

Atomic Physics

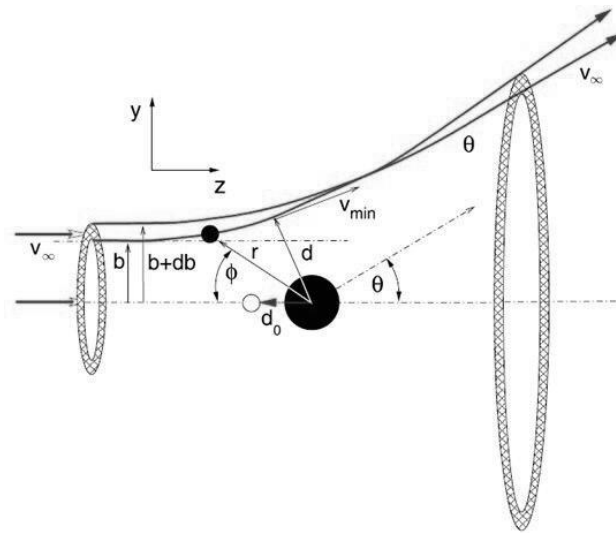
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August 18, 2020

Chapter 1

Rutherford's Alpha Particle Scattering Experiment



According to Coulomb's Law:

$$F = \frac{1}{4\pi\epsilon_0} \cdot \frac{Z_1 Z_2 e^2}{r^2} = \frac{C}{r^2}$$

$$C = \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0}$$

$$F_y = F \sin \phi = \frac{C}{r^2} \sin \phi$$

Law of momentum and angular momentum

$$mv_y = \int F_y dt$$

$$mr^2 \dot{\phi} = mv_\infty b$$

Then we integrate

$$\begin{aligned}
v_y &= \frac{1}{m} \int \frac{C}{r^2} \sin \phi \, dt = \frac{1}{m} \int \frac{C}{r^2} \sin \phi \frac{dt}{d\phi} \, d\phi = \frac{1}{m} \int \frac{C}{r^2} \sin \phi \frac{r^2}{v_\infty b} \, d\phi = \frac{C}{mv_\infty b} \int_0^{\pi-\theta} \sin \phi \, d\phi \\
&= \frac{C}{mv_\infty b} (1 + \cos \theta)
\end{aligned}$$

Now we need to relate θ with b , Since

$$v_y = v_\infty \sin \theta$$

We have

$$\frac{C}{mv_\infty b} (1 + \cos \theta) = v_\infty \sin \theta$$

So that

$$\cot \frac{\theta}{2} = \frac{1 + \cos \theta}{\sin \theta} = \frac{mv_\infty^2 b}{C} = \frac{2E_0 b}{C}$$

Note that this trigonometry transform is used

$$\frac{1 + \cos \theta}{\sin \theta} = \frac{2 \cos^2 \frac{\theta}{2}}{2 \sin \frac{\theta}{2} \cos \frac{\theta}{2}} = \cot \frac{\theta}{2}$$

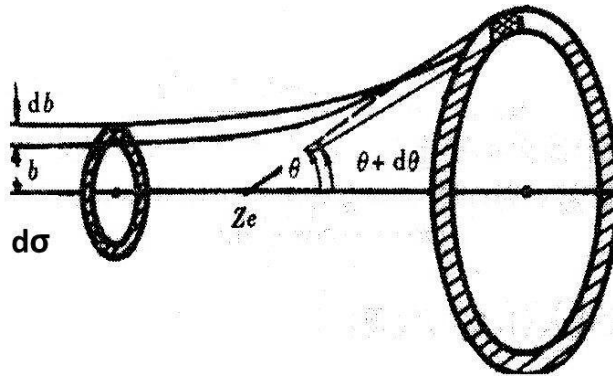
Finally

$$b = \frac{C}{2E_0} \cdot \cot \frac{\theta}{2} = \frac{1}{4\pi\epsilon_0} \frac{Z_1 Z_2 e^2}{2E_0} = \frac{1}{4\pi\epsilon_0} \cdot \frac{Z_1 Z_2 e^2}{mv_\infty^2} \cdot \cot \frac{\theta}{2}$$

