, or 3.1415926535 or 0.551 ... joule. Supposed it is moving with 1-joule energy, you can give it an extra 0.24563166 joule by hitting it with the cue stick by that amount of energy. The ball will have 1.24563166 joule. The energy value is continuous.

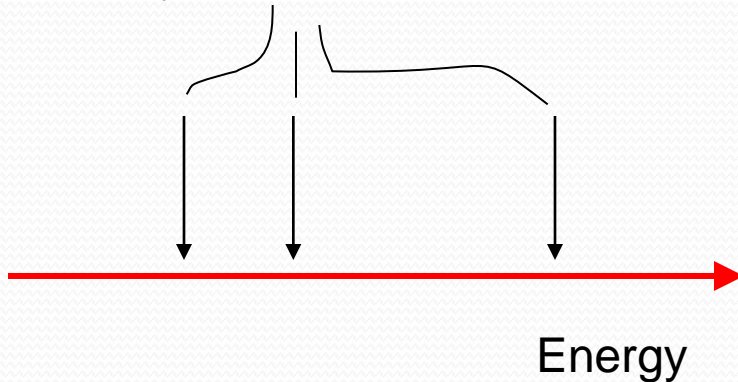
Let's shrink the table down to a very small size, and let the billiard ball become as small and light mass as an electron. Can you still do the same thing to its energy?

Answer: NO. If you don't hit the ball (electron) with the right amount of energy, IT WON'T CHANGE. Supposed it is moving with 1×10^{-19} Joule, and you want it to be moving with 1.014×10^{-19} Joule which happens not to be a value that it's happy with. You can hit it as many times as you want with 0.014×10^{-19} Joule, and nothing will happen. The ball just ignores your cue stick.

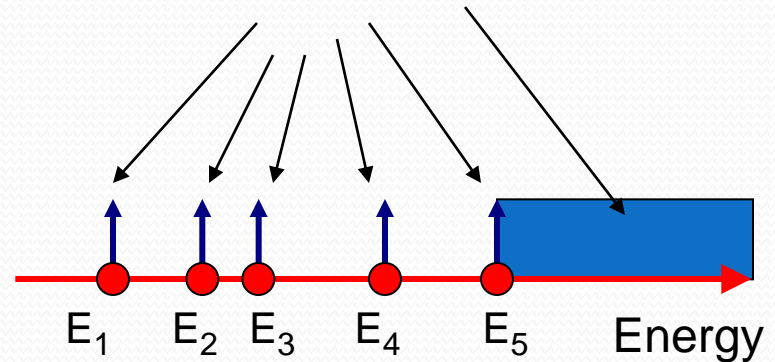
The reason is that the energy of the quantum ball now is not continuous, but **quantized into discrete values**

Quantization of energy

Continuous energy: it can be any value on the axis



Discrete (or quantized energy): it can ONLY be at certain values on the axis



Key concept of the quantum world:

- The energy can have discrete values: referred to as quantization
- But it doesn't have to be always discrete! It can be continuous also, and can be a mixed of discrete and continuum
- How many discrete levels can a system have?

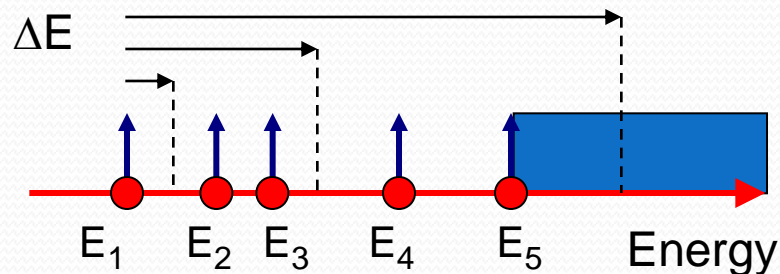
How does a quantum billiard ball behave?



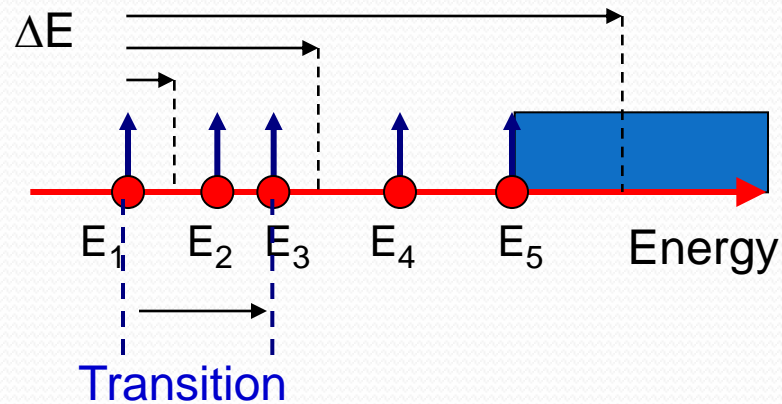
Supposed that the quantum ball has energy E_1
If we hit it with a cue stick, what will happen?

Answer:

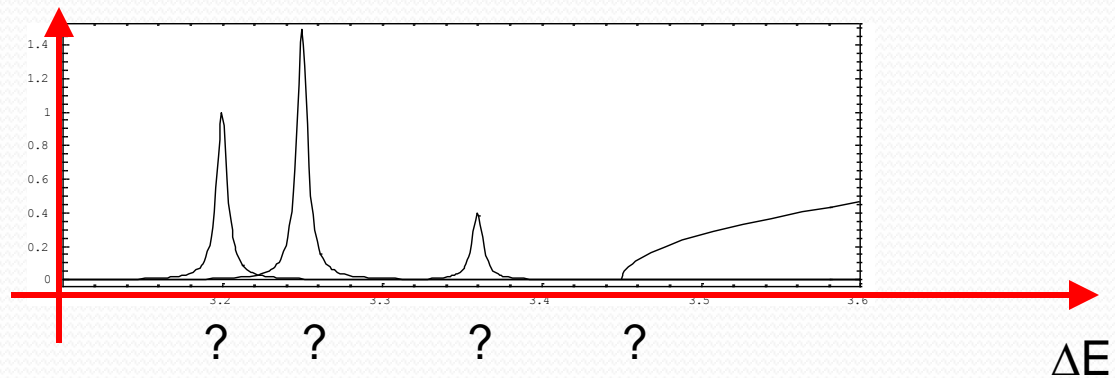
It depends, if the cue stick hits it with an energy ΔE such that $E_1 + \Delta E$ does not coincide with any of the quantized levels or $\geq E_5$, it won't change! The quantum ball just ignores the cue stick. This is the major difference between quantum physics and classical physics.



How does a quantum billiard ball behave?

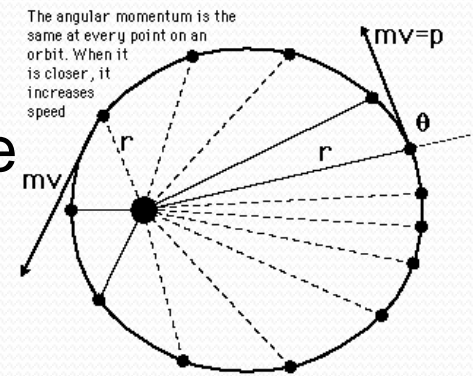


Absorption
or energy transferred



General concept of quantization – quantum number

- Quantization applies not just to energy. Many fundamental physical quantities are also quantized
- *What is quantized electric charge? (e)*
- *Are the masses of objects quantized?*
 - mass of electron? proton, neutron, neutrino, photon
- A quantity that is absolutely quantized: angular momentum – *what is the unit of a.m.?*
- Other: linear momentum
- Sometimes, we associate a “number” to a quantized quantity, we call it “**quantum number**”



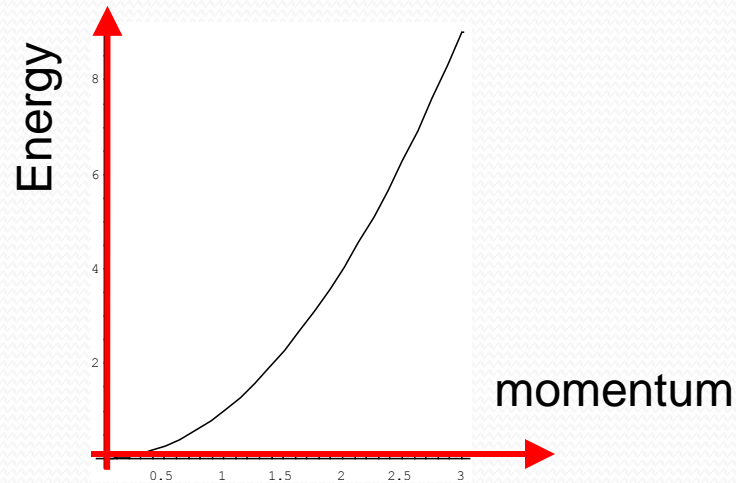
A Question

- A free electron in infinite space. Is its energy quantized?
 - No, it's not. Quantum mechanics (QM) does not say that everything has to be quantized.

A free electron has an energy value:

$$\frac{p^2}{2m}$$

where p is linear momentum, m is the mass. It's like classical mechanics. p can be continuous, and so is the energy.



A Question

- A free electron in infinite space. Is its energy quantized?
 - No ...
 - But a bound electron, one which is under the influence of a force that holds the electron to a “confined” region of space, has its energy quantized.
 - If the electron experiences a force, but the force is not enough to hold it to a finite region of space, is its energy quantized? No. So how do we know when the energy is quantized or not? We have to SOLVE the specific problem to find out. All QM says is that there is the possibility of quantization, depending on specific situations, this is different from Newtonian mechanics in which, there is no quantization at all.

Countable and Uncountable

Quantization has a major impact on physical theory. One case is the issue of countable and uncountable number of states.

How many numbers are there in the set of all integer?

How many real numbers between 0 and 1?

Are the two sets, all integers and all real number from 0-1, equal?

Are the set of real number countable?

Quantization makes the number of states (or physical conditions, or solutions) countable.

Is this some arcane, irrelevant math? No, it is a crucial difference between quantum and classical theory, and basically led to the discovery of the quantum theory: Max Planck's black body radiation theory

The Origin of the Quantum Theory:

The black-body problem

Any hot object emits electromagnetic waves; we call this thermal radiation.

