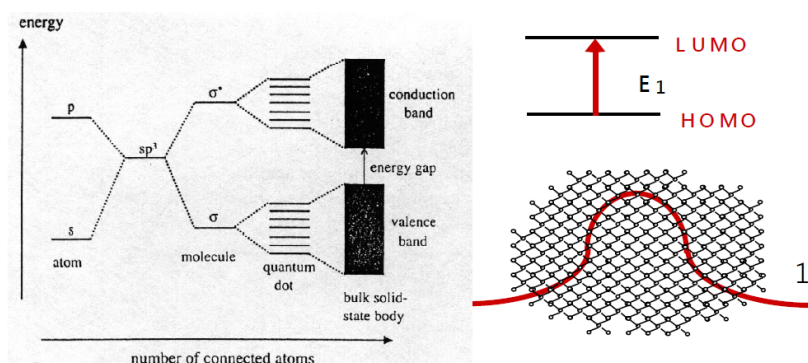


5. Quantum Nature of the Nano-world (Fundamental of Quantum mechanics)

What is the definition of nanomaterials ??

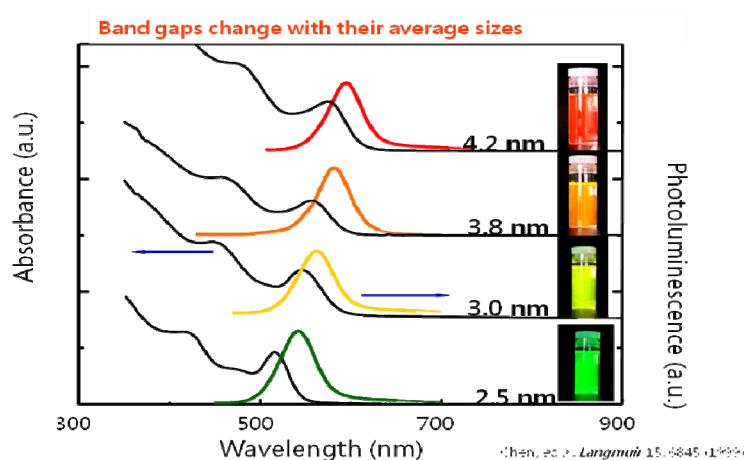
- (i) **Original:** “[quantum](#) size effect” where the electronic properties of solids are altered with great reductions in particle size
- (ii) **New (by European Union):** On 18 October 2011, the [European Commission](#) adopted the following definition of a nanomaterial:^[2]
A natural, incidental or manufactured material containing particles, in an unbound state or as an aggregate or as an agglomerate and where, for 50% or more of the particles in the number size distribution, one or more external dimensions is in the size range $1\text{ nm} - 100\text{ nm}$.

Quantum confinement effect



$$E(R) = E_g + \frac{\hbar^2 \pi^2}{2 R^2} \left[\frac{1}{m_e} + \frac{1}{m_h} \right] - \frac{1.8 e^2}{\epsilon R}$$

m_e and m_h : effective masses
 ϵ : bulk optical dielectric coefficient



Need to consider the effect of Quantum Mechanics !!

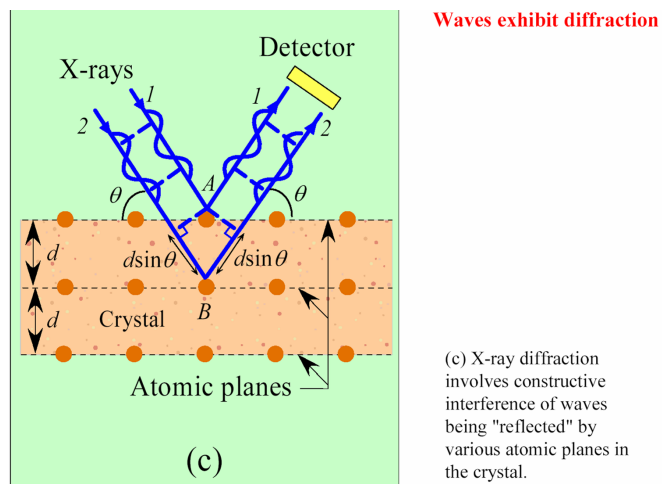
Elementary Quantum Mechanics

1. Matter Wave (by de Broglie)
2. Schrodinger equation
3. Partical in a box
4. Hyrdogen atoms

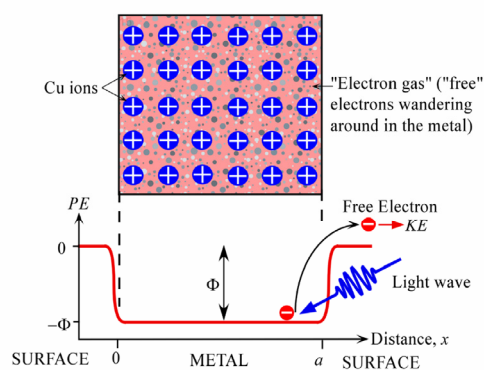
Matter Wave

Duality of Light: Wave or Particle

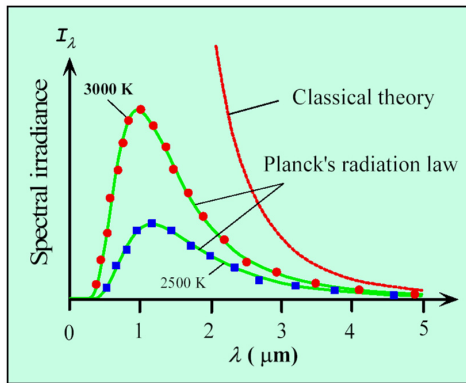
Wave: Diffraction, EM wave



Particle: Photoelectric effect, Blackbody radiation, Compton effect

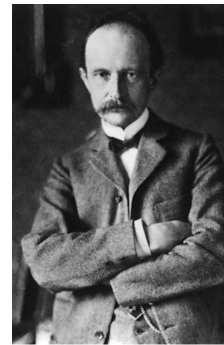
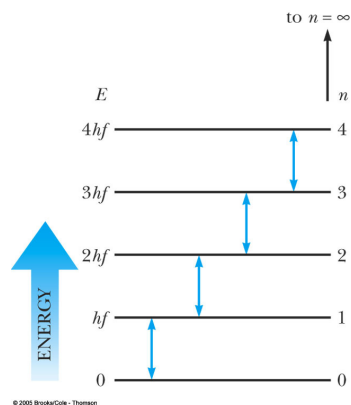


The PE of an electron inside the metal is lower than outside by an energy called the workfunction of the metal. Work must be done to remove the electron from the metal.



What did Plank do ??? (Quantization of energy OR Quanta)

Classical: $\overline{E} = kT$ (continuous)



Planck: $E = nhf$ (discrete), $n=0,1,2,3,\dots$

The result is consistent with experimental observation !!!