\Rightarrow

$$\cot \frac{\theta}{2} = 4\pi\epsilon_0 \frac{mv_\infty^2}{Z_1 Z_2 e^2} b \quad (1.1)$$

Now we begin to find the relation between db and $d\Omega$



$$d\sigma = 2\pi b \, db = \pi \left(\frac{1}{4\pi\epsilon_0} \right)^2 \left(\frac{Z_1 Z_2 e^2}{mv_\infty^2} \right)^2 \frac{\cos \frac{\theta}{2}}{\sin^3 \frac{\theta}{2}} d\theta$$

$$\Omega = 2\pi (1 - \cos \theta)$$

$$d\Omega = 2\pi \sin \theta d\theta = 4\pi \sin \frac{\theta}{2} \cos \frac{\theta}{2} d\theta$$

Then we found $\frac{d\sigma}{d\Omega}$ is only related with θ

$$\frac{d\sigma}{d\Omega} = \left(\frac{1}{4\pi\epsilon_0} \right)^2 \left(\frac{Z_1 Z_2 e^2}{2mv_\infty^2} \right)^2 \sin^{-4} \frac{\theta}{2} \quad (1.2)$$

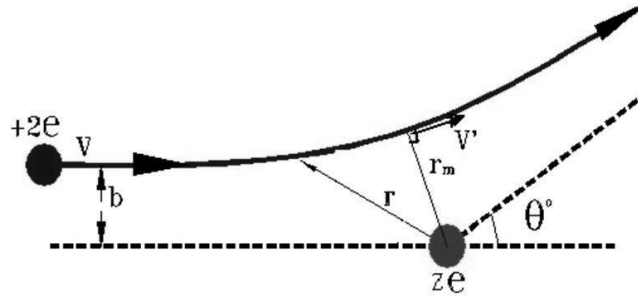
As for a thin gold leaf, we assume there's only one layer of atoms, the density of atoms is N , the area and thickness of gold leaf are A and t

When n particles passed through the gold leaf, dn of them ended up in $d\Omega$

$$\frac{dn}{n} = \frac{NAtd\sigma}{A} = Ntd\sigma = Nt \left(\frac{1}{4\pi\epsilon_0} \right)^2 \left(\frac{Z_1 Z_2 e^2}{2mv_\infty^2} \right)^2 \sin^{-4} \frac{\theta}{2} d\Omega$$

$$\frac{dn}{d\Omega} \sin^4 \frac{\theta}{2} = nNt \left(\frac{1}{4\pi\epsilon_0} \right)^2 \left(\frac{Z_1 Z_2 e^2}{2mv_\infty^2} \right)^2 = \text{const} \quad (1.3)$$

For alpha particles, $Z_1 = 2$. We can also take the closest distance between the 2 particles as the radius of a particle.



What we have already known are:

$$\frac{1}{2}MV^2 = \frac{1}{2}MV'^2 + \frac{2Ze^2}{4\pi\epsilon_0 r_m}$$

$$MVb = MV'r_m$$

$$b = \frac{1}{4\pi\epsilon_0} \cdot \frac{2Ze^2}{MV} \cdot \cot \frac{\theta}{2}$$

We solve r_m with the equation we known.

$$\frac{1}{4\pi\epsilon_0} \cdot \frac{2Ze^2}{M} \cdot \cot \frac{\theta}{2} = V'r_m$$

$$\frac{1}{2}MV^2 = \frac{1}{2}M \left(\frac{1}{4\pi\epsilon_0} \cdot \frac{2Ze^2}{Mr_m} \cdot \cot \frac{\theta}{2} \right)^2 + \frac{2Ze^2}{4\pi\epsilon_0 r_m}$$

$$\frac{1}{2}MV^2 r_m^2 - \frac{2Ze^2}{4\pi\epsilon_0} r_m - \frac{1}{2}M \left(\frac{1}{4\pi\epsilon_0} \cdot \frac{2Ze^2}{M} \cdot \cot \frac{\theta}{2} \right)^2 = 0$$