Find examples of this around you

“red hot” objects in a furnace, the sun, the universe (3K background radiation). Do you think living thing emit radiation? How about us? Do you think we get cancer from our own thermal radiation?

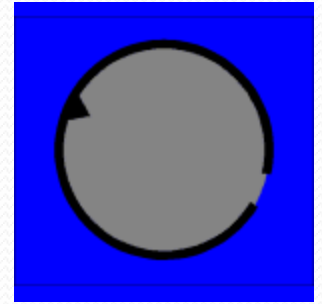
People have studied this in 19th century and observed that the hotter the object is, the **brighter** is the radiation, and also “redder” (**shorter wavelength**)

How does the glow change as you heat up an object?

Do you think the RGB color we see from the TV screen thermal radiation? Why so and if not, why not?

Black-body radiation

Hotter object -> Brighter radiation: Stefan's law



$$\frac{\text{Thermal Radiation Power}}{\text{Radiating area}} = \epsilon \sigma T^4$$

emissivity Stefan-Boltzmann constant temperature

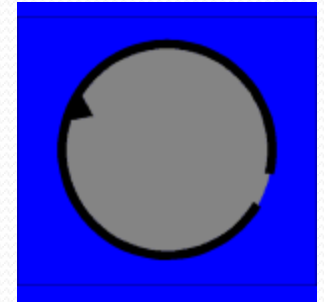
A perfectly absorbing object has emissivity=1. It absorbs all radiation falling on it, thus, it is a perfectly black object, called black-body.

In real life, very hard to make a black body, one way to make it close to it is a cavity

As shown, any light falling into the cavity aperture is most likely absorbed, thus, the radiation from the aperture should be like black-body

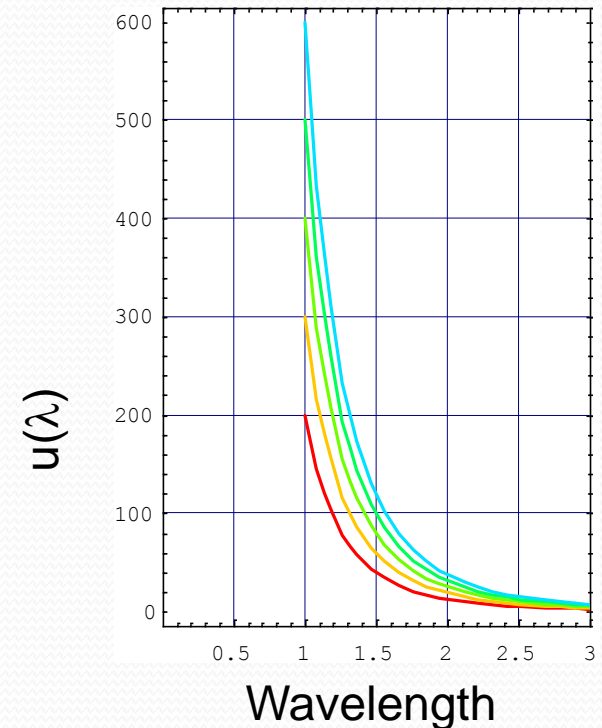
Black-body radiation

Hotter object -> color shifts to shorter wavelength
Rayleigh –Jeans' law based on Maxwell's theory



$$u(\lambda) = \frac{8\pi}{\lambda^4} k_B T$$

Spectral density $\rightarrow u(\lambda)$
Wavelength $\rightarrow \lambda^4$
Boltzmann constant $\rightarrow k_B$
temperature $\rightarrow T$



What is the problem of this? What is this object color?

Ultraviolet catastrophe! Where does it go wrong?

Planck quantum theory

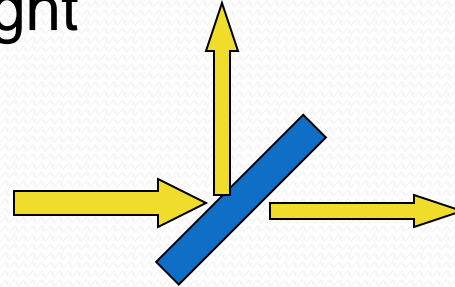
Planck proposed a bold concept of "quantum of action"

$$A = p \cdot x$$

Later, Einstein coined the corpuscular theory of light:

"photon" is the most fundamental light particle

- The concept of indivisible light



Does an electromagnetic wave carry energy?

Or power?

If so, what is the energy or power of an electromagnetic wave?

Planck quantum theory

As it turns out, the energy of an electromagnetic wave cannot be arbitrarily small, and cannot be continuous according to Planck's theory – rather, the energy of an electromagnetic wave is quantized.

The amount of energy an electromagnetic wave mode in a black-body cavity can **ONLY** have discrete value:

$$E = n h \nu$$

integer

A new fundamental constant: Planck's constant

Planck quantum theory

What happens? The number of modes suddenly go from uncountably infinite to countably infinite

With this, Planck shows that the result should be:

Planck's constant

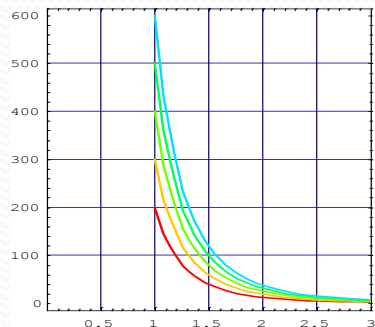
$$u(\lambda) = \frac{8\pi}{\lambda^5} \frac{ch}{e^{h\nu/k_B T} - 1}$$

wavelength

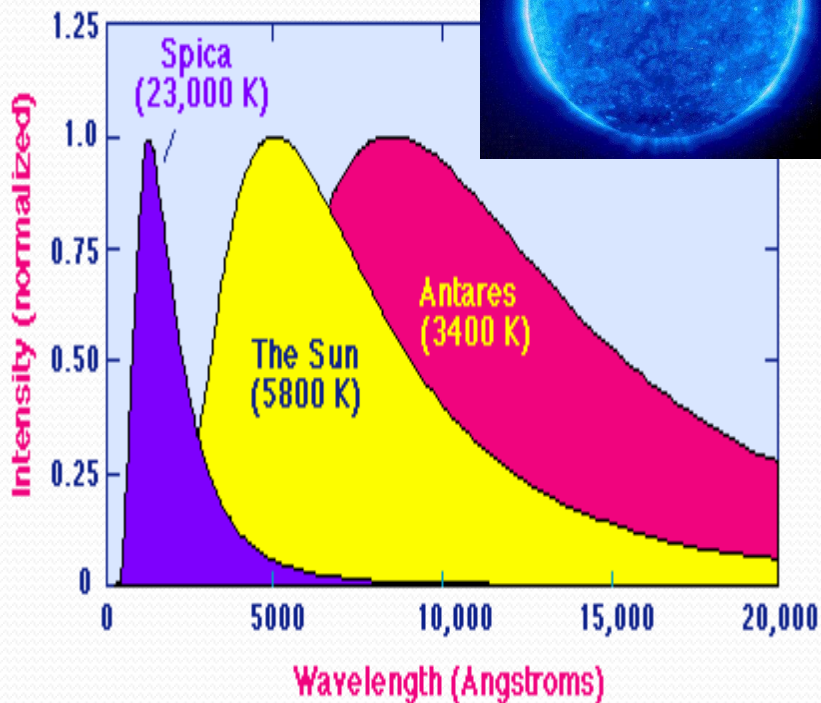
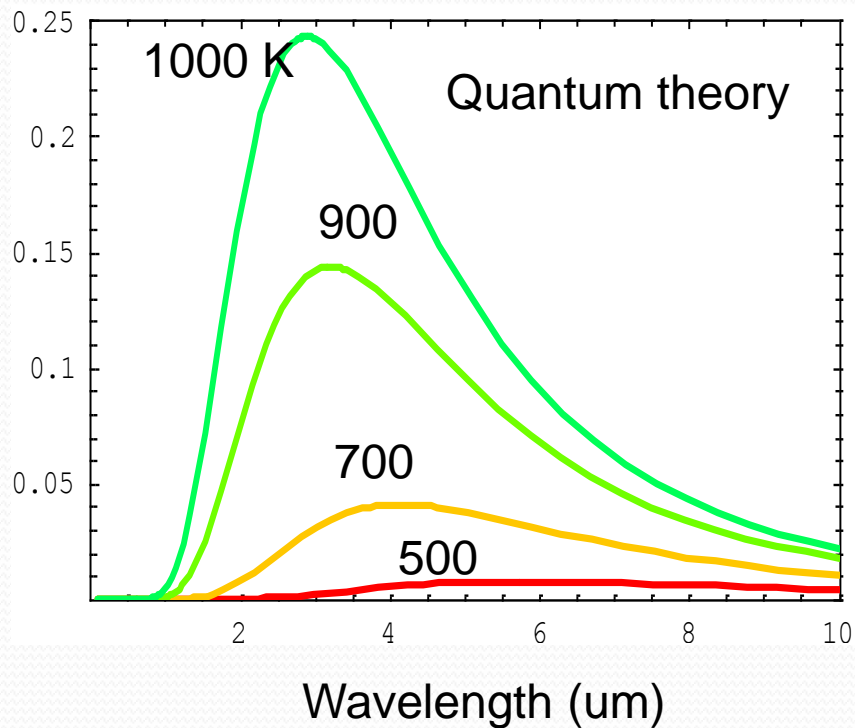
frequency

Planck's theory of black-body radiation

Classical theory



$$u(\lambda) = \frac{8\pi}{\lambda^5} \frac{ch}{e^{hv/k_B T} - 1}$$



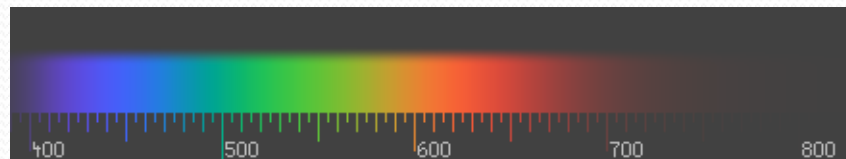
What is Planck's constant?

