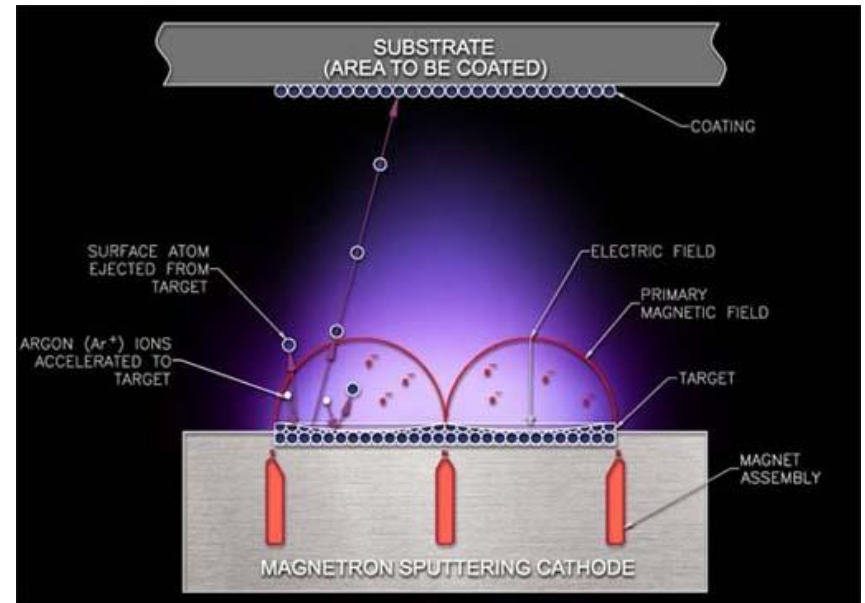


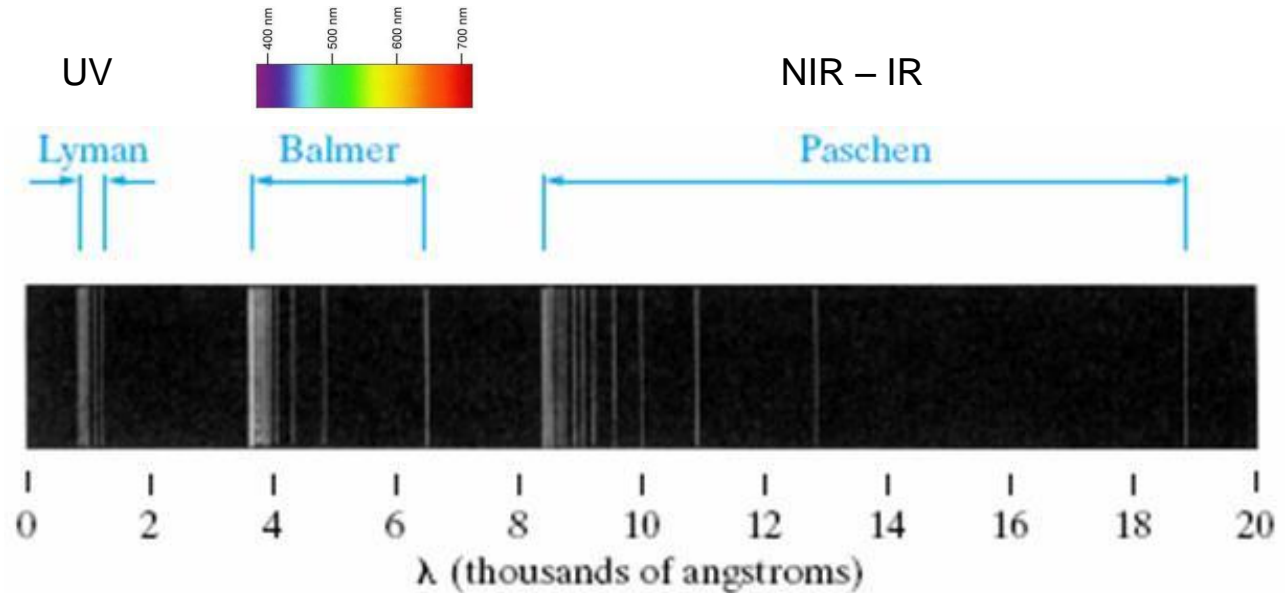
Atomic Spectra

One of the most valuable experiments of modern physics is the analysis of *absorption and emission of light by atoms*. We see this effect in a neon sign, or inside the deposition chamber of a sputtering system.



Atomic Spectra

If the *intensity of the emitted light is measured as a function of wavelength*, one finds a series of sharp lines rather than a continuous distribution of wavelengths.



Some important lines in the **emission spectrum of hydrogen**.

The lines in this figure represent the positions of observed emission peaks on the wavelength scale and they appear in several groups labeled the **Lyman, Balmer, and Paschen series** after those early investigators.