Finally

$$r_m = \frac{1}{4\pi\epsilon_0} \frac{2Ze^2}{MV^2} \left(1 + \frac{1}{\sin \frac{\theta}{2}} \right) \quad (1.4)$$

Chapter 2

The Energy and Radiation of Atoms

2.1 Rydberg Constant and Wavelength of Radiation

Wave number of Hydrogen Atoms:

$$\tilde{\nu} = \frac{1}{\lambda} = Z^2 R \left[\frac{1}{m^2} - \frac{1}{n^2} \right] \quad (2.1)$$

Where $Z = 1$

Lyman Series	$\tilde{\nu} = R \left[\frac{1}{1^2} - \frac{1}{n^2} \right]$	$n = 2, 3, 4, \dots$
Balmer Series	$\tilde{\nu} = R \left[\frac{1}{2^2} - \frac{1}{n^2} \right]$	$n = 3, 4, 5, \dots$
Paschen Series	$\tilde{\nu} = R \left[\frac{1}{3^2} - \frac{1}{n^2} \right]$	$n = 4, 5, 6, \dots$
Brackett Series	$\tilde{\nu} = R \left[\frac{1}{4^2} - \frac{1}{n^2} \right]$	$n = 5, 6, 7, \dots$
Pfund Series	$\tilde{\nu} = R \left[\frac{1}{5^2} - \frac{1}{n^2} \right]$	$n = 6, 7, 8, \dots$

Spectroscopic term

$$T(m) = \frac{Z^2 R}{m^2} \quad T(n) = \frac{Z^2 R}{n^2}$$

Then

$$\tilde{\nu} = T(m) - T(n) \quad (2.2)$$

Energy of emitted light

$$E = \frac{hc}{\lambda} = hc\tilde{\nu} = hc[T(m) - T(n)] = \frac{Rhc}{m^2} - \frac{Rhc}{n^2}$$

2.2 Bohr's Theory of Hydrogen Atoms

Energy of steady states:

$$E_n = -\frac{1}{2} \frac{Ze^2}{4\pi\epsilon_0 r_n}$$

Transition

$$h\nu = E_n - E_m$$

Angular Momentum

$$L = n \cdot \frac{h}{2\pi} = n\hbar = m_e v_n r_n$$

$$m_e \frac{v_n^2}{r_n} = \frac{Ze^2}{4\pi\epsilon_0 r_n^2}$$

So that

$$\frac{n^2 \hbar^2}{m_e r_n^3} = \frac{Ze^2}{4\pi\epsilon_0 r_n^2}$$

From which we can indicate that the radius is quantized.

$$r_n = \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2} \cdot \frac{n^2}{Z} = a_0 \cdot \frac{n^2}{Z} \quad \left(a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2} \right) \quad (2.3)$$

For hydrogen atoms, $Z = 1$. The energy is also quantized.

$$E_n = -\frac{1}{2} \frac{Ze^2}{4\pi\epsilon_0} \frac{m_e e^2}{4\pi\epsilon_0 \hbar^2} \cdot \frac{Z}{n^2} = -\frac{m_e e^4}{2 (4\pi\epsilon_0 \hbar)^2} \cdot \frac{Z^2}{n^2}$$