Planck's law: $E = nhf$ (discrete), $n=0,1,2,3,\dots$

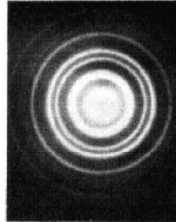
Duality of Matters:

1. Matter Wave (by de Broglie)

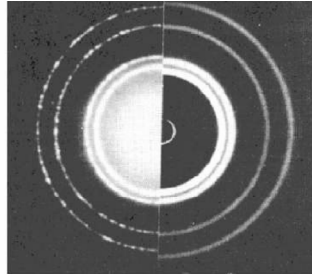
For a photon, $E = hf = pc$, $c = f\lambda$

$$p = \frac{h}{\lambda} (\text{wave} \rightarrow \text{particle})$$

$$\lambda = \frac{h}{p} (\text{particle} \rightarrow \text{wave})$$



(c) Electron diffraction pattern obtained by G. P. Thomson using a gold foil target.



(d) Composite photograph showing diffraction patterns produced with an aluminum foil by X-rays and electrons of similar wavelength. Left: X-rays of $\lambda = 0.071 \text{ nm}$. Right: Electrons of energy 600 eV.

The particle nature of matter(old quantum mechanics)

Thomson's model

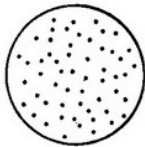
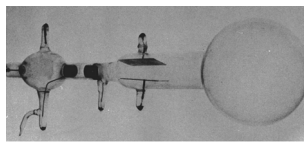


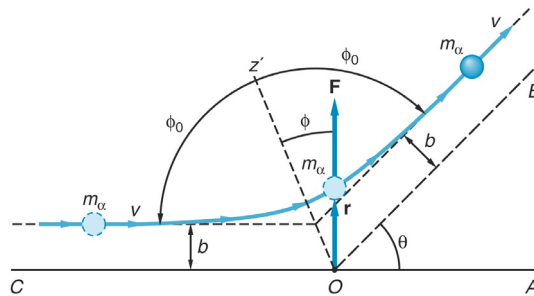
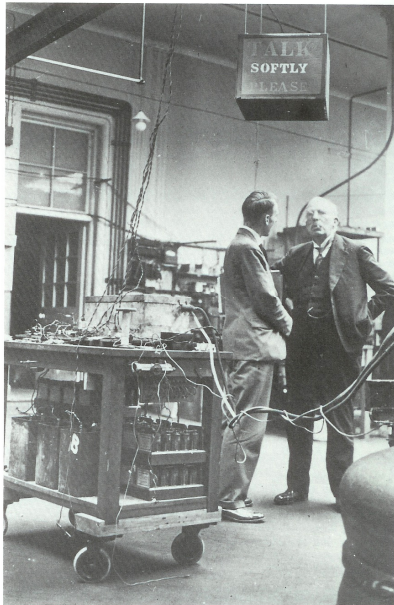
Figure 4-1 Thomson's model of the atom—a sphere of positive charge embedded with electrons.



$$\frac{e}{m} = \frac{V\theta}{B^2 \ell d}$$

Rutherford's model of the atom

In the α particle scattering experiment, a large angle of scattering is observed, which can not be observed by Thomson's model.



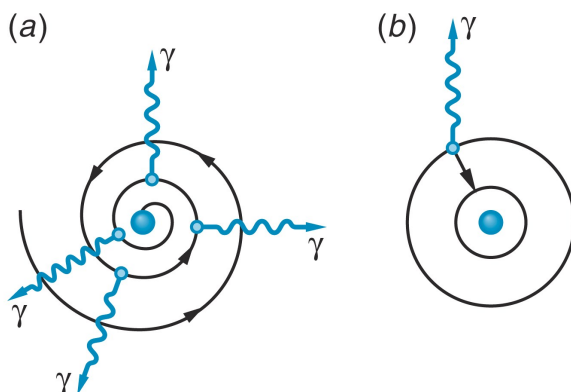
Rutherford model

All the mass and positive charge Ze were concentrated in a minute nucleus of the atom of diameter 10^{-14} m and Z electrons must circle the nucleus in some way.

Problem of stability (planet model)

Accelerating electrons \rightarrow electromagnetic radiation \rightarrow lose energy \rightarrow atoms will collapse to nuclear dimensions ???

Why are atoms stable ??? \rightarrow Bohr's model



Atomic spectra:

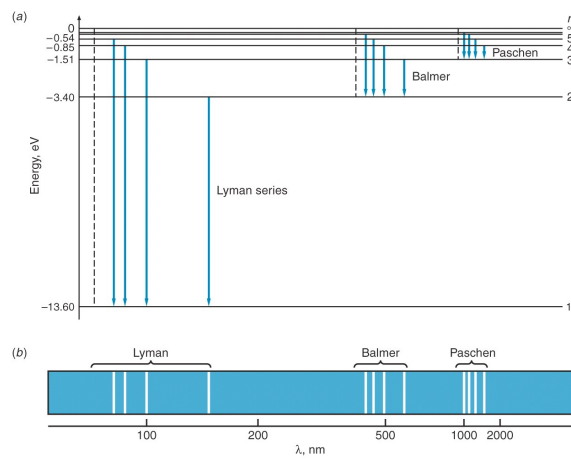
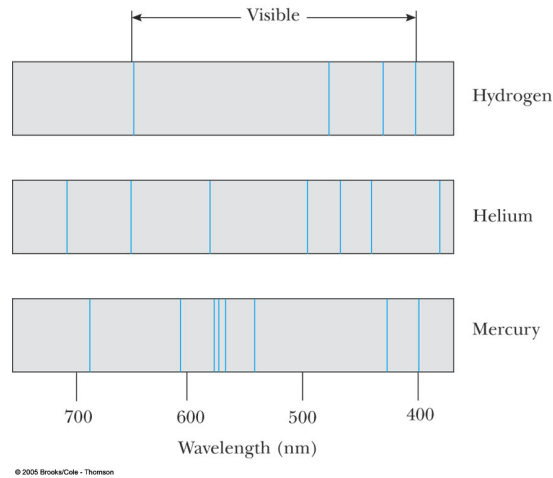
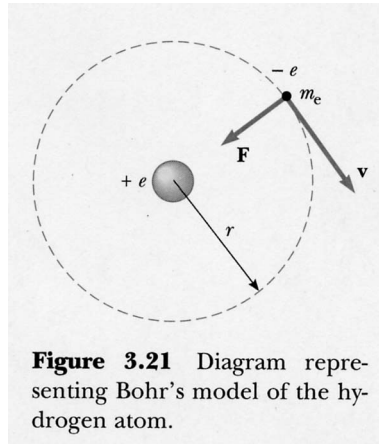