$$h = 6.63 \times 10^{-34} \text{ Joule sec.}$$

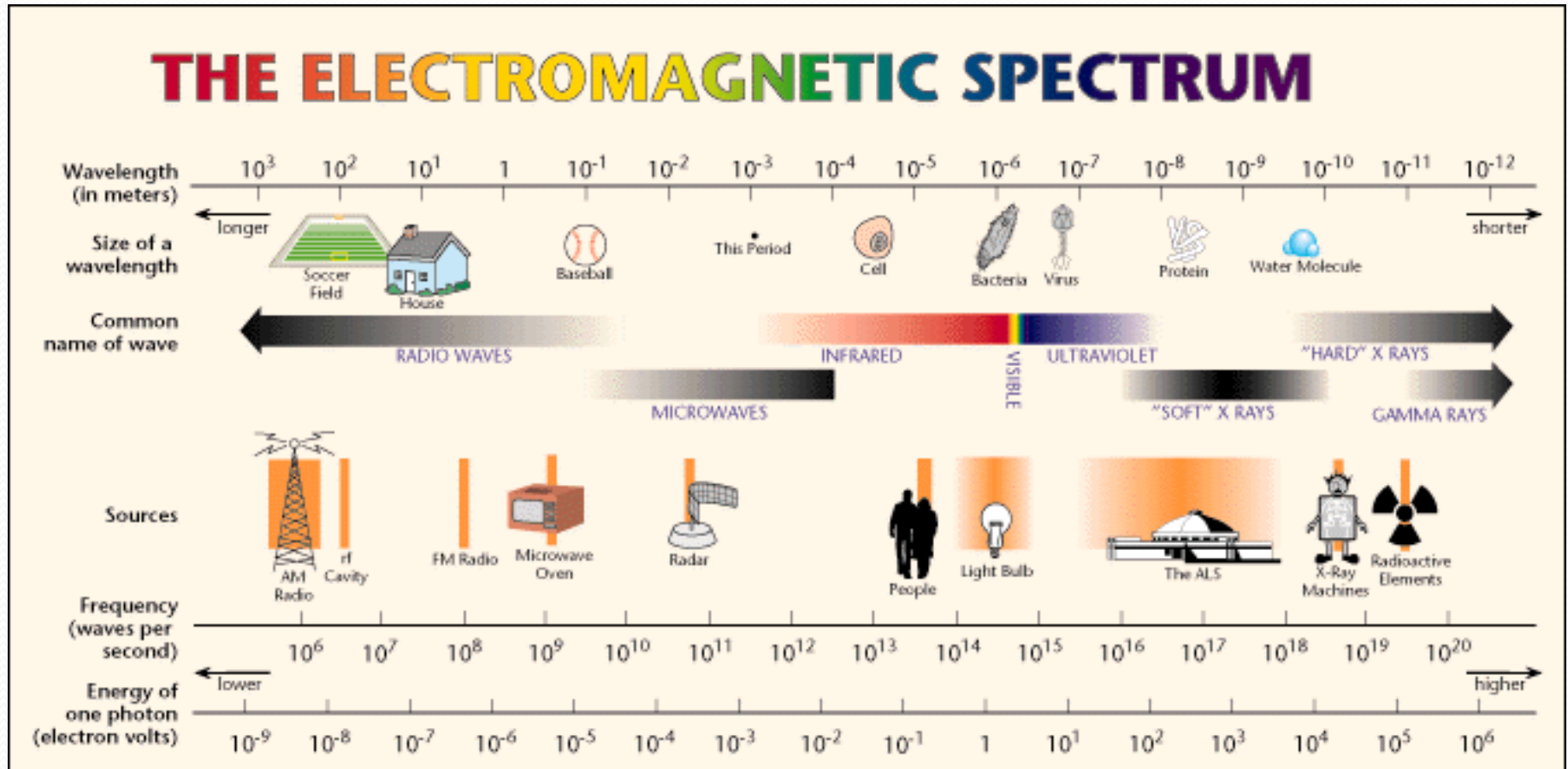
Energy of a photon of frequency ν :

$$E = h\nu = h \frac{\omega}{2\pi} = \hbar\omega \quad \text{where } \hbar \equiv \frac{h}{2\pi}$$

Link photon energy to the color of light

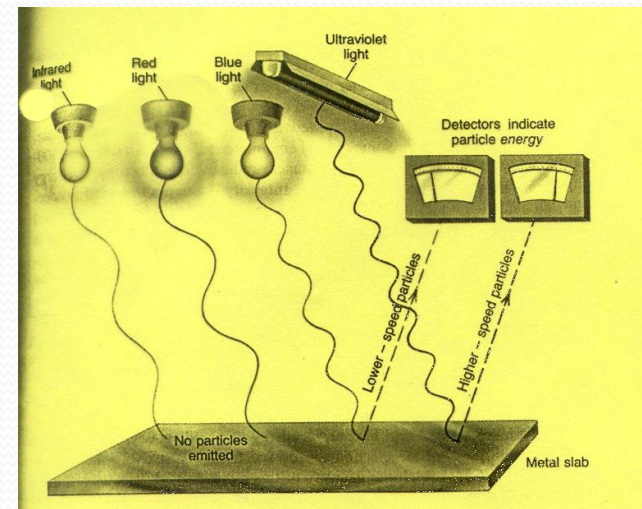
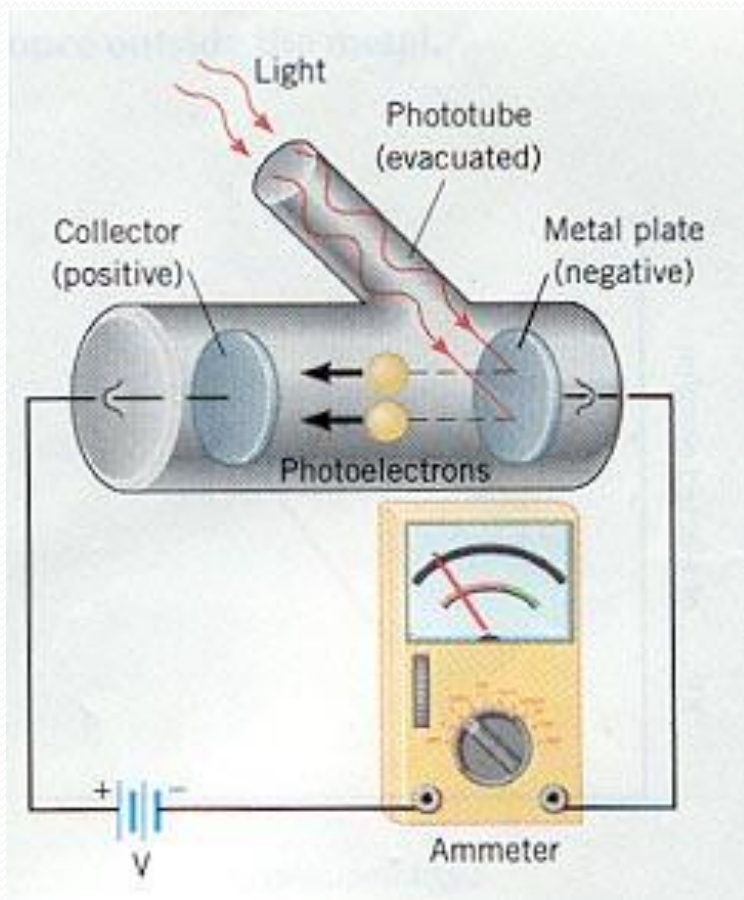


The electromagnetic spectrum



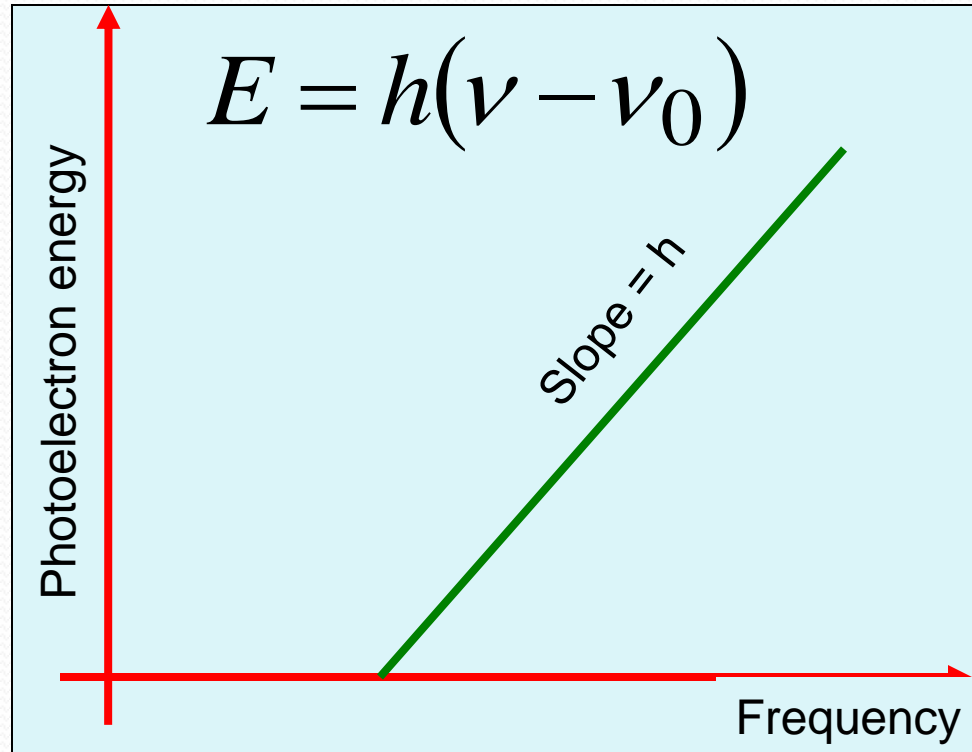
Second crucial evidence of the Quantum theory: photoelectric effect