The velocity is also quantized

$$v_n = \frac{n\hbar}{m_e r_n} = \frac{n\hbar}{m_e} \frac{m_e e^2}{4\pi\epsilon_0 \hbar^2} \cdot \frac{Z}{n^2} = \frac{e^2}{4\pi\epsilon_0 \hbar} \cdot \frac{Z}{n} = \frac{Z\alpha c}{n}$$

$$\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c} = \frac{1}{137}$$

Calculate the value of Rydberg Constant

$$E = -\frac{m_e e^4}{2 (4\pi\epsilon_0 \hbar)^2} \cdot \frac{Z^2}{n^2} = -\frac{2\pi^2 m_e e^4}{(4\pi\epsilon_0 \hbar)^2} \cdot \frac{Z^2}{n^2}$$

$$\frac{hc}{\lambda} = E_2 - E_1 = \frac{2\pi^2 m_e e^4 Z^2}{(4\pi\epsilon_0 \hbar)^2} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$

$$\tilde{\nu} = \frac{1}{\lambda} = \frac{2\pi^2 m_e e^4 Z^2}{(4\pi\epsilon_0)^2 h^3 c} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$

\Rightarrow

$$R = \frac{2\pi^2 m_e e^4}{(4\pi\epsilon_0)^2 h^3 c}$$

2.3 Rydberg Constant of Different Atoms

In previous sections, we assumed that the nucleus is fixed at a point, with the electron surrounded. But in fact, the nucleus's mass is not infinity, and it moves as well. So that for different atoms, the Rydberg Constants varies. In a two-body system, we define the Reduced Mass of a system as

$$\mu = \frac{Mm}{M+m}$$

And we replace the Reduced Mass with m_e

$$\begin{aligned} R_\infty &= \frac{2\pi^2 m e^4}{(4\pi\epsilon_0)^2 h^3 c} \\ R_A &= R_\infty \cdot \left[\frac{1}{1 + \frac{m}{M}} \right] \end{aligned} \tag{2.4}$$

2.4 Sommerfeld's Quantize Condition

For any coordinate q and its momentum p

$$\oint p \, dq = nh$$

holds

2.5 Quantized Magnetron

$$\begin{aligned} \mu &= iA \\ i &= \frac{e}{\tau} \\ A &= \int_0^{2\pi} \frac{1}{2} r \cdot r \, d\phi \\ &= \frac{1}{2} \int_0^\tau r^2 \omega \, dt \\ &= \frac{1}{2m} \int_0^\tau m r^2 \omega \, dt \\ &= \frac{p_\phi}{2m} \tau \end{aligned}$$

Consider that

$$\int_0^{2\pi} p_\phi \, d\phi = 2\pi p_\phi = nh$$

We have

$$\mu = \frac{e}{2m} p_\phi = \frac{eh}{4\pi m} \cdot n$$

Let

$$\mu_B = \frac{eh}{4\pi m} = \frac{e}{2m} \hbar \tag{2.5}$$

Then μ_B is the minimum unit of magneton.

Chapter 3

Basics of Quantum Mechanics

3.1 De Broglie Wave

$$\lambda = \frac{h}{p} = \frac{h}{mv} \quad (3.1)$$

3.2 Uncertainty Principle

$$\Delta p \Delta q \geq \frac{\hbar}{2} \quad \Delta E \Delta t \geq \frac{\hbar}{2} \quad (3.2)$$

3.3 Wave Function

$$\psi = \psi_0 \exp \left[\frac{i}{\hbar} (\vec{p} \cdot \vec{r} - Et) \right] \quad (3.3)$$

$$\begin{cases} \nabla \psi = -i \frac{\vec{p}}{\hbar} \psi \\ \nabla^2 \psi = -\frac{p^2}{\hbar^2} \psi \\ \frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} E \psi \end{cases} \quad (3.4)$$

Three properties

- limited
- Normalized
- Continuous

3.4 Schrodinger Equation

$$\frac{p^2}{2m} + V = E \quad \Rightarrow \quad \frac{p^2}{2m} \psi + V \psi = E \psi$$

\Rightarrow

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi = i \hbar \frac{\partial \psi}{\partial t} \quad (3.5)$$

