



【Chapter 6 Schrödinger Equation for H atom】

【6.1 Schrödinger Equation for H atom】

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

electric potential energy $U = \frac{-e^2}{4\pi\epsilon_0 r}$

∵ U is function of r, rather than x,y,z

- ⇒ { 1. Express U in terms of x,y,z
- ⇒ { 2. Express Schrödinger Equation in terms of r,θ,φ, (see fig 6.1)

Owing to the symmetry of physical situation

⇒ choose spherical polar coordinates.

r = length of radius vector from O to P

$$= \sqrt{x^2 + y^2 + z^2}$$

θ = angle between radius vector and z axis

$$= \cos^{-1} \frac{z}{\sqrt{x^2 + y^2 + z^2}} \quad (\text{zenith angle})$$

ψ = angle between the projection of radius vector in x-y plane and

the x axis

$$= \tan^{-1} \frac{y}{x} \quad (\text{azimuth angle})$$

*In spherical polar coordinates, Schrödinger Equation

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \varphi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \varphi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \varphi}{\partial \phi^2} + \frac{2m}{\hbar^2} (E - U) = 0$$

substituting U & multiplying $r^2 \sin^2 \theta$

⇒

$$\sin^2 \theta \frac{\partial}{\partial r} \left(r^2 \frac{\partial \varphi}{\partial r} \right) + \sin \theta \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \varphi}{\partial \theta} \right) + \frac{\partial^2 \varphi}{\partial \phi^2} + \frac{2mr^2 \sin^2 \theta}{\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0 r} + E \right) \varphi = 0$$

----- (6.4)

⇒ solve eq(6.4) for $\varphi \Rightarrow$ get three quantum number

*A particle in a three-dimensional box needs three quantum numbers for its description

∴ there are three sets of B.C., φ must be zero at the walls of box in x,y,z.

In H atom, the e' motion is restricted by the inverse-square E field
⇒ but e' is nevertheless free to move in 3-D ⇒ need 3 quantum number.

【6.2 Separation of Variables】

The advantage of writing Schrödinger Equation in spherical polar coordinates for H atom is that it may be separated into three independent eq.s, each involving only a single coordinate.

i.e. we would like to have

$$\varphi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$$

$$\Rightarrow \frac{\partial \varphi}{\partial r} = \Theta\Phi \frac{\partial R}{\partial r} = \Theta\Phi \frac{dR}{dr}$$

$$\Rightarrow \frac{\partial \varphi}{\partial \theta} = R\Phi \frac{\partial \Theta}{\partial \theta} = R\Phi \frac{d\Theta}{d\theta}$$

$$\Rightarrow \frac{\partial^2 \varphi}{\partial \phi^2} = R\Theta \frac{\partial^2 \Phi}{\partial \phi^2} = R\Theta \frac{d^2 \Phi}{d\phi^2}$$

\Rightarrow Schrödinger Equation

$$\frac{\sin^2 \theta}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{\sin \theta}{\Theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + \frac{2mr^2 \sin^2 \theta}{\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0 r} + E \right) = \frac{-1}{\Phi} \frac{d^2 \Phi}{d\phi^2}$$

This eq. can be correct only if both sides of it are equal to the same constant, since they are functions of different variables.

*It is convenient to call this constant m_e^2

$$\frac{-1}{\Phi} \frac{\partial^2 \Phi}{\partial \phi^2} = m_e^2$$

for right-hand side of eq(6.7), divided eq. by $\sin^2\theta$

$$\frac{1}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2mr^2}{\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0 r} + E \right) = \frac{m_e^2}{\sin^2 \theta} - \frac{1}{\Theta \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right)$$

Again, we have an eq. in which different variables appear on each side \Rightarrow both sides equal to the same constant. This constant is called $\ell(\ell + 1)$

$$\Rightarrow \frac{m_e^2}{\sin^2 \theta} - \frac{1}{\Theta \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) = \ell(\ell + 1)$$

$$\frac{1}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2mr^2}{\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0 r} + E \right) = \ell(\ell + 1)$$

$$\Rightarrow \begin{cases} \frac{d^2\Phi}{d\phi^2} + m_e^2\Phi = 0 \text{ eq. for } \Phi \\ \frac{1}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + \left[\ell(\ell + 1) - \frac{m_e^2}{\sin^2 \theta} \right] \Theta = 0 \text{ eq. for } \Theta \\ \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \left[\frac{2m}{\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0 r} + E \right) - \frac{\ell(\ell + 1)}{r^2} \right] R = 0 \text{ eq. for } R \end{cases}$$

\Rightarrow φ can be separated into $R\Theta\Phi$, only R is dependent on U.

【6.3 Quantum Number】

for Φ (eq(6.12)) $\Rightarrow \Phi(\phi) = Ae^{im_e\phi}$

$\therefore \Phi$ need to be single value

$$\Rightarrow \Phi(\phi) = \Phi(\phi + 2\pi)$$

$$\Rightarrow Ae^{im_e\phi} = Ae^{im_e(\phi+2\pi)}$$

$$\Rightarrow m_e = 0, \pm 1, \pm 2, \pm 3, \dots \pm \ell \quad m_e : \text{magnetic quantum number}$$

for $\Theta(\theta)$ (eq(6.13)) $\Rightarrow \ell$ is an integer equal to or greater than

$|m_e|$ (set the max of m_e)

ℓ : orbital quantum number

for $R(r)$ (eq(6.14)) E_n can be “+” or

$$E_n = \frac{-m_e^4}{32\pi^2 \epsilon_0^2 \hbar^2} \left(\frac{1}{n^2} \right) = \frac{E}{n^2} \quad n=1,2,3,\dots$$

same formula for energy levels of H atom in Bohr mode.

n : principle quantum number

n must be equal to or greater than $\ell + 1$

$$\Rightarrow \ell = 0, 1, 2, 3, \dots, (n-1)$$

$$\varphi = R_{nl} \Theta_{\ell m_e} \Phi_{m_e}$$

The wave functions R, Θ, Φ, φ are given in Table 6.1

【6.4 Principle quantum Number (Quantization of energy)】

In planetary motion, two quantities are conserved

— scalar total energy & vector angular momentum

Classically, the total energy can be any value, but it must be negative if the planet is to be trapped in solar system.