Once the hydrogen spectrum was established, scientists noticed several interesting relationships among the lines. The various series in the spectrum were observed to follow certain empirical forms:

$$\text{Lyman: } \nu = cR \left[\frac{1}{1^2} - \frac{1}{n^2} \right] \quad n = 2, 3, 4, \dots$$

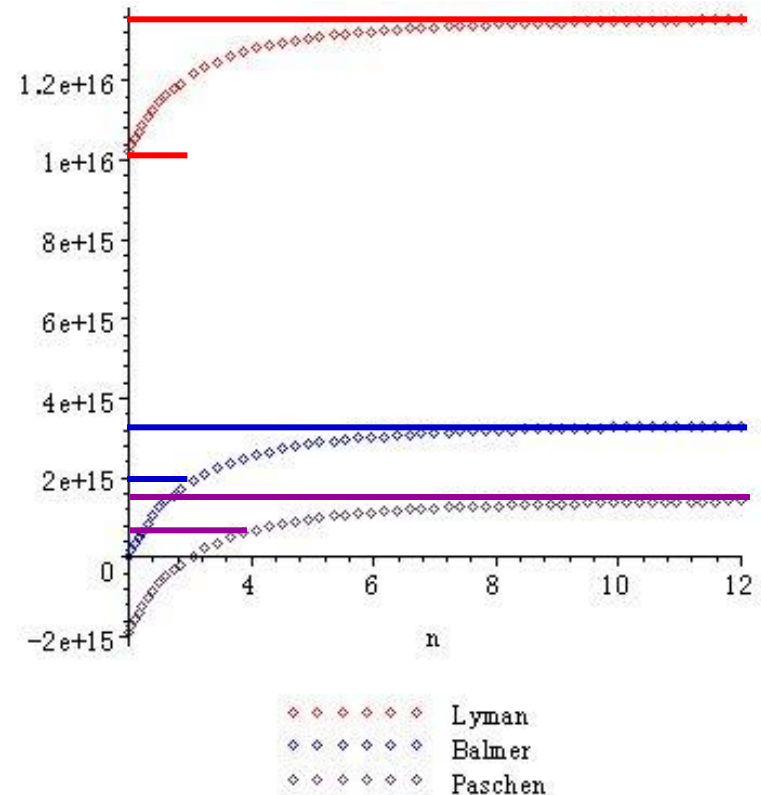
$$\text{Balmer: } \nu = cR \left[\frac{1}{2^2} - \frac{1}{n^2} \right] \quad n = 3, 4, 5, \dots$$

$$\text{Paschen: } \nu = cR \left[\frac{1}{3^2} - \frac{1}{n^2} \right] \quad n = 4, 5, 6, \dots$$

R = Rydberg constant ($R = 109,678 \text{ cm}^{-1}$).

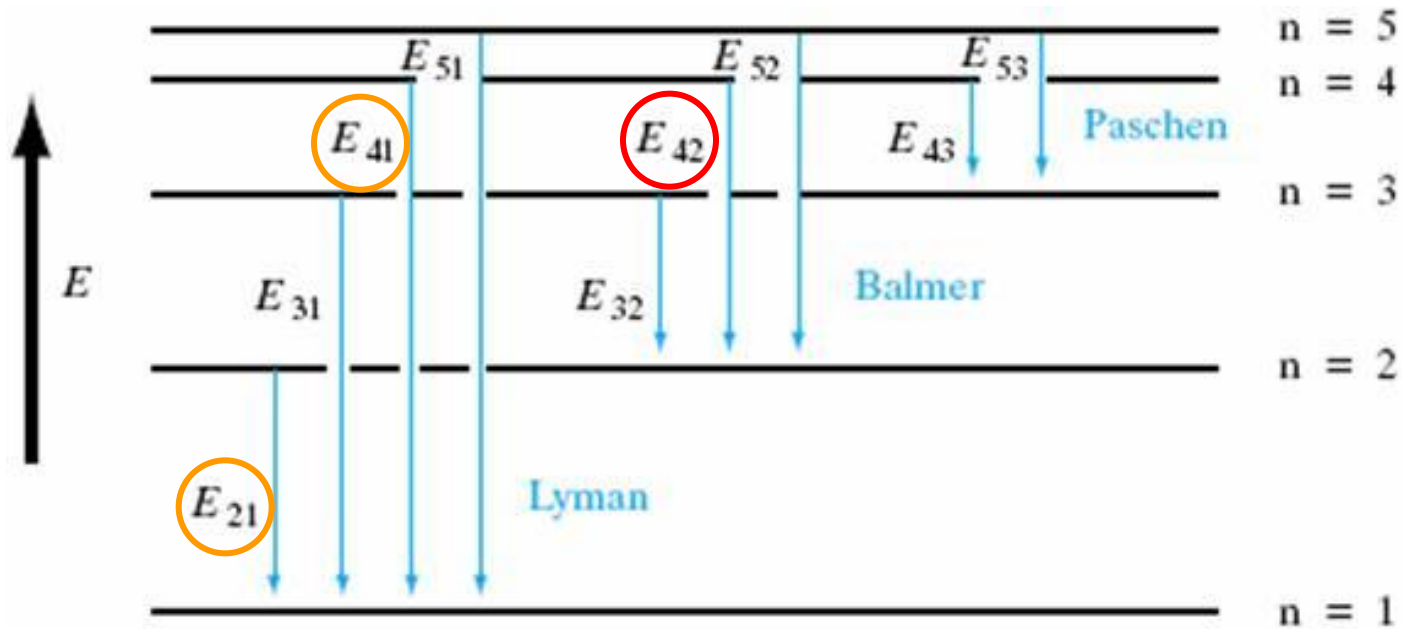
Photon energy $h\nu$ is related to wavelength by:

$$E = h\nu = \frac{hc}{\lambda}$$



Photon energies $h\nu$ plotted for successive values of the integer n .

If the photon energies $h\nu$ are plotted for successive values of the integer n , we notice that each energy can be obtained by taking sums and differences of other photon energies in the spectrum. For example, E_{42} in the Balmer series is the difference between E_{41} and E_{21} in the Lyman series.