Table 4-1 The Hydrogen Series

Names	Wavelength Ranges	Formulas
Lyman	Ultraviolet	$\kappa = R_H \left(\frac{1}{1^2} - \frac{1}{n^2} \right) \quad n = 2, 3, 4, \dots$
Balmer	Near ultraviolet and visible	$\kappa = R_H \left(\frac{1}{2^2} - \frac{1}{n^2} \right) \quad n = 3, 4, 5, \dots$
Paschen	Infrared	$\kappa = R_H \left(\frac{1}{3^2} - \frac{1}{n^2} \right) \quad n = 4, 5, 6, \dots$
Brackett	Infrared	$\kappa = R_H \left(\frac{1}{4^2} - \frac{1}{n^2} \right) \quad n = 5, 6, 7, \dots$
Pfund	Infrared	$\kappa = R_H \left(\frac{1}{5^2} - \frac{1}{n^2} \right) \quad n = 6, 7, 8, \dots$

$$\frac{1}{\lambda} = R \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right), \quad R = 1.0973732 \times 10^7 \text{ m}^{-1}$$

Bohr's model



$$L = mvr = n\hbar = \frac{nh}{2\pi}, \Rightarrow 2\pi r = \frac{nh}{mv} = \frac{nh}{p} = n\lambda$$

Bohr's postulate

- (1) e^- , nucleus \rightarrow Coulomb force.
- (2) $L = n\hbar$, $\hbar = \frac{h}{2\pi}$ (angular momentum quantized)
- (3) an electron moving in such an orbit doesn't radiate EM wave \rightarrow total energy is conserved.
- (4) Atoms can exist only in certain state, and the frequency f of an emitted photon is equal to ($hf = E' - E''$).

From the postulate:

$$\vec{F} = -\frac{Ze^2}{4\pi\epsilon_0 r^2} = -m\frac{v^2}{r}$$

$$L = mvr = n\hbar$$

$$\Rightarrow v_n = \frac{Ze^2}{4\pi\epsilon_0 n\hbar}, \text{ (speed quantized)}$$

$$\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c} \cong \frac{1}{137} \text{ (dimensionless)} \Rightarrow v_n = \frac{Z\alpha c}{n}$$

Atomic radius $r_n = \frac{n\hbar}{mv_n} = \frac{n\hbar}{m(\frac{Z\alpha c}{n})} = \frac{n^2}{Z}(\frac{\hbar}{mc\alpha})$ (quantized)

If $Z = 1, n = 1$

$$r = \frac{\hbar}{mc\alpha} = 0.53 \text{ \AA} = a_0 \text{ (Bohr's radius)}$$

$$r_n = \frac{n^2}{Z} a_0$$

Total energy of an atomic electron moving in one of the allowed orbits.

$$E = K + V, \quad K = \frac{1}{2}mv_n^2 \quad V = -\frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r_n}$$

$$\begin{aligned} \therefore E_n &= \frac{1}{2}mv_n^2 - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r_n} \\ &= \frac{1}{2}m\left(\frac{Z\alpha c}{n}\right)^2 - \frac{Ze^2}{4\pi\epsilon_0} \left(\frac{Zmc\alpha}{n^2\hbar}\right) = \frac{1}{2}m\left(\frac{Z\alpha c}{n}\right)^2 - m\left(\frac{Z\alpha c}{n}\right)^2 \\ &= -\frac{1}{2}m\left(\frac{Z\alpha c}{n}\right)^2 \end{aligned}$$

For ground state of hydrogen, $Z = 1, n = 1$

$$-\frac{1}{2}mc^2\alpha^2 = -13.6 \text{ eV}$$

$$\therefore E_n = -13.6 \frac{Z^2}{n^2} (\text{eV}), \text{ (Hydrogen-like atomic energy level)}$$

$$\because a_0 = \frac{\hbar}{mc\alpha} \quad \therefore E_n = -\frac{\hbar^2}{2ma_0^2} \frac{Z^2}{n^2}$$

The frequency of the EM radiation emitted when the electron makes a transition:

$$f_{n_2 \rightarrow n_1} = \frac{E_{n_2} - E_{n_1}}{h} = \frac{m(Z\alpha c)^2}{2h} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

$$f = \frac{c}{\lambda}, \quad \frac{1}{\lambda_{n_2 \rightarrow n_1}} = \frac{m(Z\alpha c)^2}{2hc} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) = R_y Z^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

$$R_y = \frac{m(\alpha c)^2}{2hc} = \frac{mc^2\alpha^2}{4\pi\hbar c} = 1.10 \times 10^7 \text{ m}^{-1} \quad (\text{Rydberg constant})$$

The Bohr's model can explain the atomic spectra successfully !!

De Broglie's postulate of matter waves



For a photon, $E = hf = pc$, $c = f\lambda \Rightarrow \lambda = \frac{h}{p}$

De Broglie: (Matter wave)

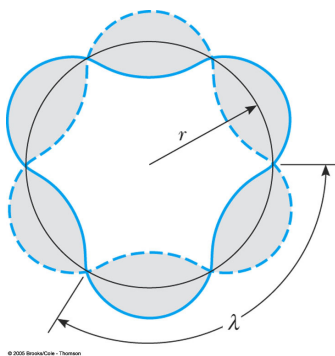
$$p = \sqrt{2mE} = mv$$

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

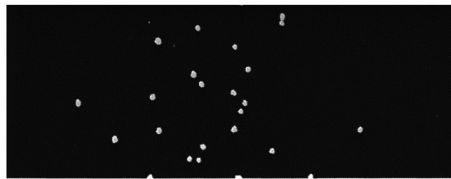
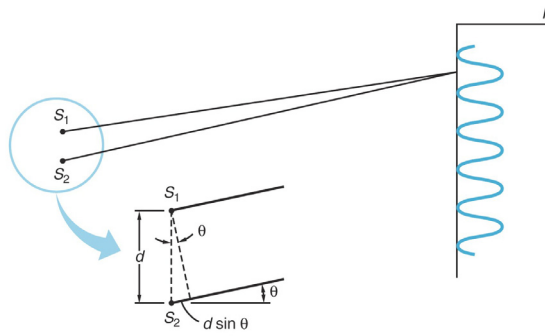
→ **Wave-like properties of particles (Matter Wave)**

Revisit Bohr's model

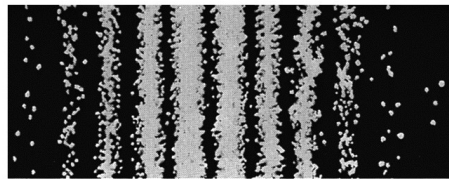
$$L = mvr = n\hbar = \frac{nh}{2\pi} , \Rightarrow 2\pi r = \frac{nh}{mv} = \frac{nh}{p} = n\lambda$$



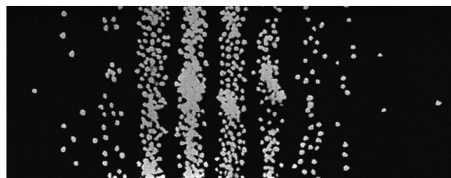
Two slit interference experiment



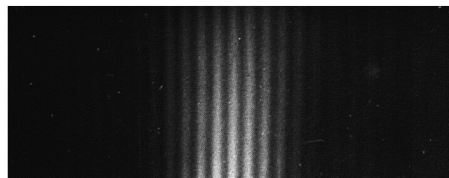
(a)



(c)



(b)

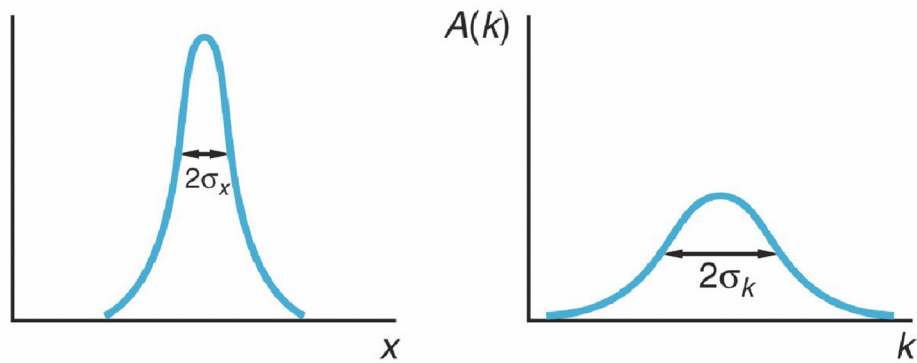


(d)

One photon at a time reaches the detector.