In Q.M. of H atom => the electron energy may have any positive value (corresponding to an ionized atom), the only negative

values are
$$E_n = \frac{E_1}{n^2}$$

=> $n \rightarrow$ Quantization of electron energy

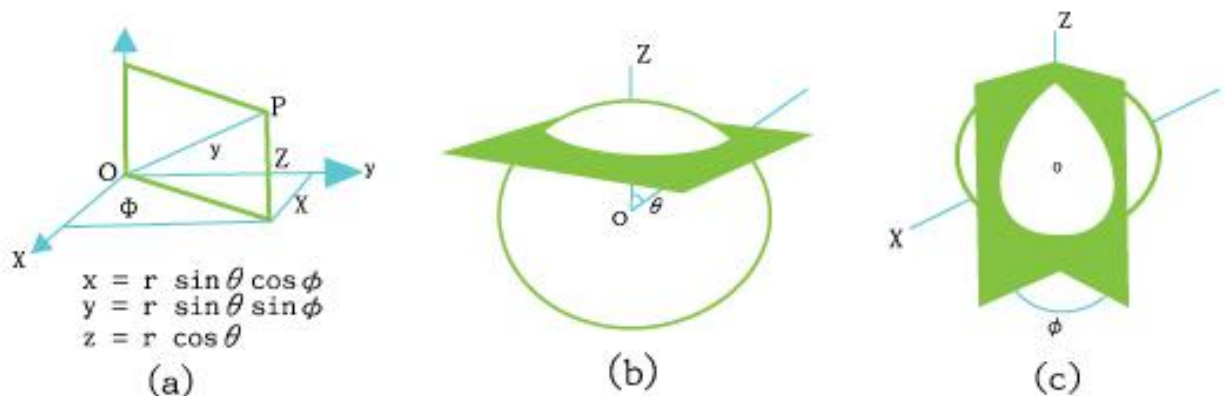


Figure 6.1 (see textbook) (a) Spherical polar coordinates. (b) A line of constant zenith angle θ on a sphere is a circle whose plane is perpendicular to the z axis. (c) A line of constant azimuth angle ϕ is a circle whose plane includes the z axis.

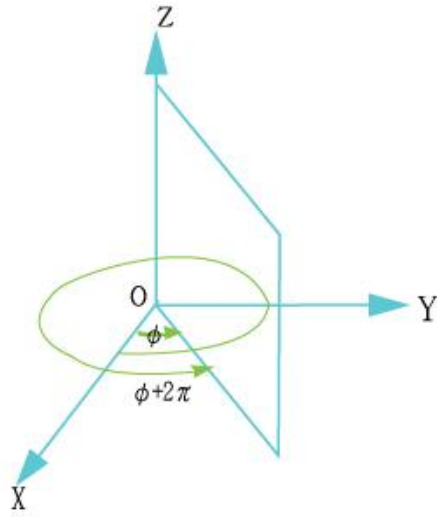


Figure 6.2 (see textbook) The angle ϕ and $\phi + 2\pi$ both identify the same meridian plane.

Figure 6.3 (see textbook) The right-hand rule for angular momentum.

【6.5 Orbital Quantum Number (Quantization of Angular Momentum Magnitude)】

eq(6.14) for R(r)

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \left[\frac{2m}{\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0 r} + E \right) - \frac{\ell(\ell+1)}{r^2} \right] R = 0$$

E includes the e' kinetic energy of orbital motion which should have nothing to do with its radial motion.

$$E = kE_{\text{radial}} + kE_{\text{orbital}} + \underline{\underline{U}}$$

$$= \frac{-e^2}{4\pi\epsilon_0 r}$$

Inserting this expression into eq(6.14)

$$\Rightarrow \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2m}{\hbar^2} \left[kE_{\text{radial}} + kE_{\text{orbital}} - \frac{\hbar^2 \ell(\ell+1)}{2mr^2} \right] R = 0 \dots (6.19)$$

$$\text{if } kE_{\text{orbital}} = \frac{\hbar^2 \ell(\ell+1)}{2mr^2}$$

⇒ eq(6.19) is a differential eq. for R(r) that involves functions of the radius r only.

$$\therefore kE_{\text{orbital}} = \frac{L^2}{2mr^2} \quad L = m v_{\text{orbital}} \cdot r$$

$$\Rightarrow kE_{\text{orbital}} = \frac{L^2}{2mr^2}$$

$$\Rightarrow \frac{L^2}{2mr^2} = \frac{\hbar^2 \ell(\ell+1)}{2mr^2}$$

$$\Rightarrow L = \sqrt{\ell(\ell + 1)}\hbar \quad (\ell=0,1,2,3,\dots,(n-1))$$

the angular momentum is quantized.

*Resignation of Angular Momentum States

$$\ell=0,1,2,3,4,5,6,\dots$$

$$s,p,d,f,g,h,i,\dots$$

d state has angular momentum $\sqrt{2(2+1)}\hbar = \sqrt{6}\hbar$

$$4s \Rightarrow n=4, \ell=0$$

$$5d \Rightarrow n=5, \ell=2$$

Magnetic Quantum Number

* Orbital quantum number ℓ determines the magnitude L of the e^- angular momentum.

* However, angular momentum is a vector \rightarrow need to specify the direction

* The way to determine the direction of $L \Rightarrow$ right-hand rule (see fig(6.3))

An e^- revolving about a nucleus is a minute current loop \rightarrow magnetic dipole.