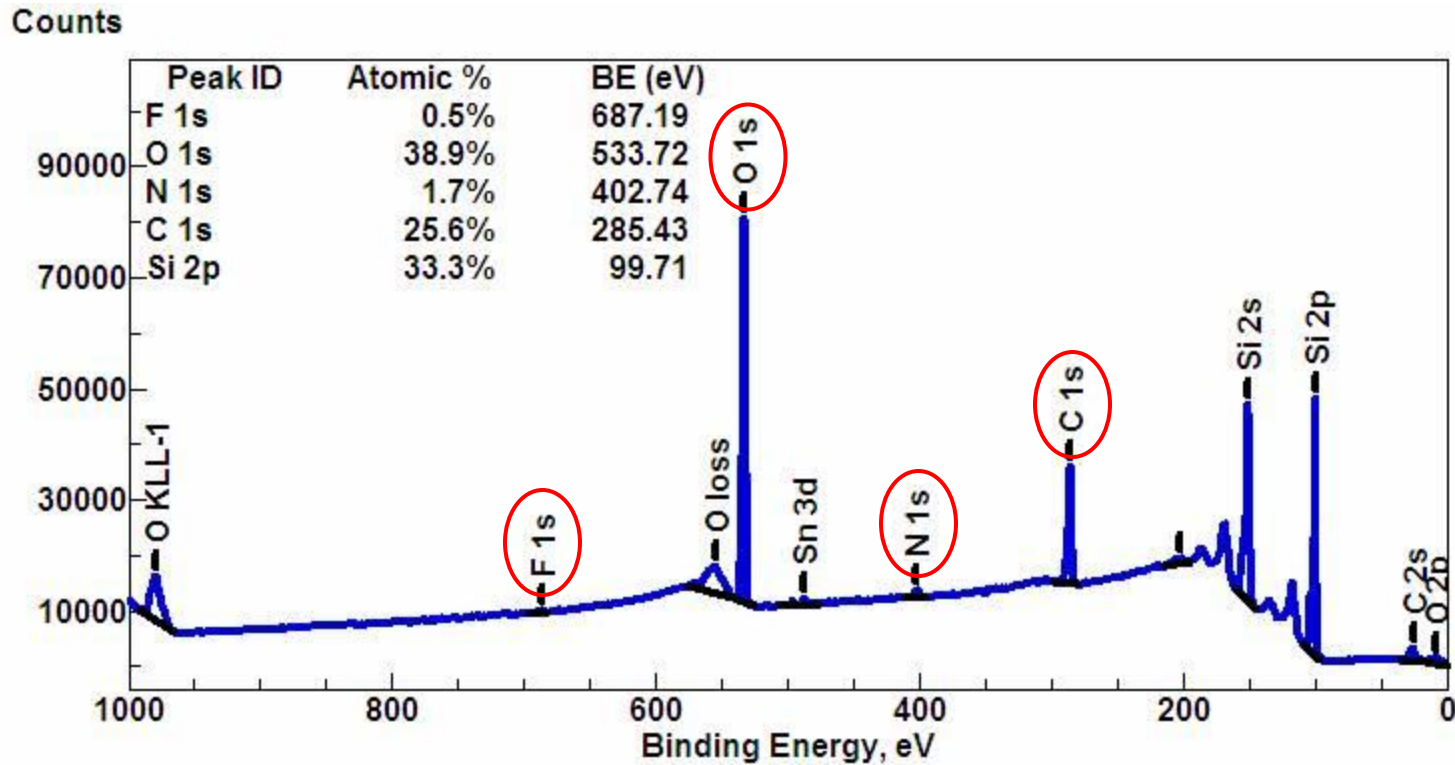


Relationships among photon energies in the hydrogen spectrum.