Frank-Hertz experiment

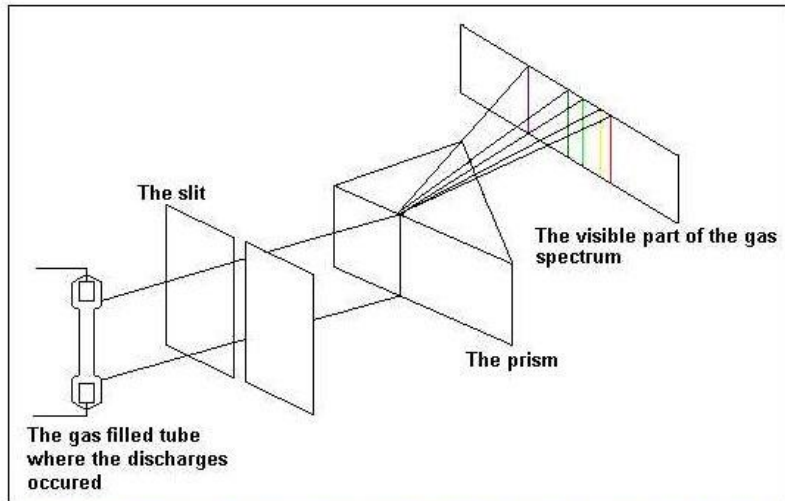


- The existence of **threshold**: photon frequency must exceed a certain value (not intensity)
- Energy of photoelectrons is proportional to frequency - NOT intensity. The proportional constant is Planck constant – (Milliken exp)

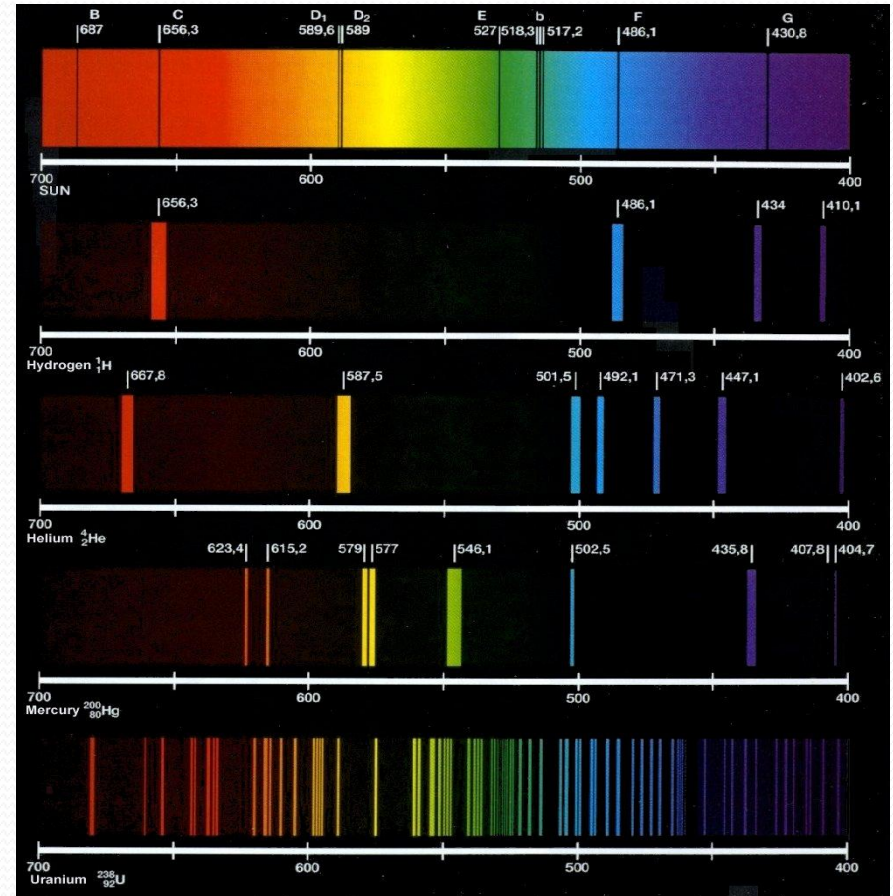
The photoelectric effect (cont.)



Discrete Lines in Atomic Vapor Spectra



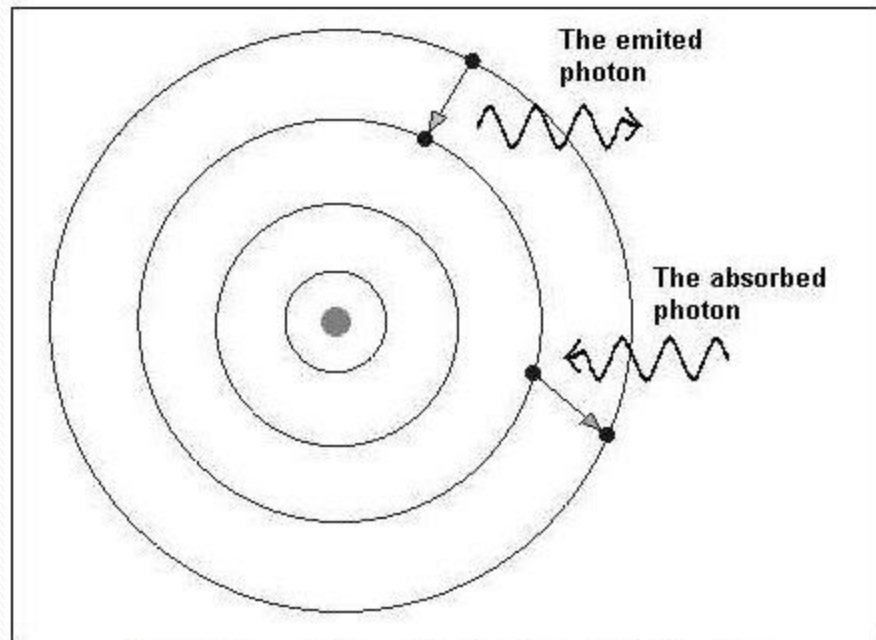
The discharges in the low pressure gas filled tube are the sources of the light which undergo refraction on the prism. We see the line spectrum of the gas.



Key concepts

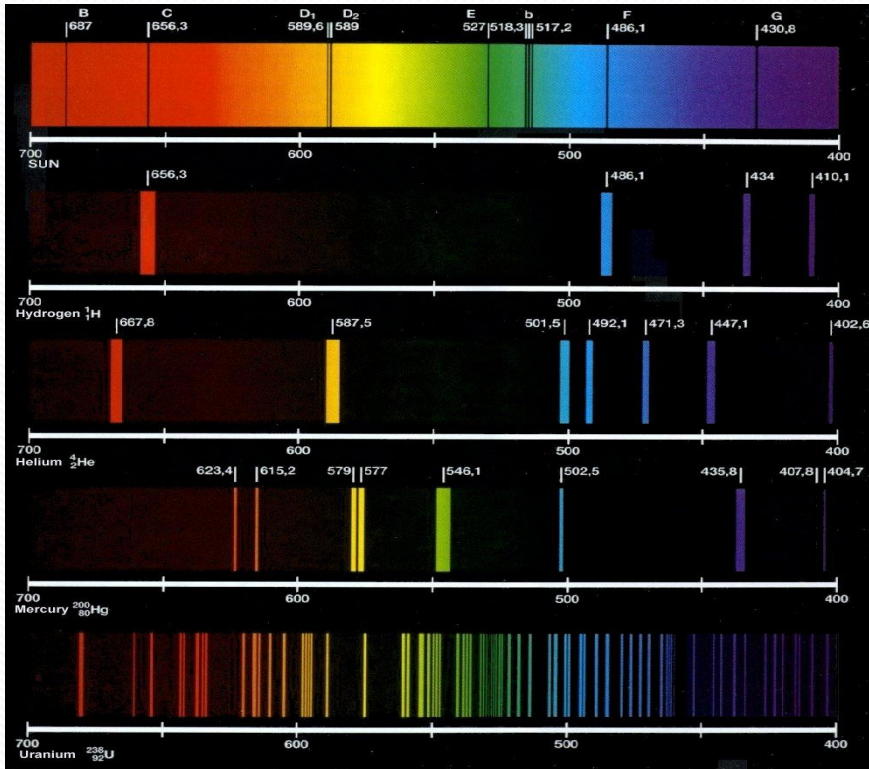
- Optical spectra
- Continuous spectra vs. quantized spectra

Where do the light come from? What do the spectra tell you?



The electron emits or absorbs the energy changing the orbits.

Atomic spectra



- Most common and natural light sources have continuous spectra.
- Atomic vapor spectra, however have discrete lines
 - *Where do the light come from? What do the spectra tell you?*
- Some exhibit simple mathematical relations: Balmer series, Lyman series, Paschen series
- Rydberg showed that all these series can be based on a “**quantized**” expression of energy:

$$E_n = -\frac{R}{n^2}$$

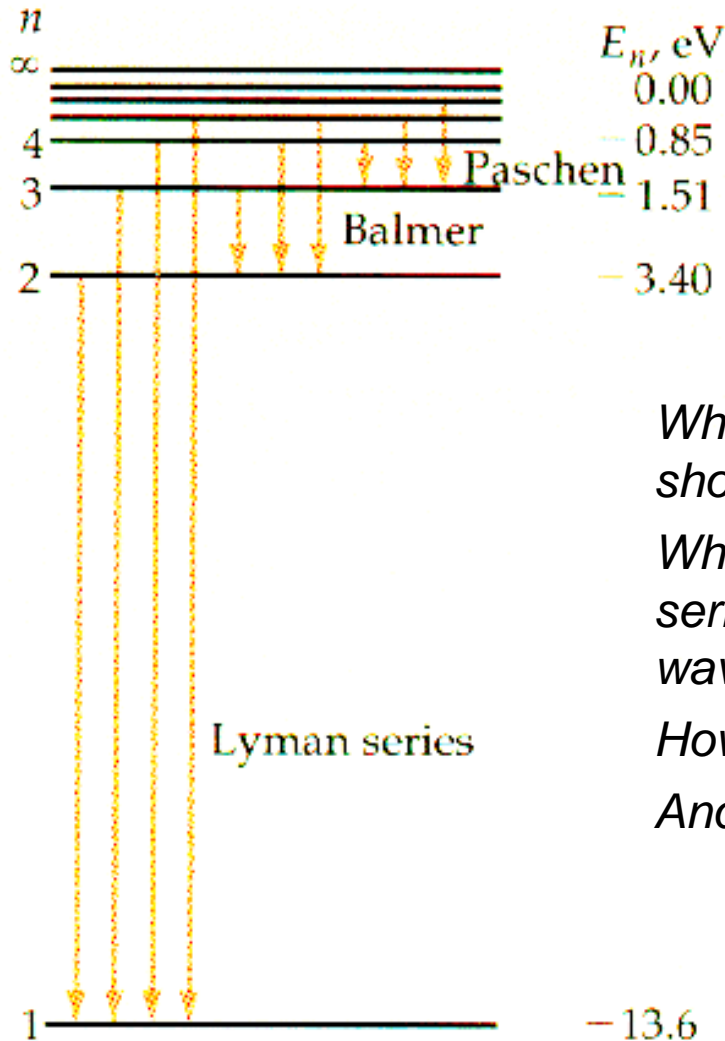
← Rydberg constant
← n = 1, 2, 3...
 quantum number

What observed is the difference energy (or transition energy):

$$E_n - E_k = R \left(\frac{1}{k^2} - \frac{1}{n^2} \right) = h\nu_{n \rightarrow k}$$

- k=2: Balmer series
- k=1: Lyman series
- k=3: Paschen

Hydrogen atom emission spectra



$$E_n - E_k = R \left(\frac{1}{k^2} - \frac{1}{n^2} \right)$$

Which series have longer wavelengths, shorter wavelengths?