\Rightarrow when an e^- that possesses angular momentum interacts with an external magnetic B field.

\Rightarrow magnetic quantum number m_ℓ specifies the direction of L by determining the component of L in the field direction.

\Rightarrow This phenomenon is space quantization.

If B direction // z direction

$$\Rightarrow L_z = m_\ell \hbar, \quad m_\ell = 0, \pm 1, \pm 2, \dots, \pm \ell$$

possible value of m_ℓ for given ℓ range from $+\ell$ to $-\ell$.

\Rightarrow number of possible orientations of the angular momentum L in the magnetic field is $2\ell + 1$

The space quantization of orbital angular momentum of H atom is shown in fig(6.4)

L can never be aligned exactly parallel or antiparallel to B

$\therefore L_z$ is always smaller than $\sqrt{\ell(\ell+1)}\hbar$

In the absence of an external magnetic field, the direction of z is arbitrary but L in any chosen direction is $m_e\hbar$.

* Why is only one component of L quantized?

L can never point in any specific direction but instead is somewhere on a cone in space such that its projection L_z is $m_e\hbar$.

Were this not so, \Rightarrow uncertainty principle would be violated.

If L were fixed in space $\Rightarrow L_x, L_y, L_z$ had definite values $\Rightarrow e'$ would be confined to a definite plane.

Ex. if L were in z direction $\Rightarrow e'$ would have to be in x-y plane

(fig(6.5)) $\Rightarrow \Delta Z=0 \Rightarrow \Delta P \rightarrow \infty$

It's impossible if it is to be part of H atom number.

\therefore only one component L_z & magnitude of L have definite value, and $|L| > |L_z|$, the e' is not limited to a single plane (see 6.5,6.6) $\Rightarrow \Delta Z$ uncertainty

\therefore the direction of L is not fixed (fig(6.6))

\Rightarrow average of L_x & $L_y = 0$ but $L_z = m_e\hbar$

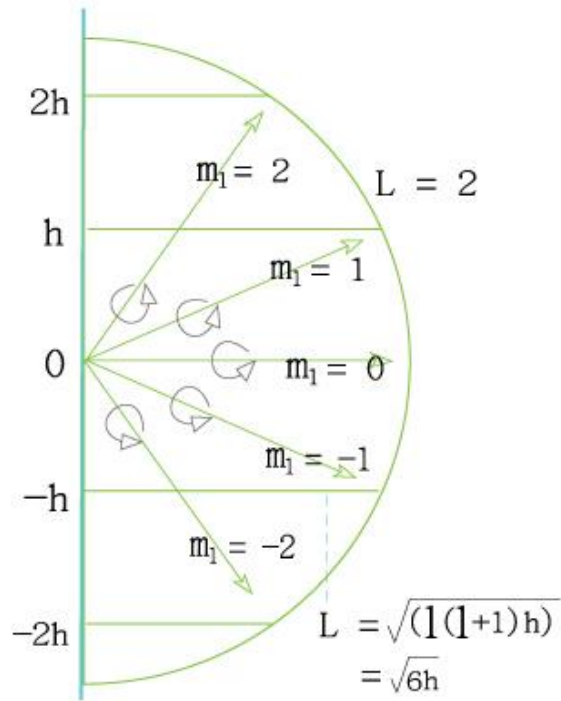


Figure 6.4 (see textbook) Space quantization of orbital angular momentum. Here the orbital quantum number is $l = 2$ and there are accordingly $2l + 1 = 5$ possible values of the magnetic quantum number m_l , with each values corresponding to a different orientation relatives to the z axis

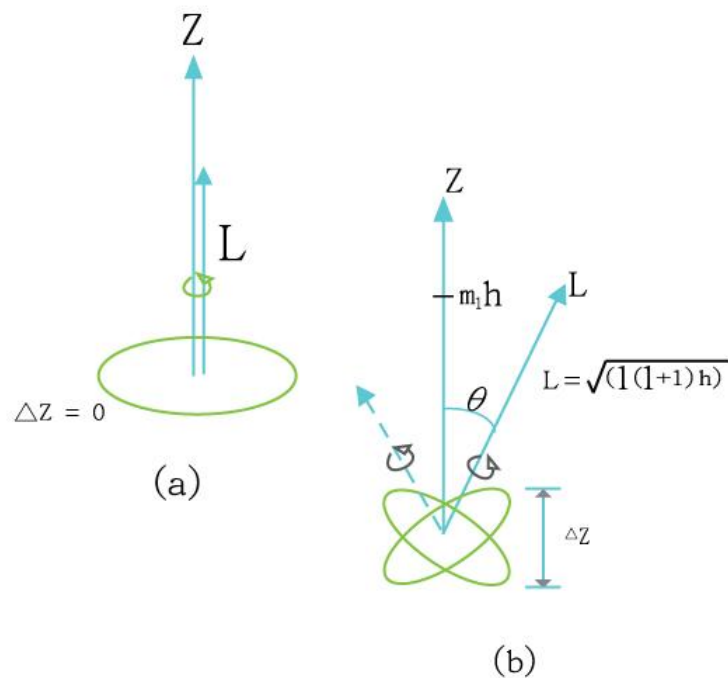


Figure 6.5 (see textbook) The uncertainty principle prohibits the angular momentum vector L from having a definite direction in space