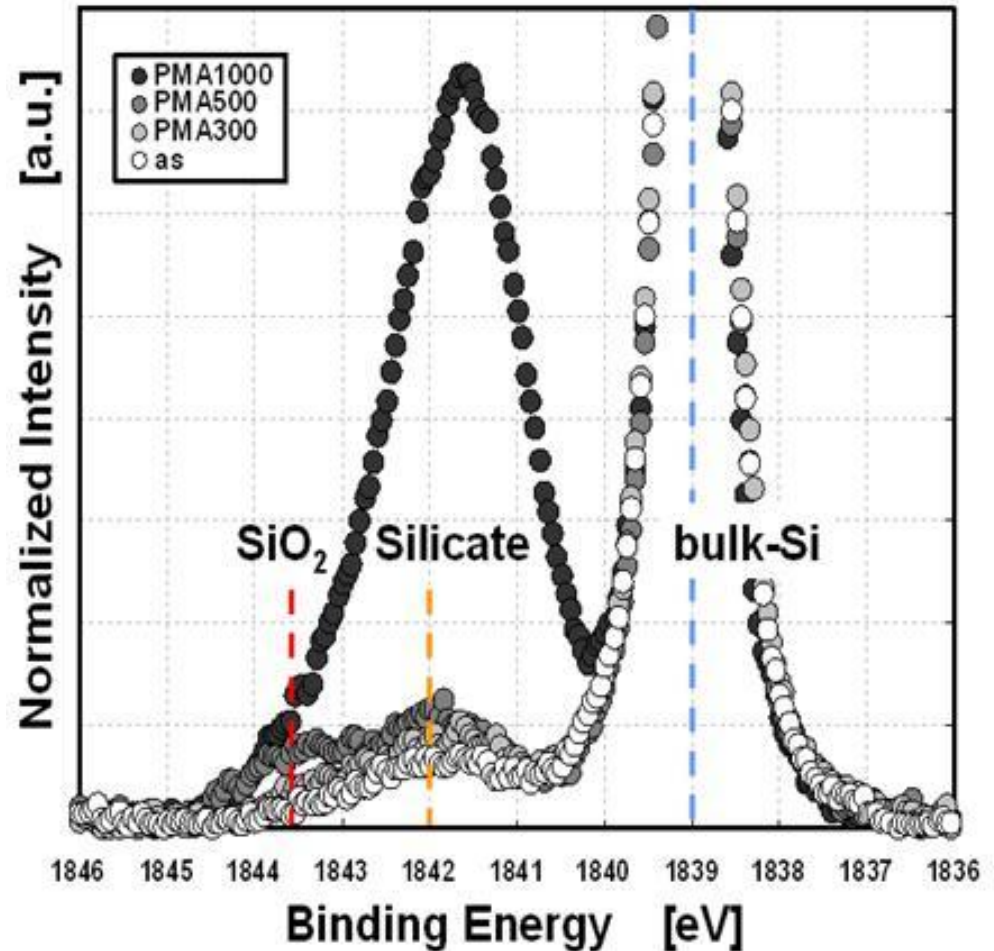
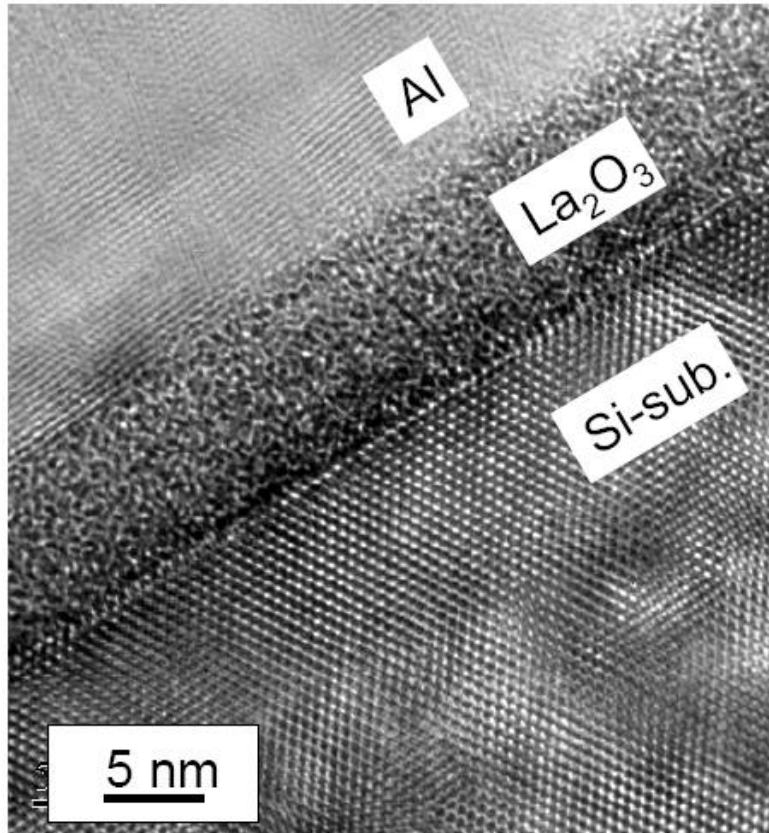
This relationship among the various series is called the **Ritz combination principle**.

X-ray photoelectron spectroscopy (XPS) is a quantitative spectroscopic technique that measures the elemental composition, empirical formula, chemical state and electronic state of the elements that exist within a material.

XPS spectra are obtained by irradiating a material with a beam of aluminium or magnesium X-rays while simultaneously measuring the kinetic energy (KE) and number of electrons that escape from the top 1 to 10 nm of the material being analyzed. XPS requires ultra-high vacuum (UHV) conditions.



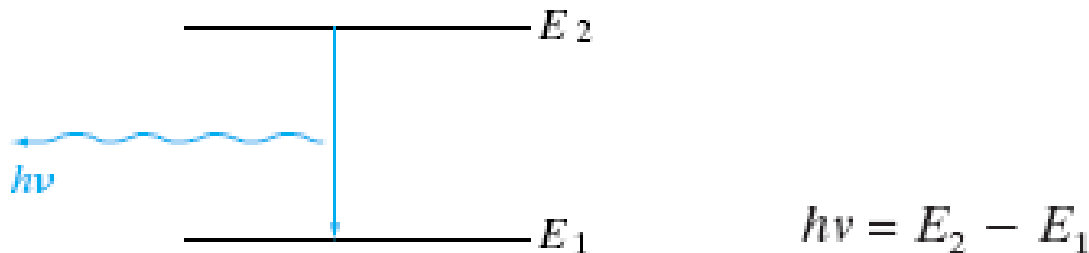
X-ray photoelectron spectroscopy (XPS) is a quantitative spectroscopic technique that measures the elemental composition, empirical formula, chemical state and electronic state of the elements that exist within a material.



The Bohr atomic model

The results of emission spectra experiments led Niels Bohr to construct a *model for the hydrogen atom*, based on the mathematics of planetary systems. To develop the model, Bohr made several postulates:

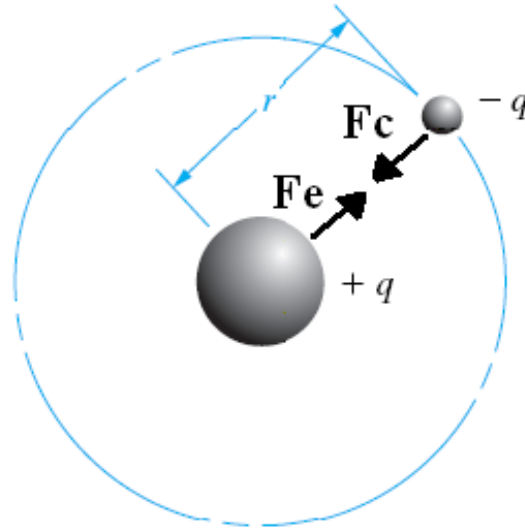
1. Electrons exist in certain stable, circular orbits around the nucleus.
2. The electron may shift to an orbit of higher or lower energy, thereby gaining or losing energy equal to the difference in the energy levels (by absorption or emission of a photon of energy $h\nu$).