3. Heisenberg's Uncertainty principles:

The more precisely the position is determined, the less precisely the momentum is known $\Delta x \Delta p \geq \hbar$



4. Schrodinger equation (1-D)

$E(\text{total}) = K(\text{kinetic}) + V(\text{potential})$

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

$(|\psi|^2 dx = \text{probability})$

Time independent Schrodinger Equation:

$$H = \frac{p^2}{2m} + V = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$

$$\hat{H}\psi_E = E\psi_E$$

$$\langle \text{Energy} \rangle = \int_{-\infty}^{\infty} \psi_E^* \hat{H} \psi_E dx$$

$$= \int_{-\infty}^{\infty} \psi_E^* E \psi_E dx = E \int_{-\infty}^{\infty} \psi_E^* \psi_E dx = E$$

$$\langle \text{Energy}^n \rangle = \langle \hat{H}^n \rangle$$

$$= \int_{-\infty}^{\infty} \psi_E^* \hat{H}^n \psi_E dx = E^n$$

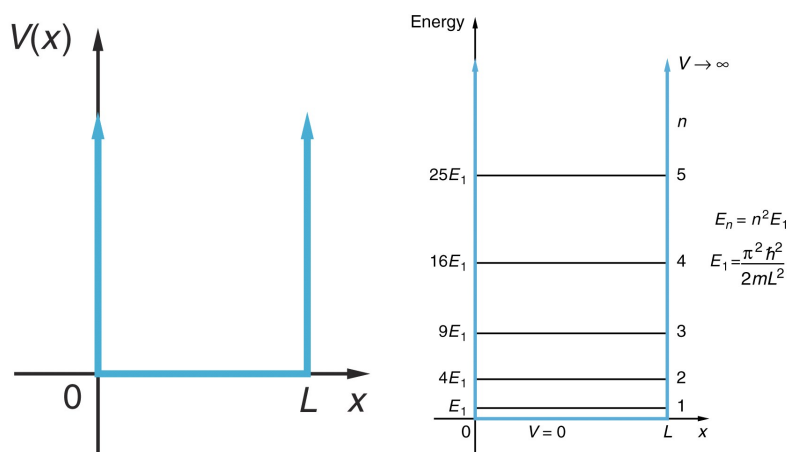
$$\sigma = \sqrt{\langle h^2 \rangle - \langle h \rangle^2} = \Delta \quad (\text{Standard deviation})$$

$$\Rightarrow \Delta E = \langle \text{Energy}^2 \rangle - \langle \text{Energy} \rangle^2 = 0 \quad (\text{Time independent Sch. Eq.})$$

→ Eigenvalue and eigenfunction

Solution of Schrodinger Equation:

1. Infinite potential well

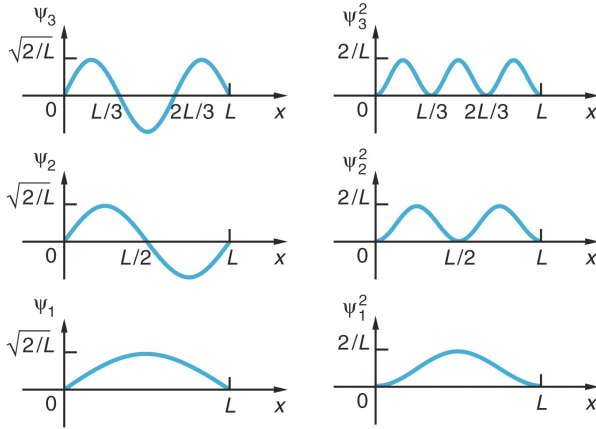


$$V(x) = \begin{cases} 0 & \text{for } 0 < x < L \\ \infty & \text{otherwise} \end{cases}$$

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

$$\Rightarrow \psi_n(x) = A \sin \frac{n\pi}{L} x \quad , \quad \text{Normalize } \int_{-\infty}^{\infty} \psi_n^* \psi_n dx = 1 \Rightarrow A = \sqrt{\frac{2}{L}}$$

$$\therefore \psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x \quad , \quad E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} = \frac{n^2 \hbar^2}{8mL^2} \quad , \quad n = 1, 2, 3, \dots$$



for $n = 1$

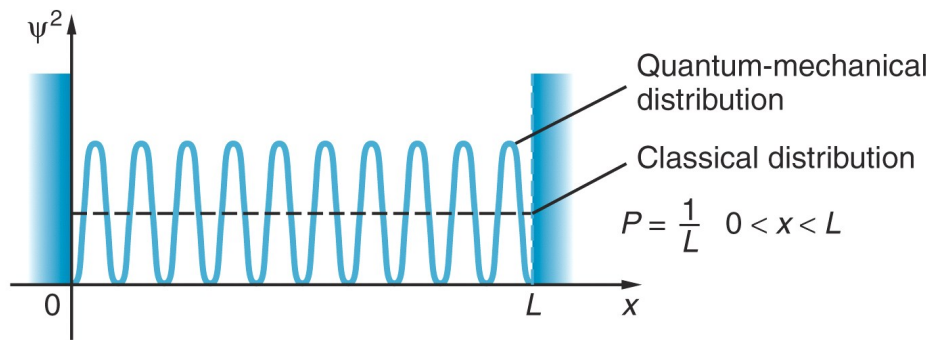
$$\langle x \rangle = \frac{2}{L} \int_0^L x \sin^2 \frac{\pi x}{L} dx = \frac{L}{2}$$

$$\langle p \rangle = \frac{2}{L} \int_0^L \sin \frac{\pi}{L} x (-i\hbar \frac{d}{dx}) \sin \frac{\pi}{L} x dx = 0$$

$$\langle p^2 \rangle = \frac{2}{L} \int_0^L \sin \frac{\pi}{L} x (-i\hbar \frac{d}{dx})^2 \sin \frac{\pi}{L} x dx = \frac{\pi^2 \hbar^2}{L^2}$$