What wavelength range is the Lyman series? What do we typically call that wavelength range?

How about Balmer series?

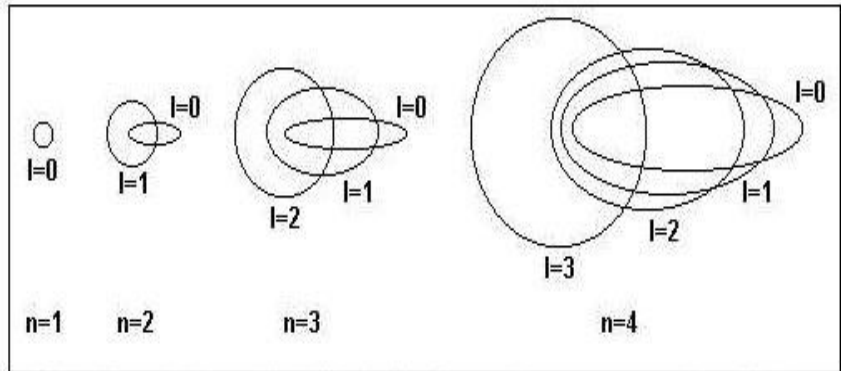
And Paschen series?

Birth of the Quantum Theory

- Evidences were mounting that energy of light, electrons in atoms are quantized
- Discovery of fundamental particles smaller than atom
- Quantized charges
- Classical physics: Newtonian mechanics, Maxwell electromagnetic theories could not account for quantum phenomena

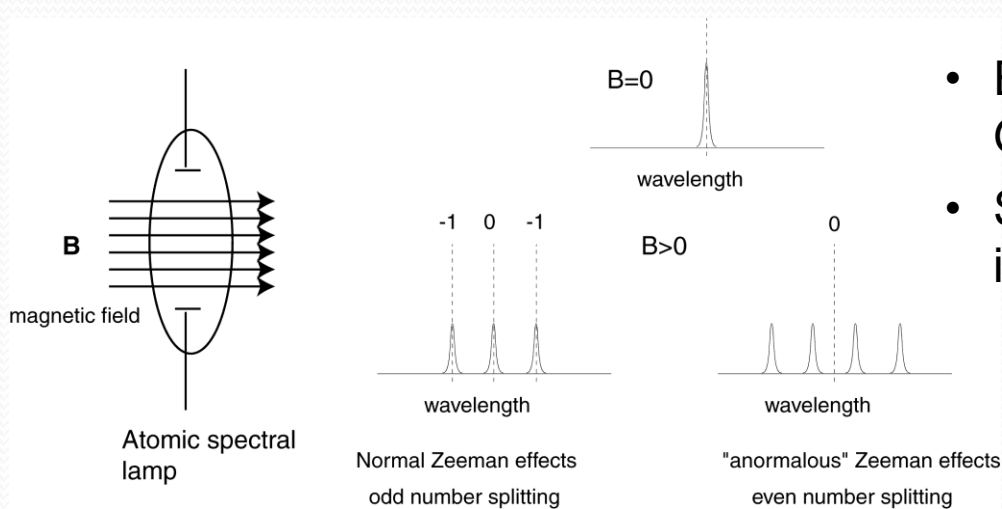
Evolution of Quantum Mechanics

- Old quantum theory: Bohr-Sommerfeld's atomic model. Newtonian mechanics for electron motion relative to the proton. Postulate: angular momentum is quantized, which leads to energy quantization and orbital quantum number
- Unfortunately, it did not take long to see that the model could not explain many other phenomena.
- Magnetic quantum number and Anomalous Zeeman effect: atomic spectral lines split under a magnetic field. The split does not conform to Bohr-Sommerfeld model.
- Discovery of electron spin. Zeeman split into even, rather than odd number of lines: anomalous Zeeman effect
- Old quantum theory appeared artificial with many postulates. Birth of the new quantum mechanical theory: DeBroglie: wave-particle duality, Heisenberg: uncertainty principle, Schroedinger: wave equation



The allowed electronic orbits for the four main quantum numbers by the Bohr-Sommerfeld model.

Anomalous Zeeman Effect



- Electron has spin $\frac{1}{2}$: Uhlenbeck & Goudsmit
- Spin-orbit coupling: $L + \frac{1}{2} \rightarrow J$ in $\frac{1}{2}$ increment: $3/2, 5/2, \dots$

If **angular orbital quantum number** is l , then the number of magnetic quantum level is:

$$m_L = -l, -l + 1, \dots, l - 1, l \quad \text{Example: } l=2, m_L=-2, -1, 0, 1, 2$$

The number of **magnetic quantum states** is $2l + 1$

What is l if the number of **magnetic quantum states** is even?

For example: 2: $2s + 1 = 2 \Rightarrow s = \frac{1}{2}$

Electron has a spin (no classical analog), and it is $1/2$

➔ **Classical theory, old quantum theory are untenable!
A new, systematic approach (not piecemeal) is needed**

Relevance of Quantum Theory to Solid State Electronics

- Essential to semiconductor physics is the concept of **energy bands (band theory)** and the energy **band-gap, density-of-state**: *explained only with quantum theory*
- Behavior of electrons (individual): **band theory** explains the electron conduction behavior in semiconductors (*classical conduction theory – Drude model – is insufficient*) – conduction in nearly-filled band: **hole model**
- Behavior of electrons (**ensemble**): **Pauli exclusion principle** and **Fermi-Dirac statistics** describes electron **ensemble statistical behavior**
- Quantum mechanical transition theory: semi-classical quantum electrodynamics (as opposed to quantum electrodynamics) explains **optical transitions** in semiconductor
- Quantization of elementary excitations in condensed matters: phonons, plasmons, excitons, and polaritons... quantum mechanical excitation and relaxation theory

A Primer to Quantum Mechanics

What is it?

It is a set of rules and equations (like Newton's laws) that allow us to calculate and predict the behavior of a quantum mechanical system

Overview of Topics

- Concept of wave-particle duality; Heisenberg uncertainty principle
- Wave mechanics: DeBroglie wavelength, electron diffraction, Schroedinger equation
- Basic concepts of wave mechanics
- Examples:
 - Quantum wells
 - The hydrogen atom
- Particle spin and statistics; Fermi-Dirac statistics

Heisenberg's uncertainty principle

- It is linked to Planck's hypothesis of quantum of action:

$$\Delta x \cdot \Delta p \geq h$$

$$\Delta E \cdot \Delta t \geq h$$

- This principle completely decouples the modern quantum mechanics from the old concept, including Bohr's model.
 - It says that it is fundamentally impossible and there is no need for a theory to be able to specify exactly the position (x) AND momentum (p) of a particle more accurately than the uncertainty given above.
 - For that matter, any other pair of quantities whose product has the unit of action (energy x time or position x momentum) obey the same principle. e. g. we know that angular momentum is quantized
-
- Heisenberg theory: matrix approach to quantum mechanics

Wave-particle duality

- De Broglie observed that an electromagnetic wave has particle-like behavior, which is the photon
- So, can a particle (such as an electron) behave like a wave?

De Broglie came up with a hypothesis (1924): the wavelength associated with a particle of momentum p is:

$$\lambda = \frac{h}{p}$$

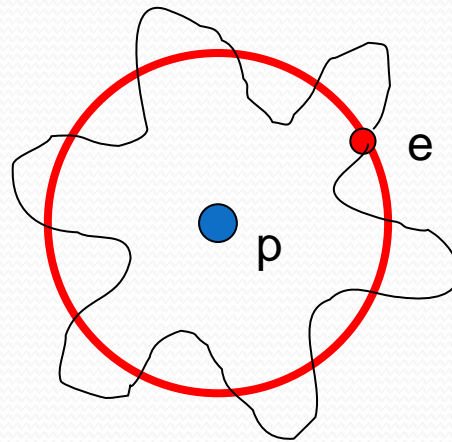
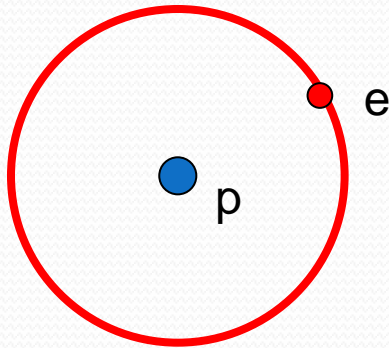
Where does this come from? He observed that for light:

$$E = mc^2 = h\nu = h\frac{c}{\lambda}$$
$$mc = \frac{h}{\lambda} \quad \text{or} \quad p_{\text{photon}} = \frac{h}{\lambda}$$

If this is the relation of photon momentum to its wavelength, then why not the same for a particle to its wavelength?

Wave-particle duality (cont.)

- As it turned out, the orbit of Bohr-Sommerfeld's atom (old quantum theory) is an exact integral multiple of the De Broglie's electron wavelength! This must be onto something, because it is such a natural explanation for the Bohr-Sommerfeld's atom quantization model



$$2\pi r = n\lambda = n\frac{h}{p}$$
$$pr = L = n\frac{h}{2\pi} = n\hbar$$

Bohr-Sommerfeld angular momentum quantization postulate explained!