Simplified form for E is constant:

$$Hu = Eu$$

$$H = \left[-\frac{\hbar^2}{2m} \nabla^2 + V \right]$$

Chapter 4

Alkalis and Self-spin of Electrons

4.1 Four Series of Spectrum

Principle Series	$p\tilde{\nu}_n = \frac{R}{(2 - \Delta_s)^2} - \frac{R}{(n - \Delta_p)^2}$	$n = 2, 3, 4, \dots$	$P \rightarrow S$
Sharp (Second Subordinate) Series	$s\tilde{\nu}_n = \frac{R}{(2 - \Delta_p)^2} - \frac{R}{(n - \Delta_s)^2}$	$n = 3, 4, 5, \dots$	$S \rightarrow P$
Diffuse (First Subordinate) Series	$d\tilde{\nu}_n = \frac{R}{(2 - \Delta_p)^2} - \frac{R}{(n - \Delta_d)^2}$	$n = 3, 4, 5, \dots$	$D \rightarrow P$
Fundamental (Bergmann) Series	$f\tilde{\nu}_n = \frac{R}{(3 - \Delta_d)^2} - \frac{R}{(n - \Delta_f)^2}$	$n = 4, 5, 6, \dots$	$F \rightarrow D$

The Spectroscopic term of alkalis

$$T = \frac{R}{n^{*2}} = \frac{R}{(n - \Delta)^2} \quad (4.1)$$

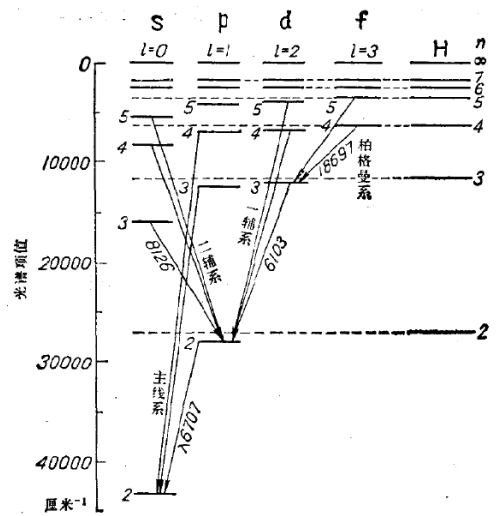


Figure 4.1: Energy Level of Lithium Atom

The wavenumbers of spectroscopic lines

$$\tilde{\nu}_n = \tilde{\nu}_\infty - \frac{R}{n^{*2}} \quad (4.2)$$

4.2 Self-spin and Orbital Angular Momentum

$$s = \frac{1}{2} \quad l = 1, 2, 3, \dots \quad j = l \pm s$$

Self-spin	$p_s = \sqrt{s(s+1)}\hbar$	$\mu_s = \frac{e}{m}p_s$
Orbital	$p_l = \sqrt{l(l+1)}\hbar$	$\mu_s = \frac{e}{2m}p_l$
Total	$p_j = \sqrt{j(j+1)}\hbar$	$\mu_j = g\frac{e}{2m}p_j$

$$\vec{p}_s + \vec{p}_l = \vec{p}_j$$

4.3 Selection Rule in Transition

$$\begin{cases} \Delta l = \pm 1 \\ \Delta j = 0, \pm 1 \end{cases}$$

Chapter 5

Atoms with Two Electrons

5.1 LS Coupling

Compound Self-spin Angular Momentum	$S = 1, 0$	$P_S = \sqrt{S(S+1)}\hbar$
Compound Orbital Angular Momentum	$L = l_1 + l_2 , l_1 + l_2 - 1, \dots, l_1 - l_2 $	$P_S = \sqrt{L(L+1)}\hbar$
Compound Total Angular Momentum	$J = L + S , L + S - 1, \dots, L - S $	$P_S = \sqrt{S(S+1)}\hbar$

5.1.1 Hund's Law

- For a given electron configuration, the term with maximum multiplicity has the lowest energy. The multiplicity is equal to $2S + 1$, where S is the total spin angular momentum for all electrons.
- For a given multiplicity, the term with the largest value of the total orbital angular momentum quantum number L , has the lowest energy.
- For a given term, in an atom with outermost subshell half-filled or less, the level with the lowest value of the total angular momentum quantum number J , (for the operator $J = L + S$) lies lowest in energy. If the outermost shell is more than half-filled, the level with the highest value of J , is lowest in energy.