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \frac{\pi \hbar}{L} \quad , \quad \Delta p \Delta x \geq \frac{\hbar}{2}$$

$$|\psi_n(x)|^2 = \frac{2}{L} \sin^2 \frac{n\pi}{L} x = \frac{2}{L} \left(\frac{1 - \cos \frac{2n\pi}{L} x}{2} \right) = \frac{1}{L} - \frac{\cos \frac{2n\pi}{L} x}{L}$$



Remark: Comparison with classical results:

(I) Potential step

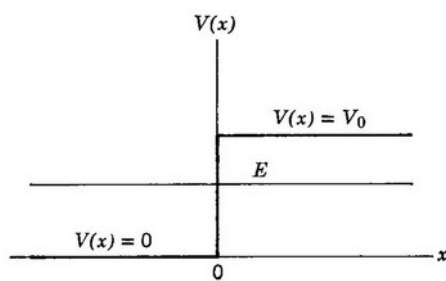
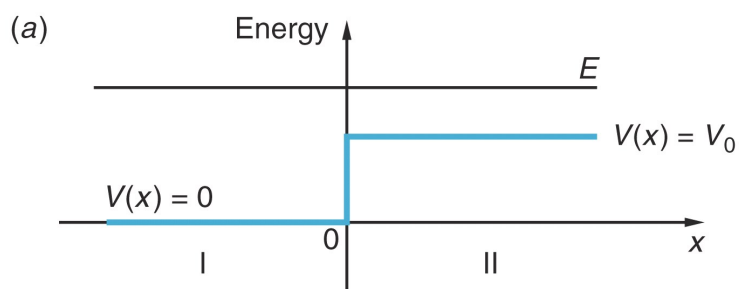
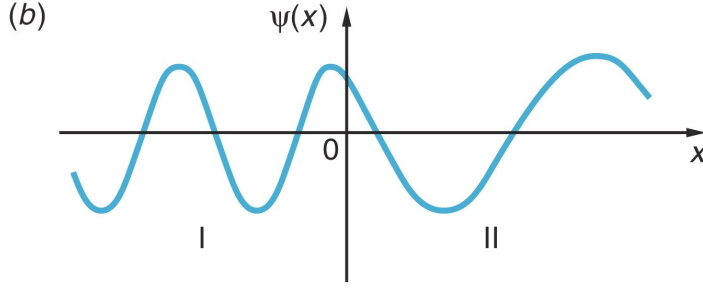


Figure 6-5 The relation between total and potential energies for a particle incident upon a potential step with total energy less than the height of the step.

$$V(x) = \begin{cases} V_0 & \text{for } x > 0 \\ 0 & \text{for } x < 0 \end{cases}$$

Case I $E > V_0$





Region I :

$$\psi_I(x) = Ae^{ik_1x} + Be^{-ik_1x} \quad , \quad k_1 = \frac{\sqrt{2mE}}{\hbar}$$

$$\therefore |\psi_{\text{incident}}|^2 = A^*A = |A|^2 \quad , \quad |\psi_{\text{reflected}}|^2 = B^*B = |B|^2$$

Region II:

$$\psi_{II}(x) = Ce^{ik_2x} + De^{-ik_2x} \quad , \quad k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$$

No reflected wave $\rightarrow D = 0$

$$|\psi_{\text{trans}}|^2 = C^*C = |C|^2$$

Boundary conditions:

$$(1) \quad \psi_I(0) = \psi_{II}(0) \quad \Rightarrow A + B = C$$

$$(2) \quad \left. \frac{\partial \psi_I}{\partial x} \right|_{x=0} = \left. \frac{\partial \psi_{II}}{\partial x} \right|_{x=0} \quad \Rightarrow k_1(A - B) = k_2C$$

$$|\psi|^2 : \frac{\text{probability}}{\text{length}} \propto \frac{\text{number}}{\text{length}}$$

$$\text{Reflection and transmission} \propto \frac{\text{number}}{\text{time}} = \frac{\text{number}}{\text{distance}} \frac{\text{distance}}{\text{time}} \propto |\psi|^2 v \quad (\text{Probability flux})$$

$$T = \frac{|\psi_{\text{tran}}|^2 v_{II}}{|\psi_{\text{in}}|^2 v_I} = \frac{|\psi_{\text{tran}}|^2 k_2}{|\psi_{\text{in}}|^2 k_1} = \frac{C^* C k_2}{A^* A k_1}$$

$$R = \frac{|\psi_{\text{ref}}|^2 v_I}{|\psi_{\text{in}}|^2 v_I} = \frac{|\psi_{\text{ref}}|^2}{|\psi_{\text{in}}|^2} = \frac{B^* B}{A^* A}$$

$$\therefore \begin{cases} A + B = C \\ A - B = \frac{k_2}{k_1} C \end{cases} \Rightarrow C = \frac{2k_1}{k_1 + k_2} A \quad , \quad B = \frac{k_1 - k_2}{k_1 + k_2} A$$

$$\Rightarrow T = \frac{4k_1 k_2}{(k_1 + k_2)^2} \quad \Rightarrow T + R = 1 \quad , \quad R \neq 0, \text{ wave property}$$

$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2}$$

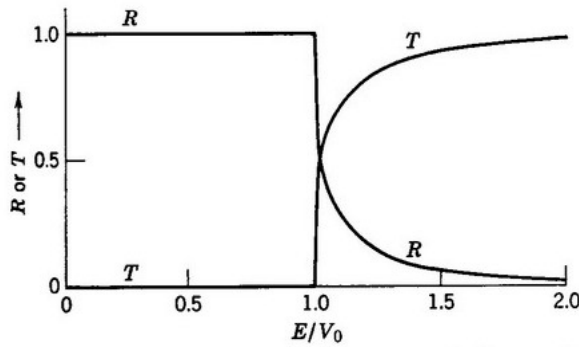


Figure 6-11 The reflection and transmission coefficients R and T for a particle incident upon a potential step. The abscissa E/V_0 is the ratio of the total energy of the particle to the increase in its potential energy at the step. The case $k_1 = 2k_2$, illustrated in Figure 6-10, corresponds to $E/V_0 = 1.33$.

Remark:

Classical: no reflection for $E > V_0$ ($R=0$)

Quantum : $R \neq 0$ for $E > V_0$, (wave property)

Case II $E < V_0$ (bound)

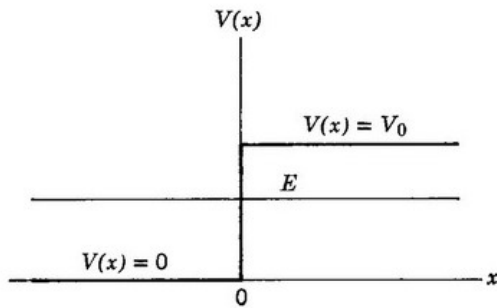


Figure 6-5 The relation between total and potential energies for a particle incident upon a potential step with total energy less than the height of the step.