3. The angular momentum p_θ of the electron in an orbit is always an integral multiple of Planck's constant divided by 2π ($h/2\pi$ is often abbreviated \hbar for convenience): $p_\theta = n \hbar$, $n = 1, 2, 3, 4, \dots$

The Bohr atomic model

If we visualize the electron in a stable orbit of radius r around the proton of the hydrogen atom, we can equate the *electrostatic force* between the charges to the *centripetal force*:



$$F_e = F_c$$

$$-\frac{q^2}{Kr^2} = -\frac{mv^2}{r} \quad (2-6)$$

where $K = 4\pi\epsilon_0$ in MKS units,
 m is the mass of the electron,
and v is its velocity.

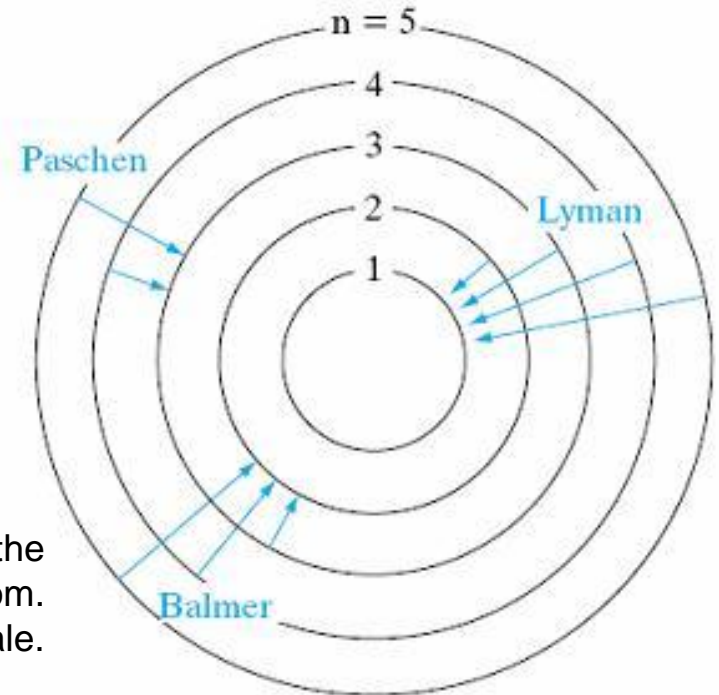
The Bohr atomic model

The total energy of the electron in the n^{th} orbit is:

$$E_n = \text{K. E.} + \text{P. E.} = -\frac{mq^4}{2K^2n^2\hbar^2}$$

$$E_n \propto (1/n^2)$$

Electron orbits and transitions in the Bohr model of the hydrogen atom. Orbit spacing is not drawn to scale.



- Whereas the Bohr model accurately describes the gross features of the hydrogen spectrum, it does not include many fine points. However, the partial success of the Bohr model was an important step toward the eventual development of the quantum theory.
- The concept that **electrons are quantized in certain allowed energy levels**, and the **relationship of photon energy and transitions between levels**, is a very important result that had been established firmly by the Bohr theory.

Quantum mechanics

The principles of quantum mechanics were developed from two different points of view at about the same time (the late 1920s). One approach, developed by **Heisenberg**, utilizes the mathematics of matrices and is called *matrix mechanics*. Independently, **Schrödinger** developed an approach utilizing a wave equation, now called *wave mechanics*.

Probability and the Uncertainty Principle

- In any measurement of the *position and momentum of a particle*, the uncertainties in the two measured quantities will be related by

$$(\Delta x) (\Delta p_x) \geq \hbar/2$$

- Similarly, the uncertainties in an *energy measurement* will be related to the uncertainty in the *time at which the measurement was made* by

$$(\Delta E) (\Delta t) \geq \hbar/2$$

$$\hbar = \frac{h}{2\pi} = 1.054\,571\,628(53) \times 10^{-34} \text{ J s} = 6.582\,118\,99(16) \times 10^{-16} \text{ eV s.}$$

- These limitations indicate that *simultaneous measurement of position and momentum or of energy and time are inherently inaccurate to some degree*. Of course, Planck's constant h is a rather small number (6.63×10^{-34} J-s), and we are not concerned with this inaccuracy in the measurement of Δx and Δp_x for a truck, for example.
- On the other hand, measurements of the *position of an electron and its speed* are seriously limited by the uncertainty principle.
- One implication of the uncertainty principle is that we cannot properly speak of *the* position of an electron, for example, but must look for the *“probability” of finding an electron at a certain position*.

The Schrödinger wave equation

- There are several ways to develop the wave equation by applying quantum concepts to various classical equations of mechanics. One of the simplest approaches is to consider a few basic postulates, develop the wave equation from them, and rely on the accuracy of the results to serve as a justification of the postulates.

1. Each particle in a physical system is described by a *wave function* $\Psi(x, y, z, t)$. This function and its space derivative ($\partial \Psi / \partial x + \partial \Psi / \partial y + \partial \Psi / \partial z$) are continuous, finite, and single valued.
2. In dealing with classical quantities such as energy E and momentum p , we must *relate these quantities with abstract quantum mechanical operators* defined in the following way:

Classical variable	Quantum operator
x	x
$f(x)$	$f(x)$
$p(x)$	$\frac{\hbar}{j} \frac{\partial}{\partial x}$
E	$-\frac{\hbar}{j} \frac{\partial}{\partial t}$

and similarly for the other two directions.