【6.7 Electron Probability Density】

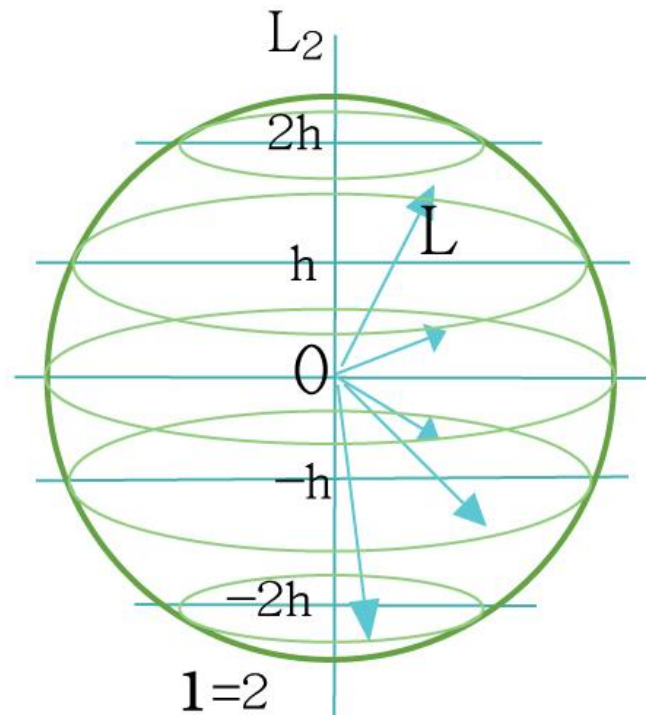


Figure 6.6 (see textbook) The angular-momentum vector \mathbf{L} precesses constantly about the z axis.

※References: Modern Physics for scientists and engineers, Stephen T. Thornton Nonclassical Physics, Randy Harris. Quantum Physics of atoms, molecules, Solids, nuclei and Particles. Eisberg & Resnick

In Bohr's model : e^- revolves around the nucleus in a circular path

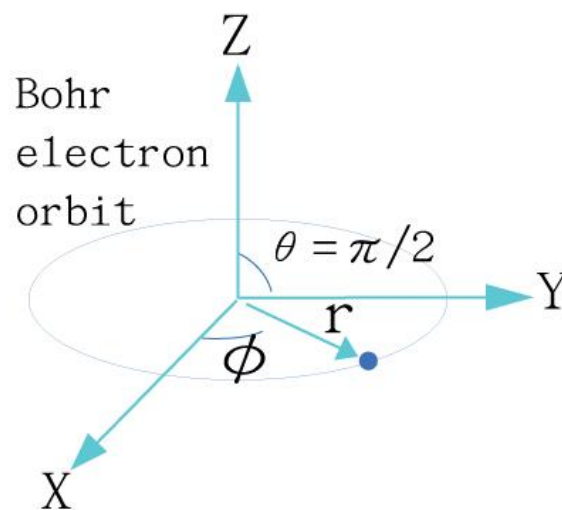


Figure 6.7 (see textbook) The Bohr model of the hydrogen atom in a spherical polar coordinates system.

※References: Modern Physics for scientists and engineers, Stephen T. Thornton Nonclassical Physics, Randy Harris. Quantum Physics of atoms, molecules, Solids, nuclei and Particles. Eisberg & Resnick

⇒ the e' would always be found a distance of $r = n^2 a_0$ from nucleus and $\theta=90^\circ$, while ψ changes with time.

Q.M. :

(1) No definite values of r, θ or ψ can be given, only relative probabilities for finding e' ⇒ wave nature of e' .

(2) We can't even think of e' as moving around the nucleus in independent of time and varies from place to place.

$$|\varphi|^2 = |R|^2 |\Theta|^2 |\Phi|^2$$

$$\because \Phi(\phi) = A e^{im_e \phi}$$

$$|\Phi|^2 = \Phi^* \Phi = A^2 e^{-im_e \phi} \cdot e^{im_e \phi} = A^2$$

The probability of finding e' is independent of ψ ⇒ probability density is symmetrical about the z axis.

* $|\theta|^2$ for s state is a constant

∴ $|\Phi|^2$ is also a constant ⇒ $|\Phi|^2$ is spherically symmetric for s state : it has the same value at a given r in all direction

* e' in other states do have angular preference. See fig(6.12)

∴ $|\Phi|^2$ is independent of ψ , we can obtain a three-dimensional picture of $|\Phi|^2$ by rotating the representation about a vertical axis.

*For 2p state $m_l = \pm 1 \Rightarrow$ like doughnut in the equatorial plane centered at nucleus. The most probable distance $= 4a_0 =$ the radius of Bohr orbit for $n=2$.

Similarly, 3d with $m_l = \pm 2$, 4f with $m_l = \pm 3$

*Bohr model predicts the most probable location of e^- in one of several possible states in each energy level.

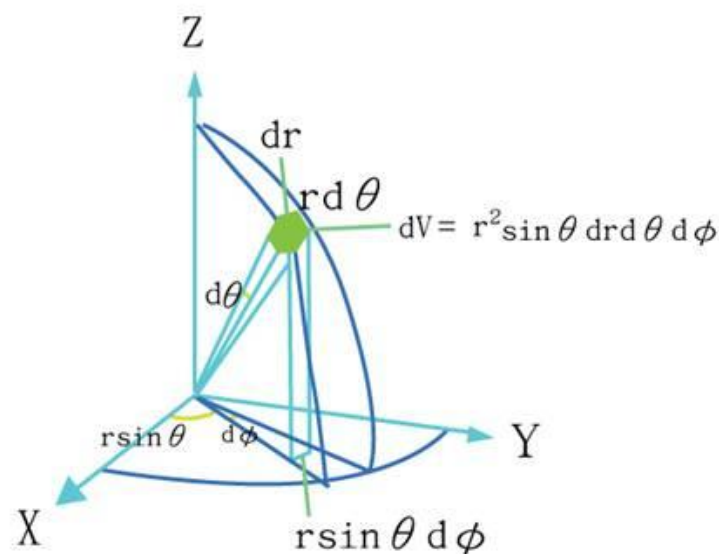
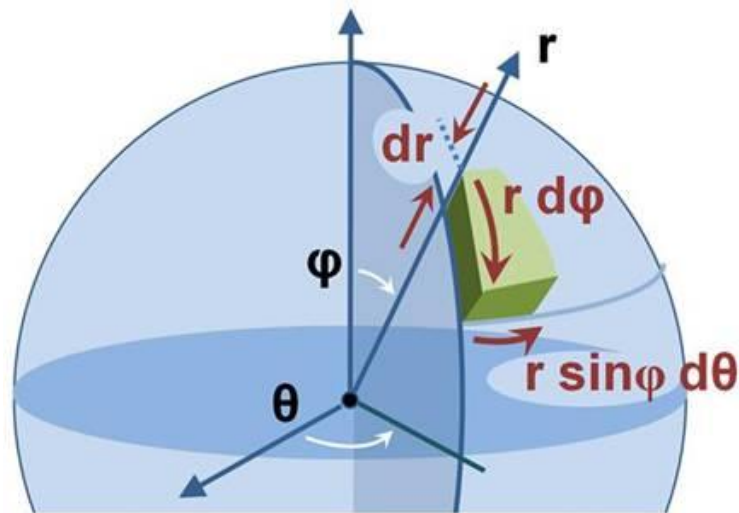