Region I : $\psi_I(x) = Ae^{ik_1x} + Be^{-ik_1x}$, $k_1 = \frac{\sqrt{2mE}}{\hbar}$

Region II: $\psi_{II}(x) = Ce^{\alpha x} + De^{-\alpha x}$, $\alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$

$$\psi_{II} \text{ cannot diverge} \Rightarrow C = 0$$

Boundary conditions:

(1) $\psi_I(0) = \psi_{II}(0) \Rightarrow A + B = D$

(2) $\left. \frac{\partial \psi_I}{\partial x} \right|_{x=0} = \left. \frac{\partial \psi_{II}}{\partial x} \right|_{x=0} \Rightarrow ik_1(A - B) = -\alpha D$

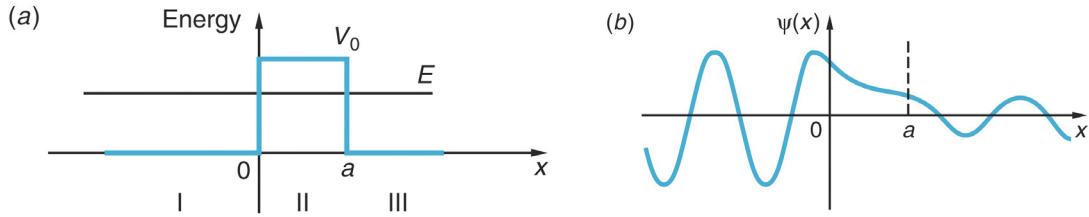
$$\Rightarrow B = -\frac{\alpha + ik}{\alpha - ik} A$$

$$\therefore |B| = \sqrt{B^* B} = \sqrt{\left(-\frac{\alpha + ik}{\alpha - ik} A\right)^* \left(-\frac{\alpha + ik}{\alpha - ik} A\right)} = \sqrt{A^* A} = |A|$$

$$R = \frac{B^* B}{A^* A} = 1, \quad T = 0$$

$$\delta = \frac{1}{\alpha} = \frac{1}{\sqrt{2m(V_0 - E)}} \quad (\text{penetration depth})$$

(II) Tunneling barrier



$$V(x) = \begin{cases} 0 & \text{for } x < 0 \quad (I) \\ V_0 & \text{for } 0 < x < a \quad (II) \\ 0 & \text{for } x > a \quad (III) \end{cases}$$

Case I $E < V_0$

$$\text{Region I : } \psi_I(x) = Ae^{ik_1 x} + Be^{-ik_1 x}, \quad k_1 = \frac{\sqrt{2mE}}{\hbar}$$

$$\text{Region II : } \psi_{II}(x) = Ce^{-\alpha x} + De^{\alpha x}, \quad \alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

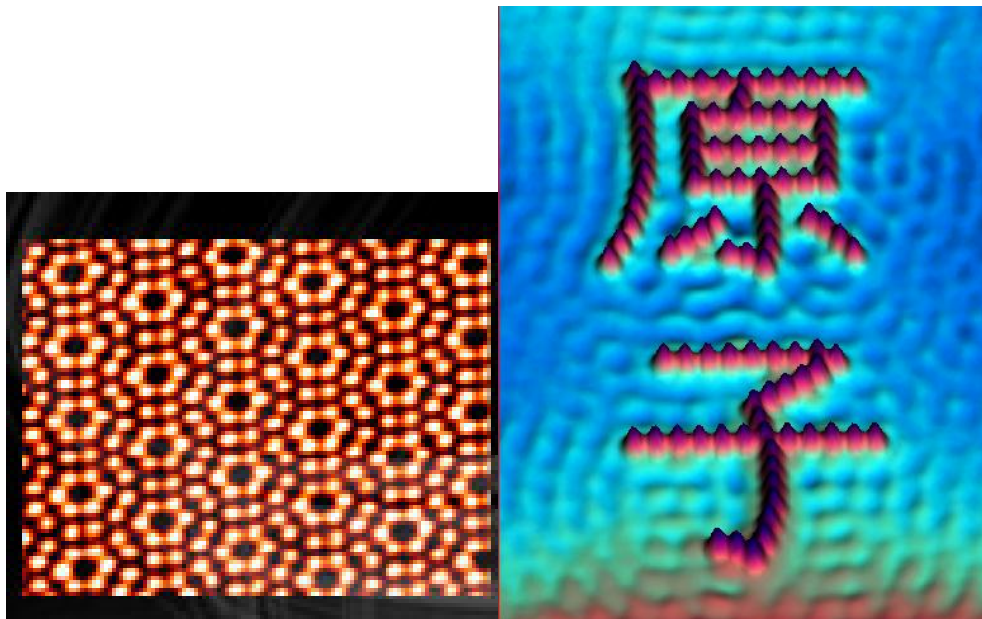
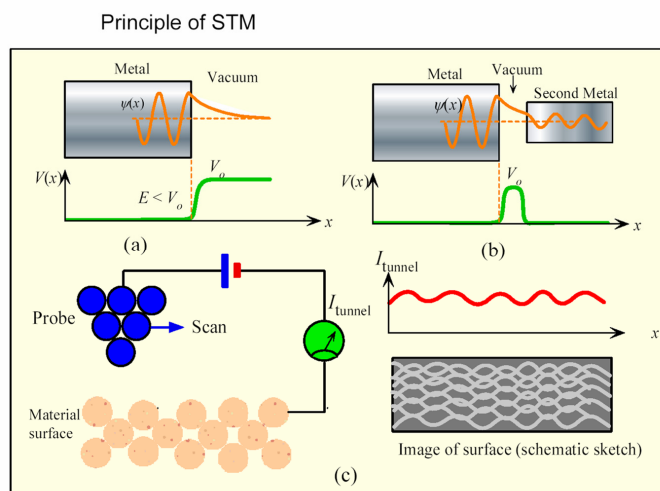
$$\text{Region III: } \psi_{III}(x) = Fe^{ik_1 x} + Ge^{-ik_1 x}, \quad k_1 = \frac{\sqrt{2mE}}{\hbar}$$

B.C. $\psi(x), \frac{\partial}{\partial x} \psi$ must be continuous at $x = 0, x = a$ and let $k = k_1$

$$\Rightarrow \begin{cases} A + B = C + D \\ ikA - ikB = \alpha D - \alpha C \\ Ce^{-\alpha a} + De^{\alpha a} = Fe^{ika} \\ (\alpha D)e^{\alpha a} - (\alpha C)e^{-\alpha a} = ikFe^{ika} \end{cases}$$