Such operators arise because in quantum mechanics you are describing nature with waves (the wavefunction) rather than with discrete particles whose motion and dynamics can be described with the deterministic equations of Newtonian physics.

3. The *probability of finding a particle with wave function Ψ* in the volume $dx dy dz$ is $\Psi^* \Psi dx dy dz$. The product $\Psi^* \Psi$ is normalized so that:

$$\int_{-\infty}^{\infty} \Psi^* \Psi dx dy dz = 1$$

Once we find the wave function Ψ for a particle, we can calculate its average position, energy, and momentum, within the limits of the uncertainty principle. Thus, a major part of the effort in quantum calculations involves solving for Ψ within the conditions imposed by a particular physical system. **The probability density function is $\Psi^* \Psi = |\Psi|^2$.**

Physical meaning of the wave function

For example, in an atom with a single electron, such as hydrogen or ionized helium, the *wave function of the electron* provides a complete description of how the electron behaves.

- The classical equation for the energy of a particle can be written:

Kinetic energy + potential energy = total energy

$$\frac{1}{2m} p^2 + V = E$$

- By using the quantum operators in three dimensions the equation is

$$\boxed{-\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi = -\frac{\hbar}{j} \frac{\partial \Psi}{\partial t}} \quad (2-24)$$

where $\nabla^2 \Psi$ is

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2}$$

- and the time-independent equation,

$$\boxed{\frac{d^2 \psi(x)}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)] \psi(x) = 0} \quad (2-27)$$

Problem: The potential well

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)]\psi(x) = 0 \quad (2-27)$$

It is quite difficult to find solutions to the Schrödinger equation for most realistic potential fields. The simplest problem is the potential energy well with infinite boundaries. Let us assume a particle is trapped in a potential well with $V(x)$ zero except at the boundaries $x = 0$ and L , where $V(x)$ it is infinitely large:

$$V(x) = 0, \quad 0 < x < L$$
$$V(x) = \infty, \quad x = 0, L$$

Inside the well we set $V(x) = 0$ in Eq. (2-27):

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} E\psi(x) = 0, \quad 0 < x < L$$



Problem: The potential well

Possible solutions to the previous eq. are $\sin kx$ and $\cos kx$, where k is $[2mE]^{1/2}/\hbar$. In choosing a solution, however, we must examine the boundary conditions. The only allowable value of Ψ at the walls is zero. Otherwise, there would be a nonzero $|\Psi|^2$ outside the potential well, which is impossible because a particle cannot penetrate an infinite barrier. Therefore, we must choose only the $\sin kx$ solution and define k such that $\sin kx$ goes to zero at $x=L$:

$$\psi = A \sin kx \quad k = \frac{\sqrt{2mE}}{\hbar}$$

Each “particle” is represented by a wavefunction $\Psi(\text{position, time})$ such that: $\Psi^*\Psi$ represents the probability of finding the particle at that position at that time.

If Ψ is to be zero at $x=L$, then k must be some integral multiple of π/L .

$$\longrightarrow k = \frac{n\pi}{L}, \quad n = 1, 2, 3, \dots \quad (2-31)$$

From the former equations we can solve for the total energy E_n for each value of the integer n :

$$\frac{\sqrt{2mE_n}}{\hbar} = \frac{n\pi}{L} \quad (2-32)$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \quad (2-33)$$

Problem: The potential well

Thus for each allowable value of n the particle energy is described by Eq. (2-33). We notice that the *energy is quantized*. Only certain values of energy are allowed. The integer n is called a *quantum number*; the particular wave function Ψ_n and corresponding energy state E_n describe the quantum state of the particle.

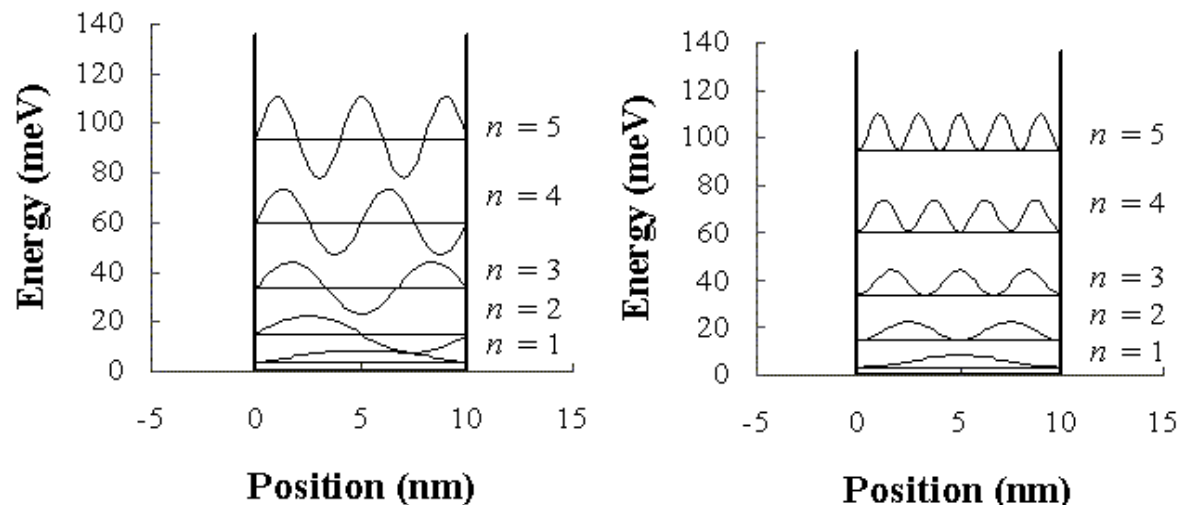
The constant A is found from postulate 3:

$$\int_{-\infty}^{\infty} \psi^* \psi dx = \int_0^L A^2 \left(\sin \frac{n\pi}{L} x \right)^2 dx = A^2 \frac{L}{2} \quad (2-34)$$