Figure 6.9 Volume element dV in spherical polar coordinates. (source:wikipedia)

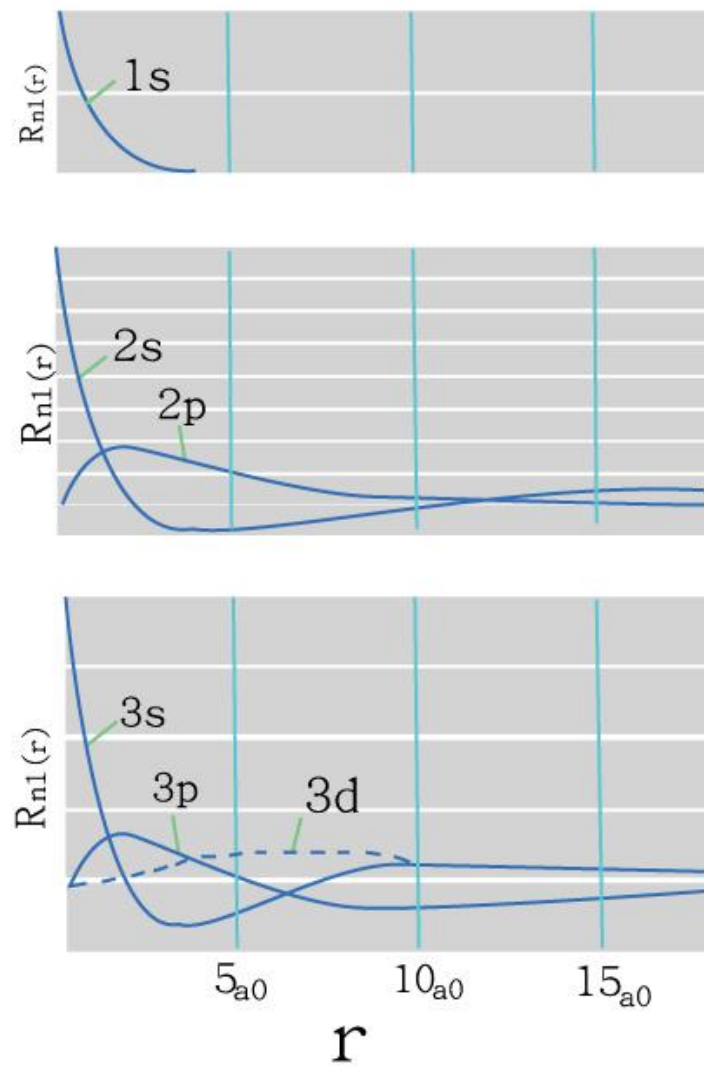


Figure 6.8 (see textbook) The variation with distance from the nucleus of the radial part of the electron wave function in hydrogen for various quantum states. The quantity $a_0 = 4\pi\epsilon_0\hbar^2/me^2 = 0.053$ nm is the radius of the first Bohr orbit.

※References:Modern Physics for scientists and engineers, Stephen T. Thornton Nonclassical Physics, RandyHarris.Quantum Physics of atoms, molecules,Solids,nuclei and Particles. Eisberg & Resnick

R depends on r and n, ℓ

R is a max at $r = 0$ for all s states, which correspond to $L = 0$

($\because \ell = 0$)

The value of $R = 0$ at $r = 0$ for the states with $\ell > 0$.

Probability of finding e^- probability of finding e^- in the

infinitesimal volume element $dV \Rightarrow |\phi|^2 dV$

$$dV = (dr)(rd\theta)(r \sin \theta d\phi)$$

$\Rightarrow p(r)dr$ of finding e^- in spherical shell between r & $r+dr$

$$p(r)dr = \int R^2 |\Theta|^2 |\Phi|^2 dV$$

$$= r^2 |R|^2 dr \int_0^\pi |\Theta|^2 \sin \theta d\theta \int_0^{2\pi} |\Phi|^2 d\phi$$

$$= r^2 |R|^2 \quad (\because \Theta \text{ \& } \Phi \text{ are normalized function})$$

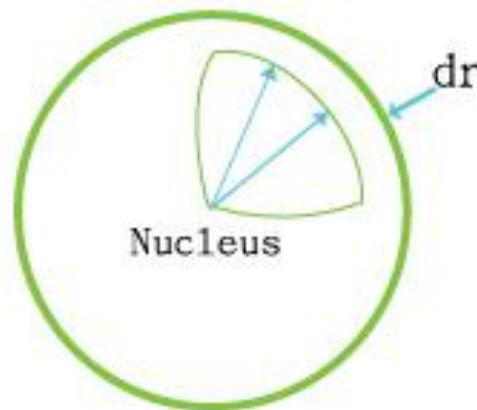


Figure 6.10 (see textbook) The probability of finding the electron in a hydrogen atom in the spherical shell between r and $r + dr$ from the nucleus is $P(r) dr$.