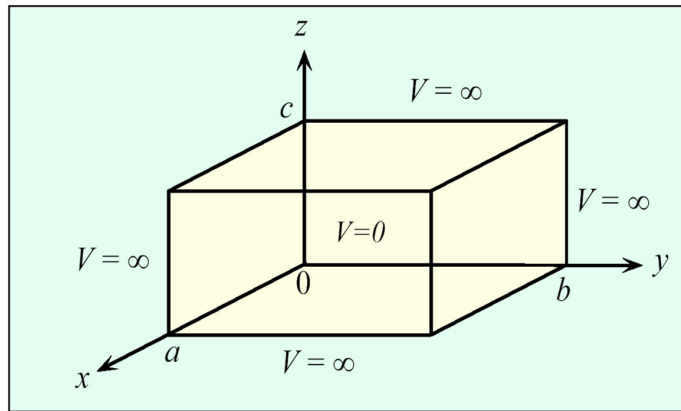
$$\begin{aligned}
\therefore T = \frac{FF^*}{AA^*} &= \left\{ 1 + \frac{1}{4} \left[\frac{V_0^2}{E(V_0 - E)} \right] \sinh^2(\alpha a) \right\}^{-1} \\
&= \left[1 + \frac{1}{16} \frac{V_0^2}{E(V_0 - E)} (e^{2\alpha a} - 2 + e^{-2\alpha a}) \right]^{-1} \\
&\cong 16 \frac{E}{V_0} \left(1 - \frac{E}{V_0} \right) e^{-2\alpha a} \quad \text{for } \alpha a \gg 1
\end{aligned}$$

Example: Scanning Tunneling Microscopy (STM)



From IBM.STM Gallery

3. Case 3. Particle in a box (3-D)



Electron confined in three dimensions by a three dimensional infinite "PE box". Everywhere inside the box, $V=0$, but outside, $V=\infty$. The electron cannot escape from the box. What is the energy and wavefunction of the electron?

Schrodinger's equation for three dimensions

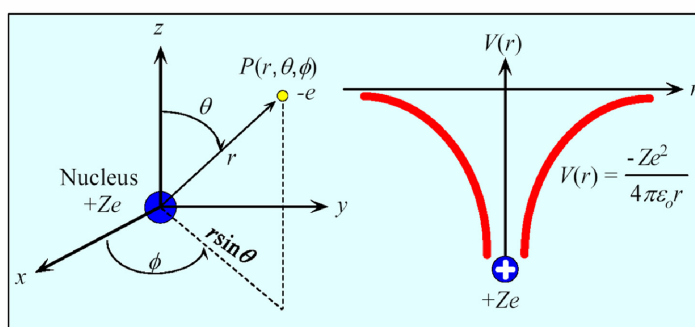
$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0$$

if $L_x = L_y = L_z = L \Rightarrow (n_x, n_y, n_z)$ correspond to one state

$$\Rightarrow E = \frac{\pi^2 \hbar^2}{2m} \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right)$$

$$(if \ L_x = L_y = L_z = L) \quad = (n_x^2 + n_y^2 + n_z^2) \frac{\pi^2 \hbar^2}{2mL^2}$$

Hydrogen Atom:



$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r},$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi - \frac{e^2}{4\pi\epsilon_0 r}\psi = E\psi, \quad \psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$$

Three quantum number (n, l, m_l)

$$\psi(r, \theta, \phi) = R_{n,l}(r)Y_{l,m_l}(\theta, \phi), \quad Y_{l,m_l}(\theta, \phi) = \Theta(\theta)\Phi(\phi)$$

$R(r)$: radial wavefunction, Y : spherical wavefunction

Electron energy in the hydrogen atom is quantized.

n is a quantum number, 1,2,3,

$$E_n = -\frac{me^4}{8\epsilon_0\hbar^2 n^2} = -\frac{(13.6\text{eV})}{n^2}$$

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2} = 0.0528\text{nm} \rightarrow \text{Bohr radius}$$

n	Principal quantum number	$n = 1, 2, 3, \dots$	Quantizes the energy of the electron, $E = -(13.58 \text{ eV})/n^2$.
ℓ	Orbital angular momentum quantum number	$\ell = 0, 1, 2, \dots, (n-1)$	Quantizes the magnitude of orbital angular momentum, L . $L = \hbar[\ell(\ell+1)]^{1/2}$
m_ℓ	Magnetic quantum number	$m_\ell = 0, \pm 1, \pm 2, \dots, \pm \ell$	Quantizes the orbital angular momentum component along a magnetic field, B_z . $L_z = m_\ell \hbar$
m_s	Spin magnetic quantum number	$m_s = \pm 1/2$	Quantizes the spin angular momentum component along a magnetic field B_z . $S_z = m_s \hbar$

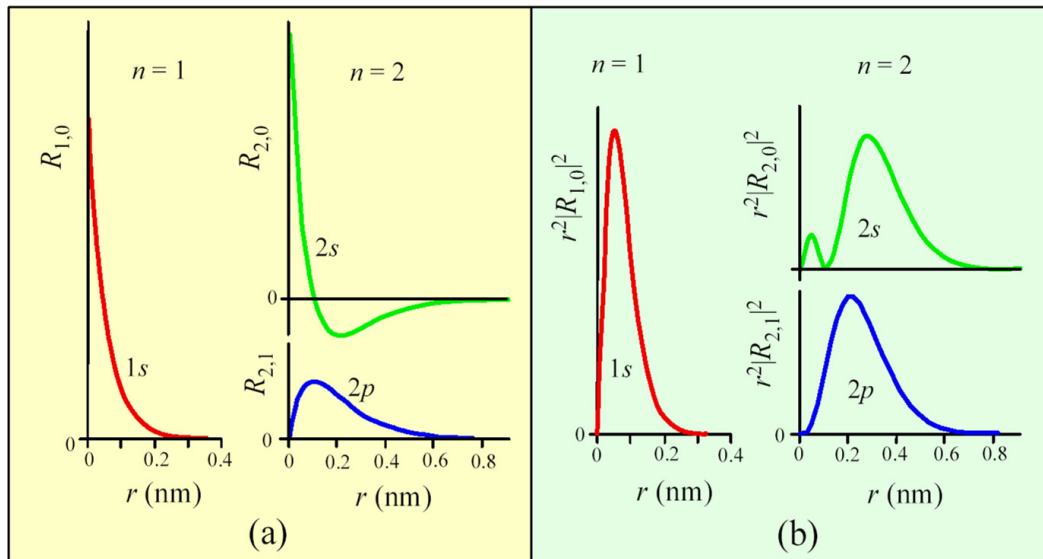
Table 3.1 Labelling of various $n\ell$ possibilities.

ℓ	0	1	2	3	4
n					
1	1s				
2	2s	2p			
3	3s	3p	3d		
4	4s	4p	4d	4f	
5	5s	5p	5d	5f	5g