Setting Eq. (2-34) equal to unity we obtain

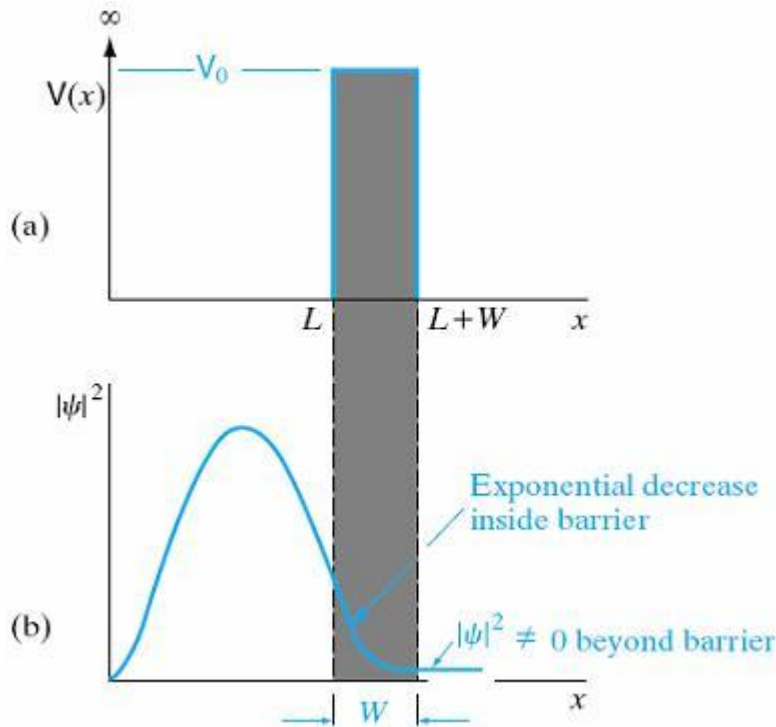
$$A = \sqrt{\frac{2}{L}}, \quad \psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x \quad (2-35)$$

The first three wave functions ψ_1, ψ_2, ψ_3 are sketched in Fig. 2-5b. The probability density function $\psi^* \psi$, or $|\psi|^2$, is sketched for ψ_2 in Fig. 2-5c.



Topic: Quantum mechanical tunneling

The wave functions are relatively easy to obtain for the potential well with infinite walls, since the boundary conditions force ψ to zero at the walls. A slight modification of this problem illustrates a principle that is very important in some solid state devices—the *quantum mechanical tunneling of an electron through a barrier of finite height and thickness*.



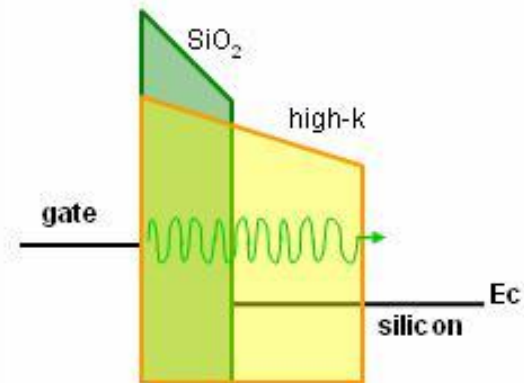
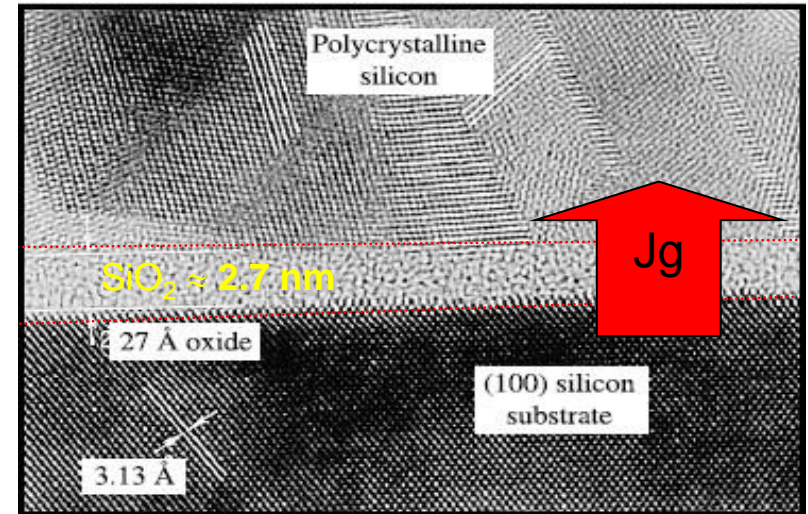
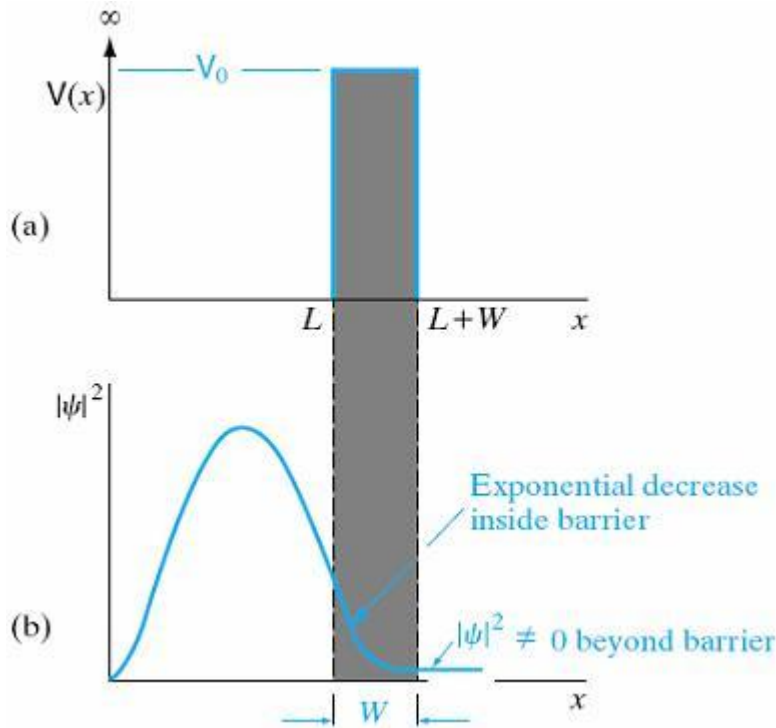
The mechanism by which the particle “penetrates” the barrier is called tunneling and this is an important effect only over very small dimensions.