Figure 6.11 (see textbook) The probability of finding the electron in a hydrogen atom at a distance between r and $r + dr$ from the nucleus for the quantum states of Fig. 6.8.

※References: Modern Physics for scientists and engineers, Stephen T. Thornton Nonclassical Physics, Randy Harris. Quantum Physics of atoms, molecules, Solids, nuclei and Particles. Eisberg & Resnick

$\text{fig}(6.11) \Rightarrow p(r)dr$ }
 $\text{fig}(6.8) \Rightarrow R$ } Curves are quite different

p is not max at $r = 0$, as R is, but has its max a definite distance from it.

The most probable value of r for $\ell s e'$ is a_0 the orbital radius of a ground-state e' in Bohr model.

However, average value of r for $\ell s e'$ is $1.5a_0$ but average value

of $\frac{1}{r}$ is $\frac{1}{a_0}$

\Rightarrow energy level for Q.M. = Bohr models

【6.8 Radiative Transitions】

In Bohr model, an atom dropping from E_m to E_n

⇒ frequency ν of radiation emitted

$$\Rightarrow \nu = \frac{E_m - E_n}{h}$$

Time-dependent wave function Ψ_n in a state of quantum number n & energy E_n is the product of a time-dependent φ_n & time-varying function

$$\nu_n = E_n/h$$

$$\varphi_n = \varphi_n e^{-(iE_n/h)t} \quad \Psi_n^* = \varphi_n^* e^{(iE_n/h)t}$$

$$\begin{aligned} \Rightarrow \langle x \rangle &= \int_{-\infty}^{\infty} x \Psi_n^* \varphi_n dx = \int_{-\infty}^{\infty} x \varphi_n^* \varphi_n e^{[iE_n/h - iE_n/h]t} dx \\ &= \int_{-\infty}^{\infty} x \varphi_n^* \varphi_n dx \end{aligned}$$

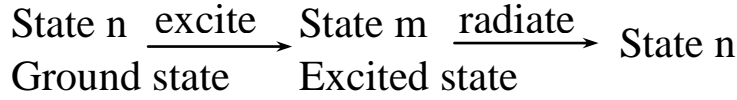
⇒ $\langle x \rangle$ is constant in time ($\because \varphi_n^*$ & φ_n are function of x)

⇒ The electron does not oscillate

⇒ No radiation

⇒ Q.M. predicts that a system in a specific quantum state does not radiate.

* consider e' shift from one state to another, e.g.



Ψ can exist in both state n & m \Rightarrow

$$\Psi = a\varphi_n + b\Psi_m$$

$$\left. \begin{array}{l} aa^* \equiv \text{probability in state n} \\ bb^* \equiv \text{probability in state m} \end{array} \right\} aa^* + bb^* = 1$$

$$\text{initially } a=1 \ \& \ b=0 \xrightarrow{\text{excite}} b=1 \ \& \ a=0 \xrightarrow{\text{radiate}} a=1 \ \& \ b=0$$

while e' is in either state \Rightarrow no radiation in the midst of transition

from m to n

\Rightarrow a, b are non-zero \Rightarrow EM waves produced

$$\begin{aligned} \langle x \rangle &= \int_{-\infty}^{\infty} x(a^*\varphi_n^* + b^*\Psi_m^*)(a\Psi_n + b\varphi_m)dx \\ &= \int_{-\infty}^{\infty} x(a^2\Psi_n^*\Psi_n + b^*a\varphi_m^*\varphi_n + a^*b\Psi_n^*\varphi_m + b^2\varphi_m^*\Psi_m)dx \\ &= a\int_{-\infty}^{\infty} x\varphi_n^*\varphi_n dx + b^2\int_{-\infty}^{\infty} x\varphi_m^*\varphi_m dx + b^*a\int_{-\infty}^{\infty} x\varphi_m^*e^{i(E_m/\hbar)t}\varphi_n e^{-i(E_n/\hbar)t} dx \\ &\quad + a^*b\int_{-\infty}^{\infty} x\varphi_n^*e^{i(E_n/\hbar)t}\varphi_m e^{-i(E_m/\hbar)t} dx \end{aligned}$$

last two terms

$$+ i \sin\left(\frac{E_m - E_n}{\hbar}\right) t \int_{-\infty}^{\infty} x[b^*a\varphi_m^*\varphi_n - a^*b\varphi_n^*\varphi_m] dx$$

$$\cos\left(\frac{E_m - E_n}{\hbar}\right)t \int_{-\infty}^{\infty} x [b^* a \varphi_m^* \varphi_n + a^* b \varphi_n^* \varphi_m] dx$$

for real part, it varies with time

$$\cos\left(\frac{E_m - E_n}{\hbar}\right)t = \cos 2\pi\left(\frac{E_m - E_n}{h}\right)t = \cos 2\pi\nu t$$

⇒ e' position oscillates at the frequency

$$\nu = \frac{E_m - E_n}{h}$$

⊙ When e' is in state n or m the expectation value of the e' position between these states, its position oscillates with ν .

⇒ like electric dipole & radiates EM waves ν .

Figure 6.13 (see textbook) Energy-level diagram for hydrogen showing transitions allowed by the selection rule $\Delta l = \pm 1$. In this diagram the vertical axis represents excitation energy above the ground state.

※References: Modern Physics for scientists and engineers, Stephen T. Thornton Nonclassical Physics, Randy Harris. Quantum Physics of atoms, molecules, Solids, nuclei and Particles. Eisberg & Resnick

【6.8 Selection Rules】

Forv, we don't need to know $\varphi_n, \varphi_m, a, b$

But if we would like to know the chance a given transition will

occur \Rightarrow we need to know $\varphi_n, \varphi_m, a, b$

If $\int_{-\infty}^{\infty} x \varphi_n \varphi_m^* dx \neq 0 \rightarrow$ allowed transition

$= 0 \rightarrow$ forbidden transition

In H atom \Rightarrow 3 quantum number needed to specify

initial(n', ℓ', m_ℓ') & final(n, ℓ, m_ℓ) states.