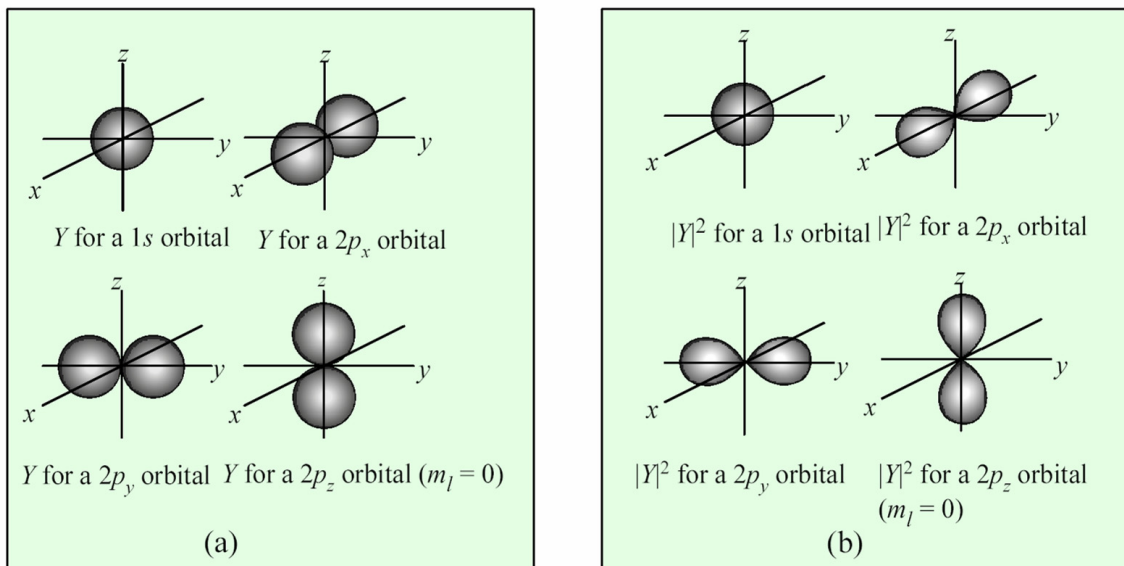
Table 3.2

The radial and spherical harmonic parts of the wavefunction in the hydrogen atom. ($a_0 = 0.0529\text{nm}$)

n	ℓ	$R(r)$	m	ℓ	$Y(\theta, \phi)$	
1	0	$(\frac{1}{a_0})^{3/2} 2 \exp(-\frac{r}{a_0})$	0		$\frac{1}{2\sqrt{\pi}}$	
2	0	$(\frac{1}{2a_0})^{3/2} (2 - \frac{r}{a_0}) \exp(-\frac{r}{2a_0})$	0		$\frac{1}{2\sqrt{\pi}}$	
2	1	$(\frac{1}{2a_0})^{3/2} (\frac{r}{\sqrt{3} a_0}) \exp(-\frac{r}{2a_0})$	0		$\frac{1}{2} \sqrt{\frac{3}{\pi}} \cos \theta$	$\left\{ \begin{array}{l} \propto \sin \theta \cos \phi \\ \propto \sin \theta \sin \phi \end{array} \right\}$ Correspond $m_\ell = -1$ and
			1		$\frac{1}{2} \sqrt{\frac{3}{2\pi}} \sin \theta e^{i\phi}$	
			-1		$\frac{1}{2} \sqrt{\frac{3}{2\pi}} \sin \theta e^{-i\phi}$	

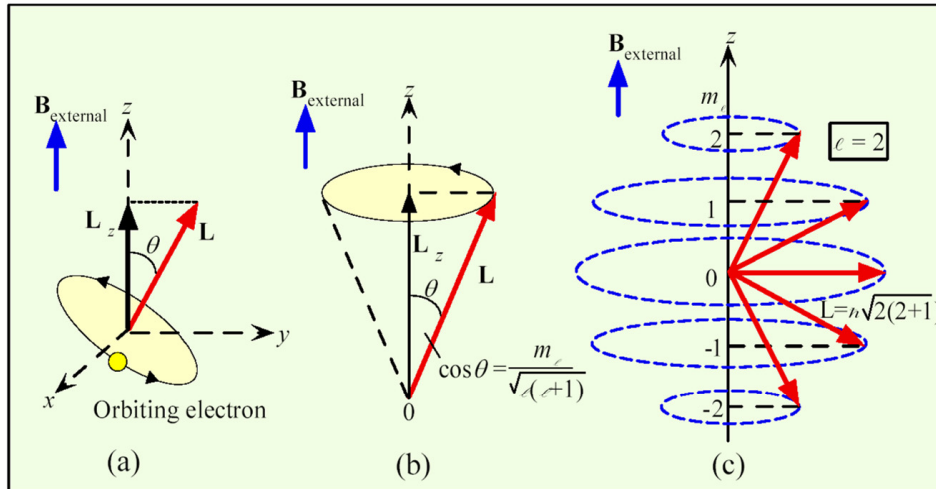


(a) Radial wavefunctions of the electron in a hydrogenic atom for various n and l values. (b) $r^2|R_{n,l}|^2$ gives the radial probability density. Vertical axis scales are linear in arbitrary units.



(a) The polar plots of $Y_{n,l}(\theta, \phi)$ for $1s$ and $2p$ states. (b) The angular dependence of the probability distribution which is proportional to $|Y_{n,l}(\theta, \phi)|^2$.

Orbitabl angular momentum and Space quantization



(a) The electron has an orbital angular momentum which has a quantized component, L_z , along an external magnetic field, $\mathbf{B}_{\text{external}}$. (b) The orbital angular momentum vector \mathbf{L} rotates about the z -axis. Its component L_z is quantized and therefore the orientation of \mathbf{L} , the angle θ , is also quantized. \mathbf{L} traces out a cone. (c) According to quantum mechanics, only certain orientations (θ) for \mathbf{L} are allowed as determined by ℓ and m_ℓ .

Orbital Angular Momentum and Space Quantization

Orbital angular momentum

$$L = \hbar [\ell(\ell + 1)]^{1/2}$$

where $\ell = 0, 1, 2, \dots, n-1$

Orbital angular momentum along B_z

$$L_z = m_\ell \hbar$$

Selection rules for EM radiation absorption and emission

$$\Delta\ell = \pm 1 \quad \text{and} \quad \Delta m_\ell = 0, \pm 1$$

Electron Spin and Intrinsic Angular Momentum S

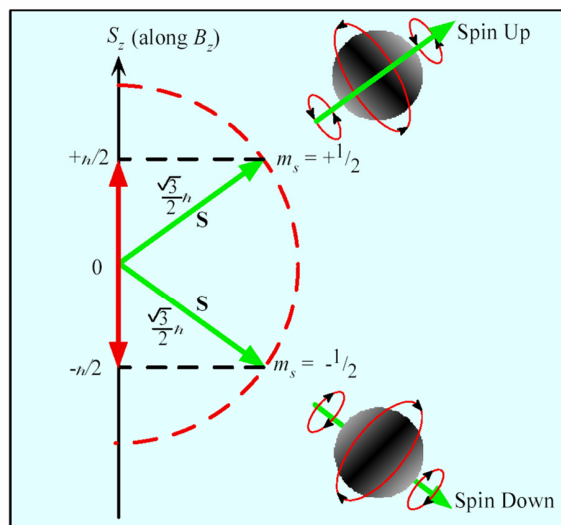
Electron spin

$$S = \hbar[s(s+1)]^{1/2} \quad s = \frac{1}{2}$$

Spin along magnetic field

$$S_z = m_s \hbar \quad m_s = \pm \frac{1}{2}$$

the quantum numbers s and m_s , are called the **spin** and **spin magnetic quantum numbers**.



Spin angular momentum exhibits space quantization. Its magnitude along z is quantized so that the angle of S to the z -axis is also quantized.