If the barrier is not infinite, the boundary conditions do not force ψ to zero at the barrier. Instead, we must use the condition that ψ and its slope $d\psi/dx$ are continuous at each boundary of the barrier. Thus ψ must have a nonzero value within the barrier and also on the other side.

Since ψ has a value to the right of the barrier, $\psi^*\psi$ exists there also, implying that there is some probability of finding the particle beyond the barrier. We notice that the particle does not go over the barrier; its total energy is assumed to be less than the barrier height V_0 .

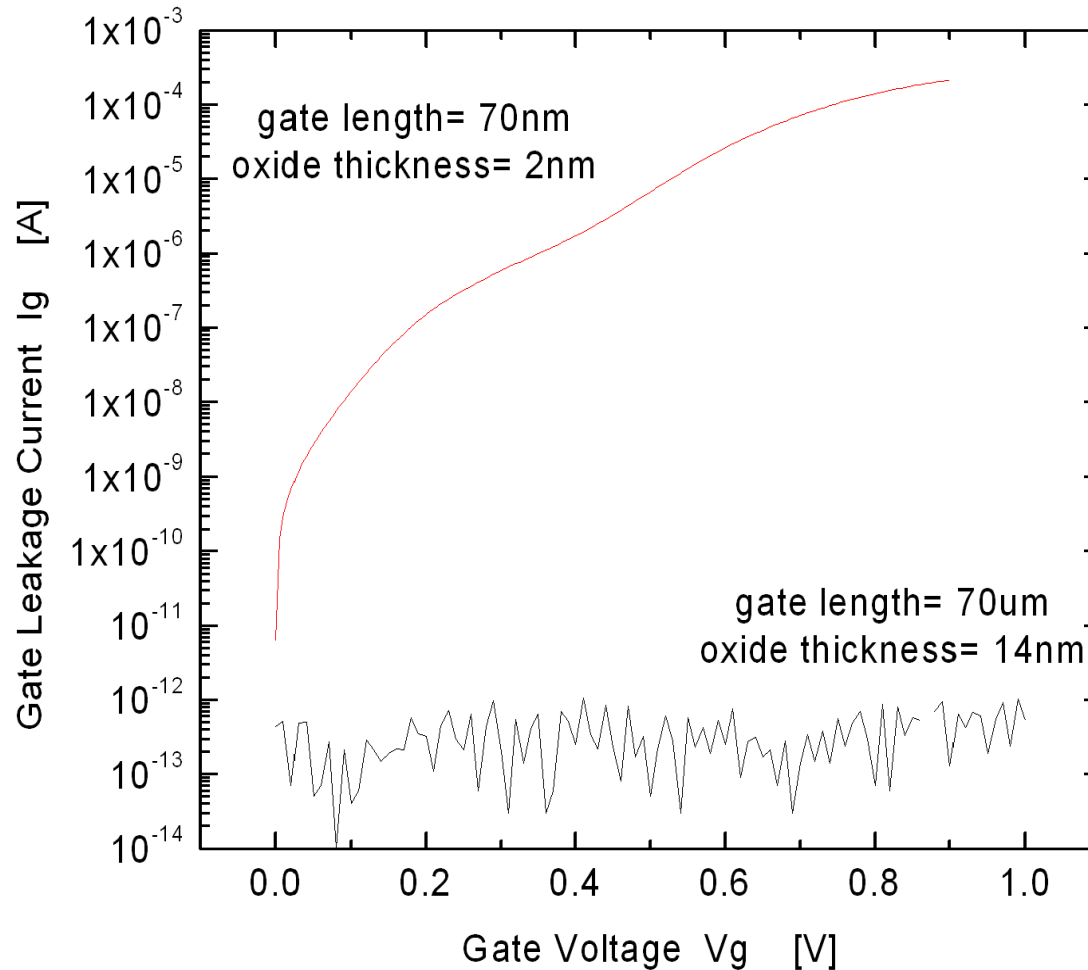
Topic: Quantum mechanical tunneling

By making the thickness W greater, we can reduce ψ on the right-hand side to the point that negligible tunneling occurs.



Topic: Quantum mechanical tunneling

Gate leakage current for long and short-channel MOSFET devices



Topic: Quantum mechanical tunneling

$J_g = 6.4 \times 10^{-3} \text{ A/cm}^2 \text{ @ EOT} = 0.47 \text{ nm}$