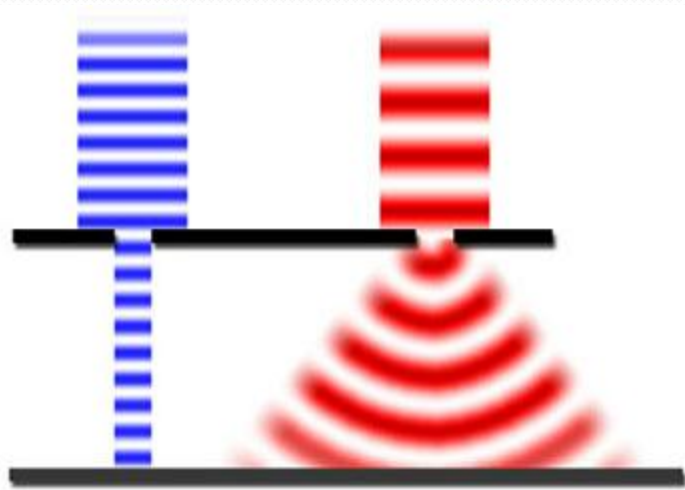
Wave-particle duality (cont.)

- This gave motivation for Schroedinger to develop a different math to model quantum mechanics: wave mechanics
- 3 years later (1927), Davidson and Germer demonstrated electron diffraction: experimentally showed that particles can indeed diffract like a wave!

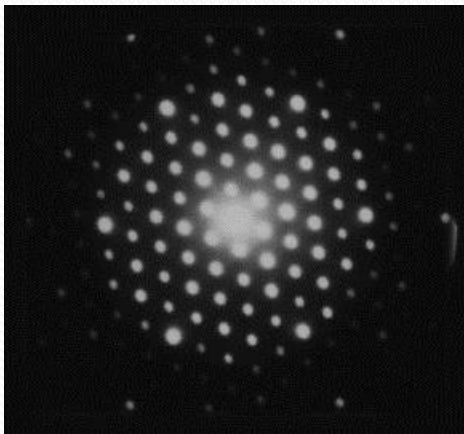
What is diffraction?

What is the difference between particle and wave?

Diffraction



Electron diffraction from a crystal



Light Diffraction by a Razor Blade

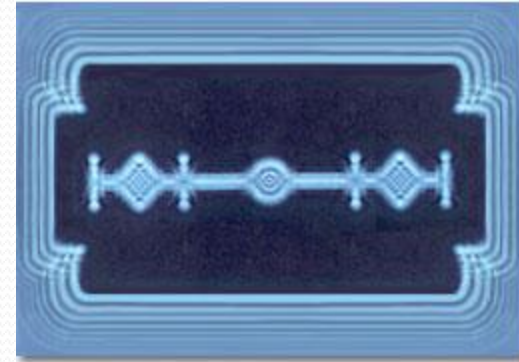
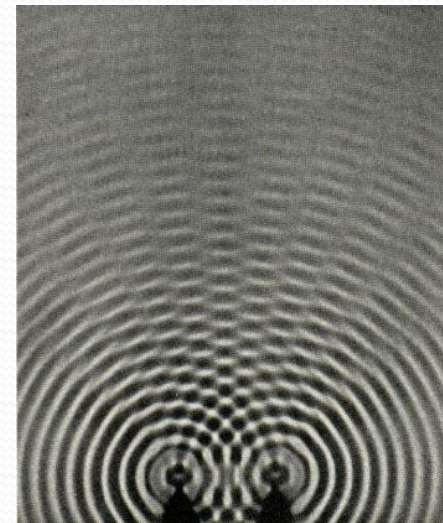


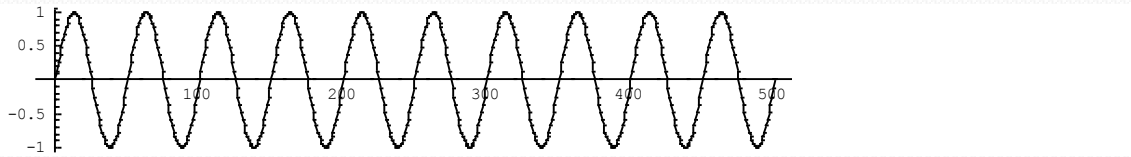
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Diffraction and Interference

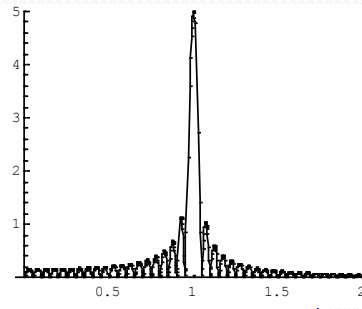
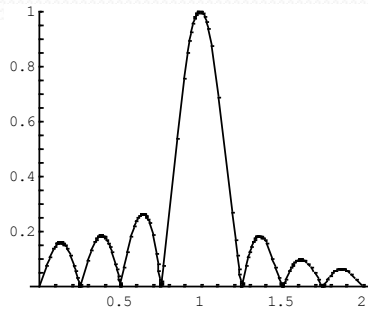
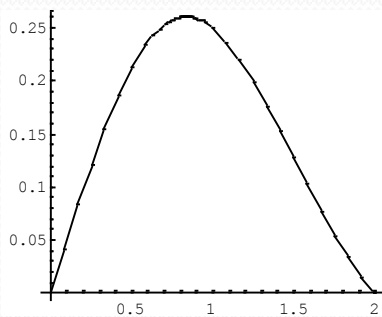


An analogy to uncertainty principle

Suppose we have a sine wave



What is its frequency?



$$\Delta \nu \cdot \Delta t \geq 1$$

$$h\Delta \nu \cdot \Delta t \geq h \Leftrightarrow \Delta E \cdot \Delta t \geq h$$

Schrodinger's equation and wave mechanics

Heisenberg's matrix-based quantum mechanics is too complicated. With De Broglie's wave theory, Schrodinger in 1926 came up with an alternative description: wave equation

The diagram shows the Schrodinger equation: $\left[\frac{\hat{\mathbf{p}}^2}{2m} + \hat{V} \right] \Psi = \hat{E} \Psi$. Red arrows point from text labels to parts of the equation: 'momentum operator' points to $\hat{\mathbf{p}}^2$; 'particle mass' points to $2m$; 'kinetic energy operator' points to the entire term $\frac{\hat{\mathbf{p}}^2}{2m}$; 'potential energy' points to \hat{V} ; 'the wave' points to Ψ ; and 'total energy operator' points to \hat{E} . A yellow dashed circle highlights the kinetic energy operator term.

$$\hat{\mathbf{p}} = \frac{\hbar}{i} \nabla \quad ; \quad \hat{V} \text{ is the potential operator (problem specific)} \quad ; \quad \hat{E} = -\frac{\hbar}{i} \frac{\partial}{\partial t}$$

What does it mean? It's an equation describing how a wave should behave. Like Maxwell's equations for EM waves

What wave is it? It's a wave from which one can extract measurable physical quantities (energy, momentum, ...) using a set of rules

What are the rules?

Wave mechanics (cont.)

What are the rules?

A physical quantity is determined only by its “expected” value, given by:

$$\bar{O}(t) = \frac{\langle \psi | \hat{O} | \psi \rangle}{\langle \psi | \psi \rangle} \equiv \frac{\int dx dy dz \psi^*(x, y, z; t) \hat{O} \psi(x, y, z; t)}{\int dx dy dz \psi^*(x, y, z; t) \psi(x, y, z; t)}$$

where \hat{O} is the operator associated with that physical quantity.

The wave itself does not necessarily have any physical meaning or is measurable

The wavefunction can be **normalized**: (if squared-integrable)

$$\int dx dy dz \psi^*(x, y, z; t) \psi(x, y, z; t) = 1$$

A common interpretation of $\psi(x, y, z; t)$ is that $|\psi(x, y, z; t)|^2$ represents the particle “probability density”.

Wave mechanics – Common basic features

- Space and time can be decoupled (solution by part)
- For the space component, many systems (problems) have eigenfunctions, which are **quantum states** associated with definite energy levels (often quantized, but not always)
- Often, they form an orthogonal basis for the vector space of all solutions
- A general solution can be expressed as a linear combination of the eigensolutions or eigenvectors
- Equivalence between Schroedinger wave mechanics and Heisenberg matrix representation: each wavefunction is a vector, and yield the matrix operators in Heisenberg representation

Example: free electron

What is a free electron?

An electron that experiences zero potential energy everywhere

The diagram shows the Schrödinger equation $\left[\frac{\hat{\mathbf{p}}^2}{2m} + \hat{\mathbf{V}} \right] \Psi = \hat{\mathbf{E}} \Psi$. Annotations include: 'momentum operator' pointing to $\hat{\mathbf{p}}^2$; 'particle mass' pointing to $2m$; 'kinetic energy operator' pointing to the entire term $\frac{\hat{\mathbf{p}}^2}{2m}$; 'potential energy' pointing to $\hat{\mathbf{V}}$; 'the wave' pointing to Ψ ; and 'total energy operator' pointing to $\hat{\mathbf{E}}$.

$\hat{\mathbf{p}} = \frac{\hbar}{i} \nabla$; $\hat{\mathbf{V}}$ is the potential operator (problemspecific) ; $\hat{\mathbf{E}} = -\frac{\hbar}{i} \frac{\partial}{\partial t}$

\mathbf{V} is zero:

$$\frac{\hat{\mathbf{p}}^2}{2m} \Psi = \hat{\mathbf{E}} \Psi \Leftrightarrow -\frac{\hbar^2}{2m} \nabla^2 \Psi = i\hbar \frac{\partial}{\partial t} \Psi$$

Example: free electron (cont.)