5.1.2 Rules of Transition

$\Delta S = 0$	$\Delta L = 0, \pm 1$	$\Delta J = 0, \pm 1 \quad (0 \rightarrow 0 \text{ forbidden})$
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5.2 jj Coupling

Self-spin Angular Momentum	$s_1 = \frac{1}{2}$	$s_2 = \frac{1}{2}$
Orbital Angular Momentum	l_1	l_2
Total Angular Momentum	$j_1 = l_1 \pm s_1$	$j_2 = l_2 \pm s_2$
Compound Total Angular Momentum	$J = j_1 + j_2 , j_1 + j_2 - 1, \dots, j_1 - j_2 $	$P_J = \sqrt{J(J+1)}\hbar$

5.3 Pauli exclusion principle

For state $nsns$ or ns^2 (for instance, $1s1s$ or $2s2s$), 3S_1 can not exist.

Chapter 6

Atoms in Magnetic Field

6.1 Magnetic Moment of Atoms

$$\mu_L = -\frac{e}{2m}p_l = -\sqrt{l(l+1)}\mu_B \quad \mu_B = \frac{e\hbar}{2\pi m} = \frac{e\hbar}{2m} \quad (\text{Bohr magneton})$$

6.2 Lande Factor

$$g = 1 + \frac{j(j+1) - l(l+1) + s(s+1)}{2j(j+1)}$$

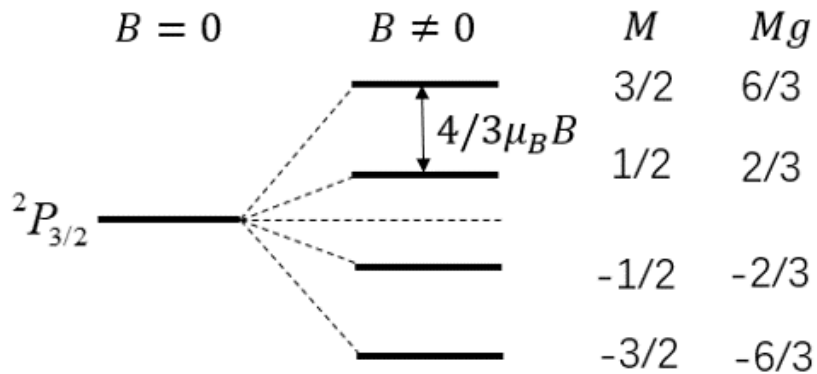
For single electron atom:

$$\mu_j = g\frac{e}{2m}p_j$$

For multi electron atom:

$$\mu_J = -g\frac{e}{2m}P_J$$

6.3 Energy of Atom in Magnetic Field



$$\Delta E = (M_2 g_2 - M_1 g_1) \mu_B B \quad M = J, J-1, J-2, \dots, -J$$

$$\Delta\tilde{\nu} = \frac{1}{\lambda'} - \frac{1}{\lambda} = [M_2g_2 - M_1g_1] \frac{Be}{4\pi mc} = [M_2g_2 - M_1g_1] L \quad L = \frac{Be}{4\pi mc}$$