\Rightarrow Allowed transition $\int_{-\infty}^{\infty} u \varphi_{n\ell m_\ell} \varphi_{n'\ell'm_\ell'}^* dV \neq 0$

(u represents either x, y or z)

$\because \varphi_{n\ell m_\ell}$ are known $\Rightarrow \int_{-\infty}^{\infty} u \varphi_{n\ell m_\ell} \varphi_{n'\ell'm_\ell'}^* dV$ can be calculated

\Rightarrow only $\begin{cases} \Delta\ell = 1 \\ \Delta m_\ell = 0, \pm 1 \end{cases}$ the transition is allowed

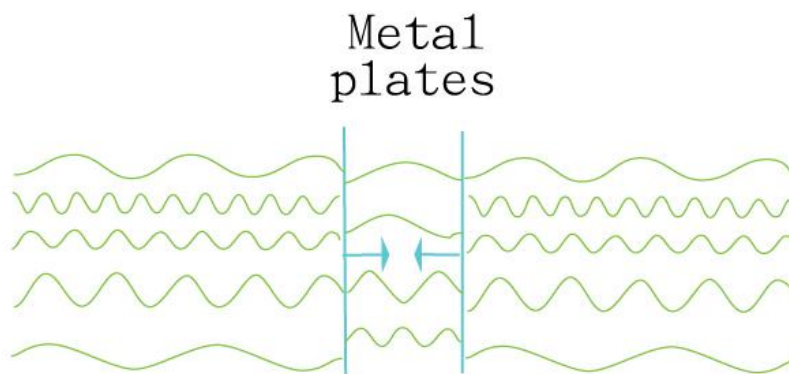


Figure 6.14 (see textbook) Two parallel metal plates exhibit the Casimir effect even in empty space. Virtual photons on any wavelength can strike the plates from the outside, but photons trapped between the plates can have only certain wavelengths. The resulting imbalance produces inward forces on the plates.

※References: Modern Physics for scientists and engineers, Stephen T. Thornton Nonclassical Physics, Randy Harris. Quantum

Physics of atoms, molecules, Solids, nuclei and Particles. Eisberg & Resnick

【6.9 Zeeman Effect】

Magnetic dipole in a magnetic field \mathbf{B}

$$\Rightarrow \text{torque } \boldsymbol{\tau} = uB\sin\theta = \mathbf{u} \times \mathbf{B}$$

U_m , by definition $U_m = 0$ when $\theta = \frac{\pi}{2}$

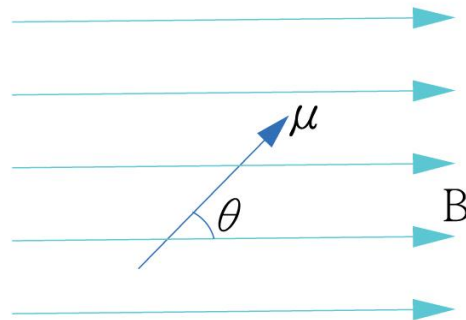
$$\Rightarrow U_m = \int_{\frac{\pi}{2}}^{\theta} \tau d\theta = uB \int_{\frac{\pi}{2}}^{\theta} \sin\theta d\theta = -uB \cos\theta = -\mathbf{u} \cdot \mathbf{B}$$

magnetic dipole tends to align itself with \mathbf{B}

The magnetic moment of the orbital e^- in H atom depends on L

The magnetic moment of a current loop

$$u = IA$$



A magnetic dipole of moment μ at the angle θ relative to a magnetic field \mathbf{B}

Figure 6.15 (see textbook) A magnetic dipole of moment \mathbf{u} at the angle θ relative to a magnetic field \mathbf{B} .

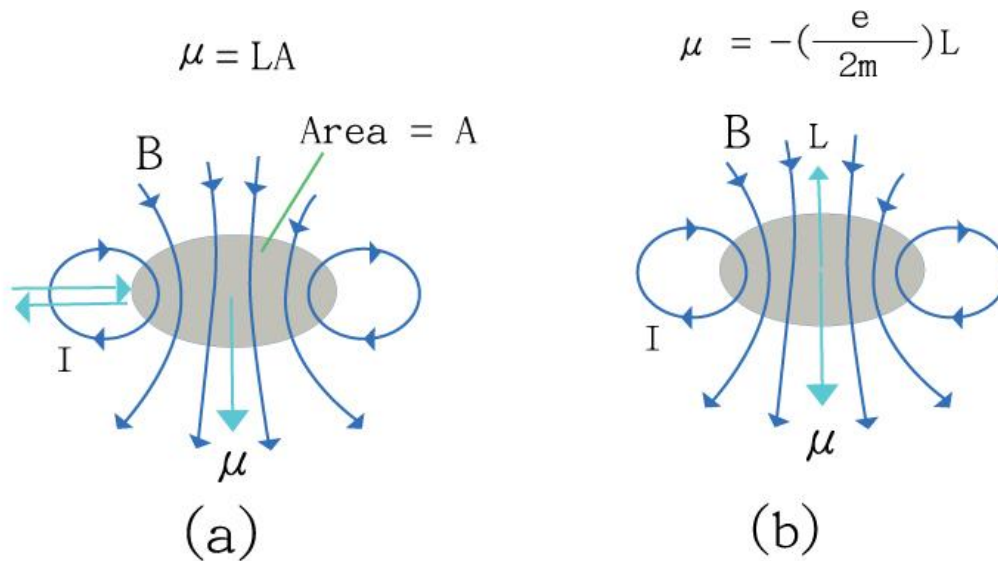


Figure 6.16 (see textbook) (a)Magnetic moment of a current loop enclosing area A. (b)Magnetic moment of an orbiting electron of angular momentum **L**.