V is zero:

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi = i\hbar \frac{\partial}{\partial t} \Psi$$

$$\nabla^2 \Psi = -\frac{2m}{\hbar} i \frac{\partial \Psi}{\partial t}$$

Let's solve for one dimension:

$$\frac{\partial^2 \Psi}{\partial x^2} = -\frac{2m}{\hbar} i \frac{\partial \Psi}{\partial t}$$

Space-time separation:

$$\Psi = \psi(x)f(t)$$

$$f(t) \frac{\partial^2 \psi}{\partial x^2} = -\psi(x) \frac{2m}{\hbar} i \frac{\partial f}{\partial t}$$

$$\nearrow f(t) \frac{\partial^2 \psi}{\partial x^2} = -k^2 f(t) \psi(x)$$

$$\searrow -\psi(x) \frac{2m}{\hbar} i \frac{\partial f}{\partial t} = -k^2 f(t) \psi(x)$$

Example: free electron (cont.)

$$f(t) \frac{\partial^2 \psi}{\partial x^2} = -k^2 f(t) \psi(x)$$

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2 \psi(x)$$

$$-\psi(x) \frac{2m}{\hbar} i \frac{\partial f}{\partial t} = -k^2 f(t) \psi(x)$$

$$-\frac{2m}{\hbar} i \frac{\partial f}{\partial t} = -k^2 f(t)$$

$$-\frac{2m}{\hbar} i \frac{\partial f}{\partial t} = -k^2 f(t) \Rightarrow f(t) = C_1 e^{-i\hbar k^2 t / 2m}$$

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2 \psi(x) \Rightarrow \psi(x) = C_2 e^{\pm ikx}$$

$$\Psi(x, t) = \psi(x) f(t) = C e^{\pm ikx} e^{-i\hbar k^2 t / 2m}$$

$$\Psi(x, t) = C e^{i(\pm kx - (\hbar k^2 / 2m)t)}$$

Example: free electron (cont.)

$$\Psi(x, t) = C e^{i(\pm kx - (\hbar k^2 / 2m)t)} \quad \text{Is a plane wave!}$$

What is its wavelength?

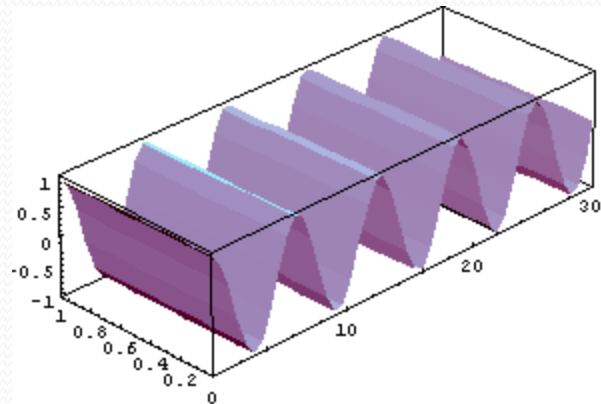
$$\Psi(x + \lambda, t) = C e^{i[\pm k(x + \lambda) - (\hbar k^2 / 2m)t]} = C e^{i[\pm kx - (\hbar k^2 / 2m)t]}$$

$$e^{i[\pm k\lambda]} = 1 \Rightarrow k\lambda = 2\pi \Rightarrow k = \frac{2\pi}{\lambda}$$

What is its frequency?

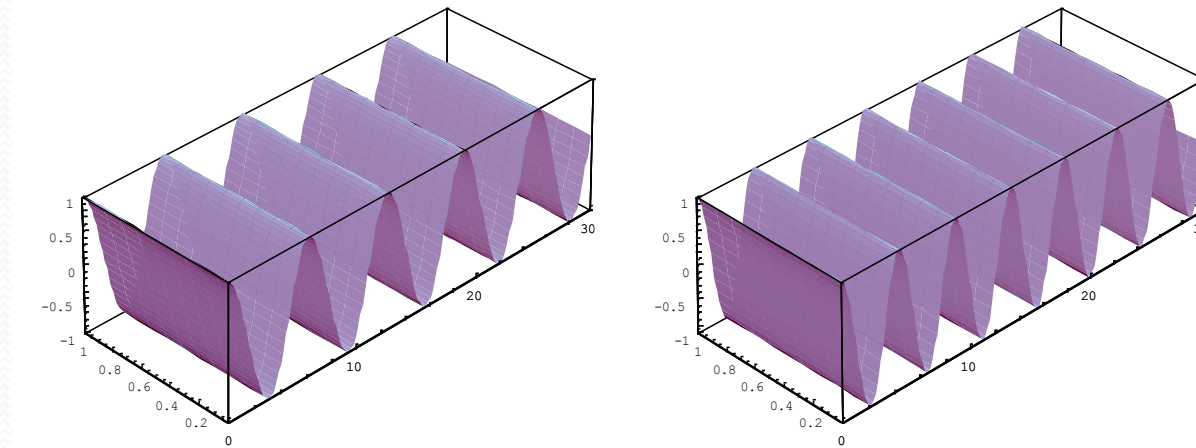
$$\omega \equiv 2\pi\nu = \frac{\hbar k^2}{2m} = \frac{1}{\hbar} \frac{\hbar^2 k^2}{2m}$$

What does it look like?



Example: free electron (cont.)

What are the differences between these two electron waves?



$$\Psi(x, t) = C e^{i(\pm kx - (\hbar k^2 / 2m)t)}$$
 is an electron plane wave!

What is its momentum? $\hat{\mathbf{p}} = \frac{\hbar}{i} \nabla \Rightarrow p_x = \frac{\hbar}{i} \frac{\partial}{\partial x}$

$$p_x = \frac{\hbar}{i} \frac{\partial}{\partial x} C e^{i[\pm kx - \omega t]} = \pm \hbar k C e^{i[\pm kx - \omega t]}$$

It's the DeBroglie's hypothesis!

$$p_x = \pm \hbar k = \pm \hbar \frac{2\pi}{\lambda} = \pm \frac{h}{\lambda}$$

Example: free electron (cont.)

$\Psi(x, t) = C e^{i(\pm kx - (\hbar k^2 / 2m)t)}$ is an electron plane wave!

What is its energy? $\hat{E} = i\hbar \frac{\partial}{\partial t} C e^{i[\pm kx - (\hbar k^2 / 2m)t]} = \frac{\hbar^2 k^2}{2m} \Psi$

$$E = \frac{\hbar^2 k^2}{2m} = \hbar\omega$$

It's the quantum hypothesis!

What is the relationship between energy and momentum?

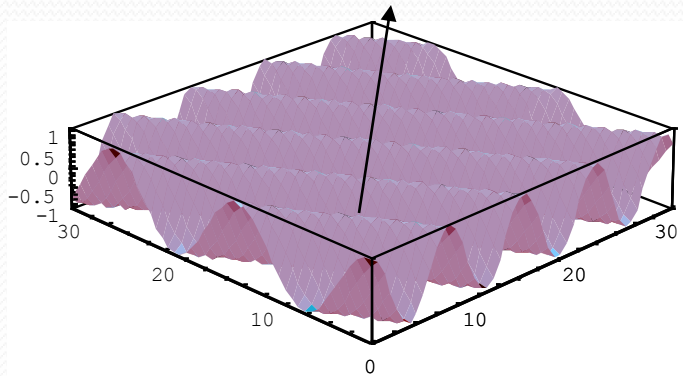
$$p = \hbar k \qquad E = \frac{\hbar^2 k^2}{2m} \qquad E = \frac{p^2}{2m}$$

Relevance of electron plane-wave to solid state electronics:

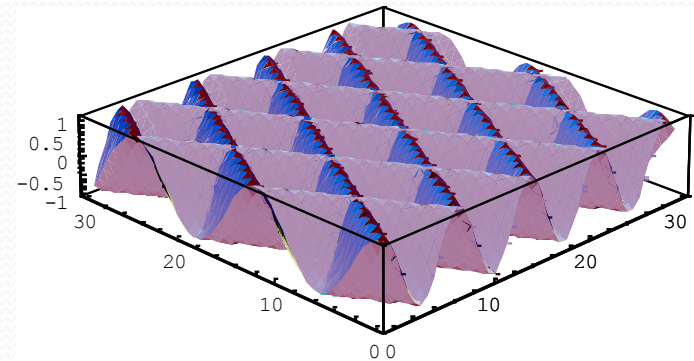
- In many crystalline semiconductors, electrons behave as if they are free (sort of!) and therefore, simple plane wave solutions can be applied in many problems
- Simple relationship between energy and momentum allows simple calculation

A small test

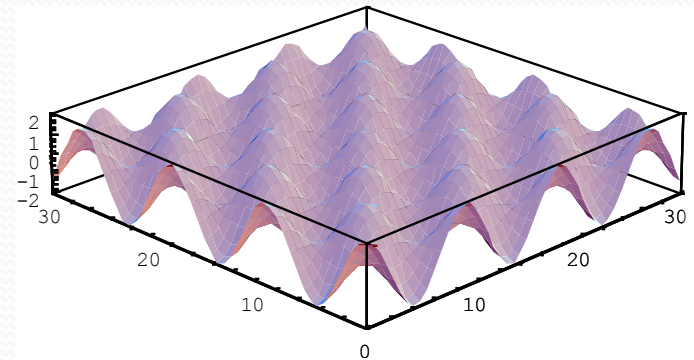
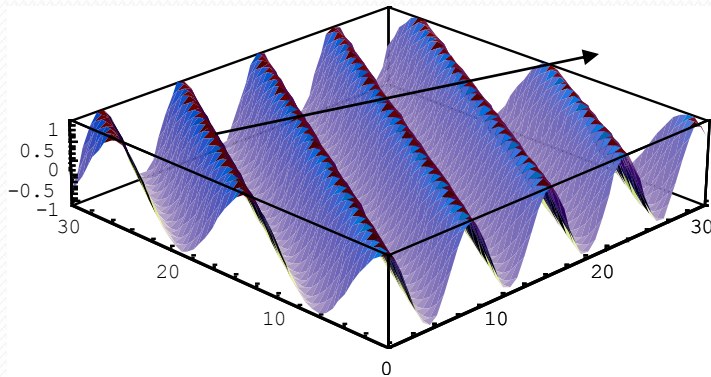
An electron wave with momentum k_1



What is the sum of the two electron waves?