${}^2P_{3/2}$	\longrightarrow ${}^2S_{1/2}$					
M	3/2	1/2	-1/2	-3/2		
M_2g_2	6/3	2/3	-2/3	-6/3		
			X		/	
M_1g_1		1	-1			
<hr/>						
	-5/3	-3/3	-1/3	1/3	3/3	5/3

$$\Delta\tilde{\nu} = \Delta\left(\frac{1}{\lambda}\right) = \left(-\frac{5}{3}, -\frac{3}{3}, -\frac{1}{3}, \frac{1}{3}, \frac{3}{3}, \frac{5}{3}\right)L$$

6.4 Selection Rule

$$\begin{aligned} \Delta M = 0 &\Rightarrow \pi \\ \Delta M = \pm 1 &\Rightarrow \sigma \end{aligned}$$

π beam cannot be observed in the perspective which is parallel to B , both beam can be observed in the perspective perpendicular to B .

6.5 Abnormal Zeeman effect

$$\Delta\tilde{\nu} = [M_2g_2 - M_1g_1] L \neq \pm L \Rightarrow M_2g_2 - M_1g_1 \neq \pm 1$$

Chapter 7

Shell Structure

7.1 Pauli Exclusion Principle

For each two electrons in atom, n , l , m_l and m_s cannot all be same.

For each n , l can be $0, 1, 2, \dots, n-1$

For each l , m_l can be $l, l-1, \dots, -l$

For each m_l , m_s can be $\frac{1}{2}$ or $-\frac{1}{2}$

7.2 Maximum Electrons Allowed for Each Shell and Sub-shell

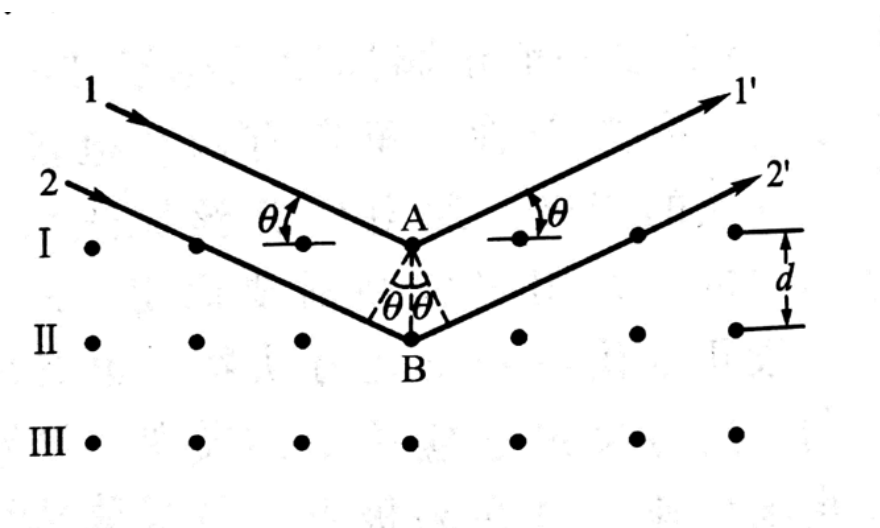
For shell: $N_n = 2n^2$

For sub-shell: $N_l = 2(2l+1)$

Chapter 8

X-ray

8.1 X-ray Diffraction



$$n\lambda = 2d \sin \theta$$

Chapter 9

Molecules

9.1 Oscillation Energy

Spectrum: near infrared

$$\frac{1}{\lambda} = \tilde{\nu} = \frac{1}{2\pi c} \sqrt{\frac{K}{m}} \qquad m = \frac{m_1 m_2}{m_1 + m_2}$$

9.2 Rotation Energy

Spectrum: far infrared

$$\Delta E_r = \frac{h^2}{8\pi^2 I} 2J \qquad \Delta \tilde{\nu} = \frac{h}{8\pi^2 I c} 2J = 2B \qquad B = \frac{h}{8\pi^2 I c}$$

9.3 Oscillation Combines Rotation

$$\tilde{\nu} = \tilde{\nu}_0 \pm (2BJ)$$