※References:Modern Physics for scientists and engineers, Stephen T. Thornton Nonclassical Physics, RandyHarris.Quantum Physics of atoms, molecules,Solids,nuclei and Particles. Eisberg & Resnick

If e' makes f rev/s in a circular orbit of r

$$\Rightarrow I = -ef \Rightarrow u = -ef\pi r^2$$

$$L = mvr = m(2\pi fr)r = 2\pi mfr^2$$

$$\vec{u} = -\left(\frac{e}{2m}\right)\vec{L} \quad - : \text{negative charge}$$

$(-e/2m) : \text{gyromagnetic ratio}$

$$U_m = \left(\frac{e}{2m}\right)LB \cos \theta$$

$$L = \sqrt{l(l+1)}\hbar$$

⇒ magnetic energy $U_m = m_\ell \left(\frac{e\hbar}{2m} \right) B$

$$\frac{e\hbar}{2m} : \text{Bohr magneton}$$

$$\begin{aligned} u_B &= 9.274 \times 10^{-24} \text{ J/T} \\ &= 5.788 \times 10^{-5} \text{ eV/T} \end{aligned}$$

⇒ In a magnetic field, the energy of a particular atomic state depends on m_ℓ & n .

⇒ A state of total quantum number n breaks up into several substates when the atom is in a magnetic field. Their energy are slightly more or less than the energy of the state in the absence of field.

⇒ Individual spectral lines “splitting” into separate lines

⇒ Zeeman Effect

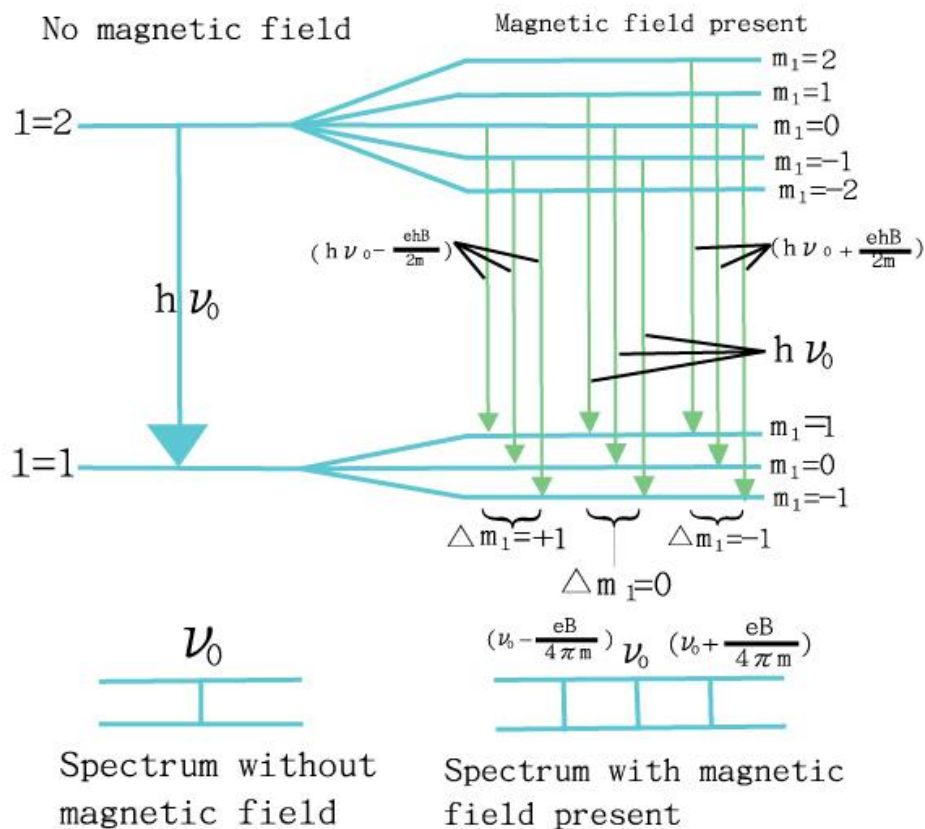


Figure 6.17 (see textbook) The normal Zeeman effect.

※References:Modern Physics for scientists and engineers, Stephen T. Thornton Nonclassical Physics, RandyHarris.Quantum Physics of atoms, molecules,Solids,nuclei and Particles. Eisberg & Resnick

The spacing of lines depends on magnitude of field

m_l have $2l + 1$ values

$\therefore l$ split into $2l + 1$ substates in magnetic field energy

difference is $u_B B$

$\therefore \Delta m_l = 0, \pm 1$ (selection rule)

\Rightarrow spectral line from transition between 2 states of different

l to be split into 3 components.

* Normal Zeeman Effect consists of splitting of a spectral line of

$$\nu_0 \text{ into } \left\{ \begin{array}{l} \nu_1 = \nu_0 - \frac{eB}{4\pi m} = \nu_0 - u_B \cdot \frac{B}{h} \\ \nu_2 = \nu_0 \\ \nu_3 = \nu_0 + \frac{eB}{4\pi m} = \nu_0 + u_B \cdot \frac{B}{h} \end{array} \right.$$

ex 6.4

A sample of a certain element is placed in a 0.3T magnetic field & suitably excited. How far apart are the Zeeman components of 450nm spectra line of this element?

Sol.

$$\Delta \nu = \frac{eB}{4\pi m}$$

$$\nu = \frac{c}{\lambda} \quad d\nu = -c \frac{d\lambda}{\lambda^2}$$

$$\Rightarrow \Delta \lambda = \frac{\lambda^2 \Delta \nu}{c} = \frac{eB \lambda^2}{4\pi m c} = 2.83 \times 10^{-12} m = 0.00283 nm$$