An electron wave with momentum k_2



Example: semiconductor quantum well

$$E = \frac{p^2}{2m}$$

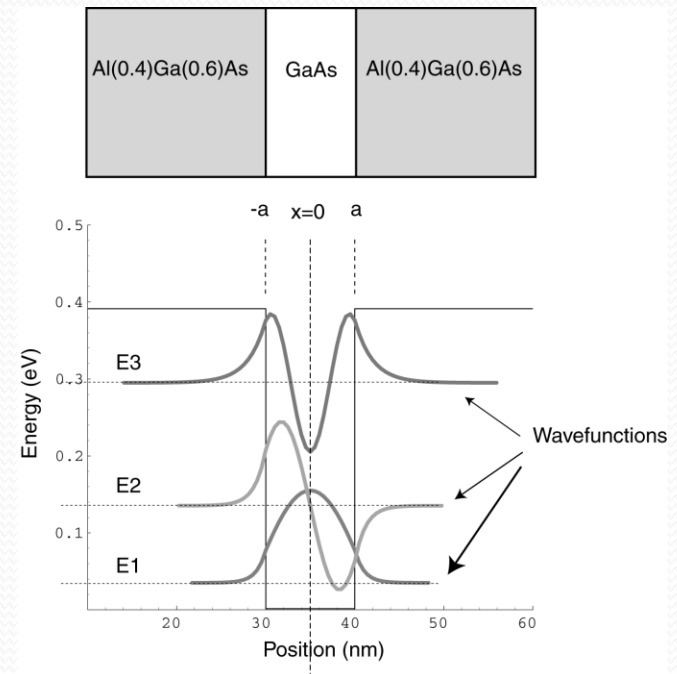
It looks like quantum mechanics produces the same results as classical mechanics for free electrons

So, why do we need quantum mechanics?

Example:

Semiconductor quantum wells

- Application: diode lasers used in printers, CD players; 2D HEMT (high-electron mobility transistor)
- Consist of layers of different semiconductor alloys
- Electrons behave like in a simple potential well, called “quantum well”



Example: hydrogen-like atom

The Schroedinger equation

$$\nabla^2 \psi + \frac{2m}{\hbar^2} \left(E + \frac{Ze^2}{r} \right) \psi = 0$$

We can get rid of constants by using the "natural" unit:

$$\text{Length: } a_B = \frac{\hbar^2}{me^2} \quad \text{Energy: } Ry = \frac{e^2}{2a_B}$$

Use spherical coordinate: it's the natural symmetry of the problem

$$\nabla^2 \psi = \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right) \psi$$

Separation of radial and angular variables

$$\psi = R(r)Y(\theta, \phi)$$

$$\frac{r^2}{R} \left(\frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} + \left(E + 2 \frac{Z}{r} \right) R \right) = J = -\frac{1}{Y} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \right]$$

Hydrogen-like atom (cont.)

$$\frac{r^2}{R} \left(\frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} + \left(E + 2 \frac{Z}{r} \right) R \right) = J = -\frac{1}{Y} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \right]$$

For the right-hand side:
$$\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} + JY = 0$$

We can separate variables again: $Y(\theta, \phi) = e^{im\phi} P(\theta)$ m is integer, *why?*

$$\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial P}{\partial \theta} \right) - \frac{m^2}{\sin^2 \theta} + JP = 0$$

As it turns out, the solution for this equation is Legendre polynomial, with the condition

$$J = l(l+1) \quad ; \quad l \text{ must be a non-negative integer} = 0, 1, 2, \dots$$

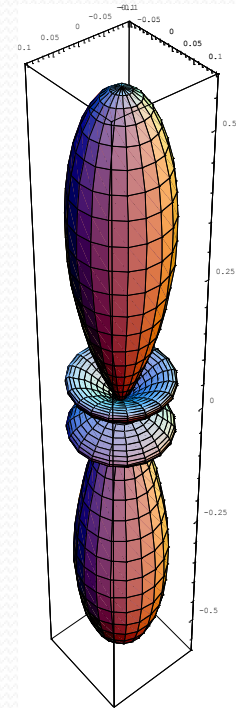
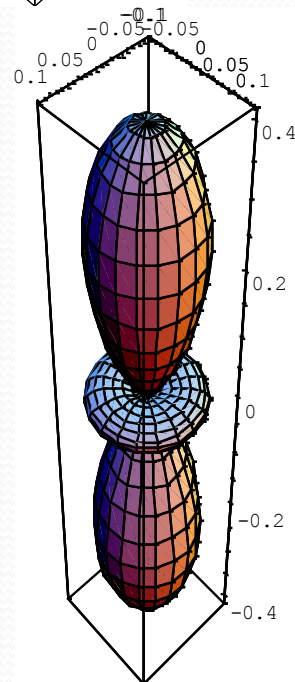
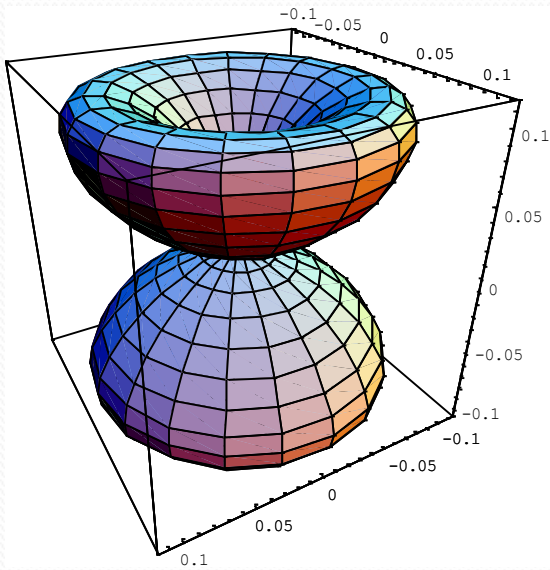
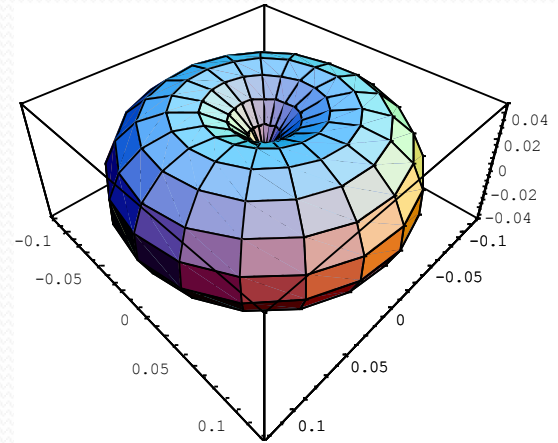
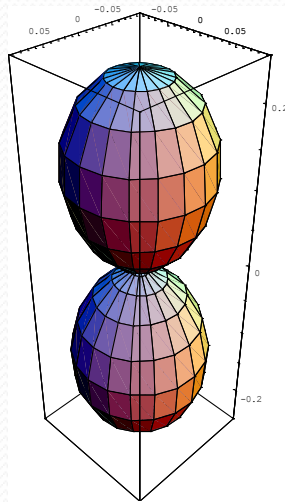
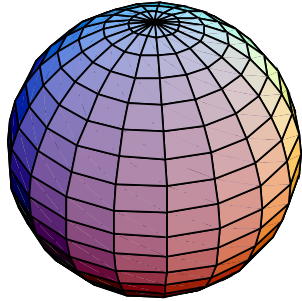
$$m \text{ must be } = -l, -l+1, \dots, l-1, l$$

Solutions for Y are called spherical harmonics:

$$Y_l^m(\theta, \phi) = \sqrt{\frac{(l-m)!}{(l+m)!} \frac{2l+1}{4\pi}} P_l^m(\cos \theta) e^{im\phi}$$

Where P is called associated Legendre polynomial

Spherical harmonics



Quantization of angular momentum

$J = l(l+1)$; l must be a non-negative integer = 0,1,2,...

m must be $= -l, -l+1, \dots, l-1, l$

l is called the **angular momentum quantum number**

m is called the **magnetic quantum number**

$$Y_l^m(\theta, \phi) = \sqrt{\frac{(l-m)!}{(l+m)!} \frac{2l+1}{4\pi}} P_l^m(\cos \theta) e^{im\phi}$$

describes the **quantum state** associated with angular momentum l and magnetic quantum number m

A quantum state can have multiple associated quantum numbers. Each quantum number usually represents a certain symmetry of the problem

Hydrogen-like atom (cont.)

$$\frac{r^2}{R} \left(\frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} + \left(E + 2 \frac{Z}{r} \right) R \right) = J = -\frac{1}{Y} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \right]$$

For the left-hand side:

$$\frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} + \left(E + 2 \frac{Z}{r} \right) R = \frac{l(l+1)}{r^2} R$$

$$\frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} + \left(E + \frac{2Z}{r} - \frac{l(l+1)}{r^2} \right) R = 0$$

The solution is:

$$R_{n,l}(r) = d_{nl} e^{-Zr/n} \left(\frac{Zr}{n} \right)^l L_{n-l-1}^{2l+1} \left(\frac{2Zr}{n} \right)$$

where L is a Laguerre polynomial, and n is a positive integer number. It is called **radial quantum number**

Most important result: E is the energy and it is:

$$E = -\frac{Z^2}{n^2} Ry$$

So, the quantum theory explains the atomic hydrogen spectra

Atomic shell structure

	0	1	2	3	4	5
	s	p	d	f	g	h
1	↓					
2	↓	→				
3	←	→	(5,10)			
4	←	←	←			
5	←	←	←	←		

For most atoms, completion of the outer most orbits:
2 S and 6 P states result in the lowest and stable
energy configuration

Particle spin and statistics

- Two types of particles: those with even spin: $J=0, 1, 2, \dots$ and those with odd spin: $J=1/2, 3/2, 5/2, \dots$
- Pauli exclusion principle: No 2 odd-spin particles can occupy the same quantum state. For even-spin particles, many particles can occupy the same quantum state
- As a result, each type has a different statistical behavior
- Even spin particles obey Bose-Einstein statistics. (Bose-Einstein condensation). They are called bosons.
- Odd-spin particles obey **Fermi-Dirac statistics**; they are called **fermions**. This statistics is essential for semiconductor theory, as we deal with electrons, which are fermions.

In a nutshell...

- Quantum theory is crucial to the understanding of semiconductors that gives us today microelectronics and optoelectronics, photonics technologies
- Yet, some aspects of electronic devices can be understood in terms of classical model concepts (*not because the classical theory is correct, but*) thanks to various quantum approximation approaches that facilitate the understandings in terms of classical behaviors (e. g. electron effective mass, holes as positive charge particles, particle diffusions,...)
- But one must be mindful of the validity limits of these approximations and Quantum theory must be applied when appropriate