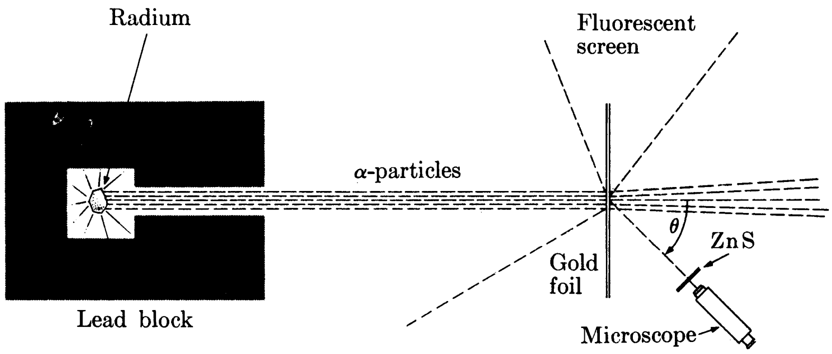
(Lecture 5) The Atomic Models

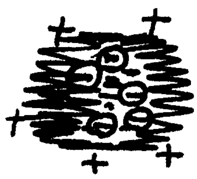
1. Rutherford Scattering Experiment

- Rutherford α-입자 산란 실험 : E. Rutherford, Geiger, Marsden 1911 년 경.
  (Experimental arrangement)



1/20,000 의 비율로 α-입자들이 90° 이상으로 편향.

2. Thomson Model of the Atom



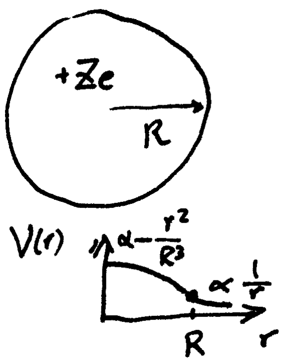
- Thomson model = “plum-pudding” model
  dispersive positive charge cloud
  + electron plum
- Analysis of Rutherford scattering in Thomson model
  +Ze 전하가 반경 R(원자 반경) 내에 균일하게 분포.

  Surface potential $V(R) = \dfrac{1}{4\pi\varepsilon_0}\dfrac{Ze}{R}$

  Center potential $V(0) = \dfrac{3}{8\pi\varepsilon_0}\dfrac{Ze}{R}$

  +ze 의 전하가 center 를 통과하는 경우의 potential 높이

  $$= \frac{3}{8\pi\varepsilon_0}\frac{zZe^2}{R} \equiv V_c$$



α-입자의 경우 z=2, Au foil Z=79,

R $\approx$ 1 Å = 10^{-10} m $\rightarrow$ V_c $\approx$ 3400 eV

E_α $\approx$ 5 MeV = 5×10^6 eV >>> V_c

$\rightarrow$ 단일 충돌에 의해서는 큰 각도로의 산란이 불가능.

$\rightarrow$ 전자와의 충돌? 전자 질량 $\approx$ (1/7500)(α-입자 질량)

다중 산란(multiple scattering) :

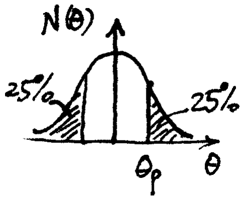
산란각의 평균 $\bar{\theta} = 0$, 산란각의 분산 $\overline{\theta^2} = \sigma^2$

산란각 θ에 대한 분포 함수 $\rightarrow$

Gaussian $N(\theta) = N(0)e^{-\theta^2/2\sigma^2}$

$\uparrow$ 산란각 θ에 대한 단위 입체각 당 산란수

N(0) : 0° 방향의 단위 입체각 당 산란수



50% 산란 각도 $\theta_p = 0.6745\sigma = 0.87°$ $\rightarrow$ $\sigma = 1.3°$

주어진 σ에 대해 $\theta = 90°$일때는

$$N(90^\circ) = N(0)\times e^{-2434} \approx N(0)\times 10^{-1057} \quad (\log_{10} e \cong 0.434)$$

3. Rutherford Model of the Atom

- Implication of large angle scattering in the Rutherford experiment

  large deflection by a single encounter

  $\rightarrow$ very intense field (force) from close encounter

  $\rightarrow$ very concentrated(=small volume) charge (at the nucleus) & electrons surrounding the nucleus

- Analysis of Rutherford scattering

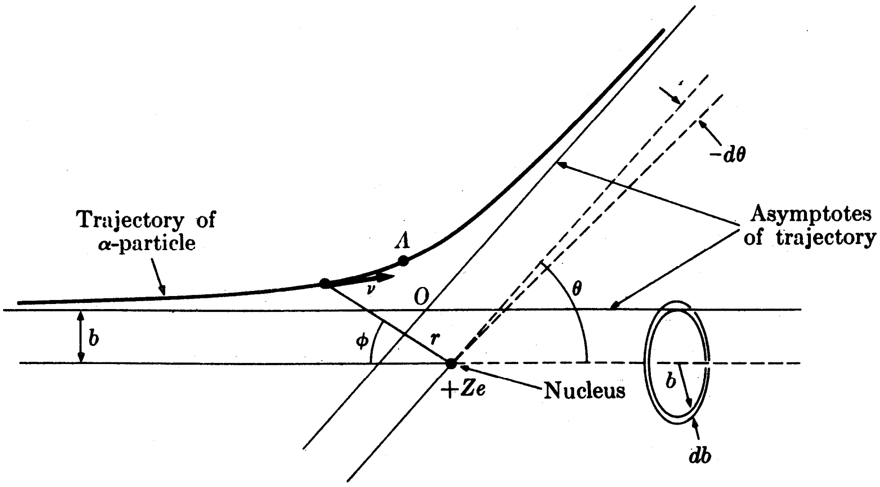
  α-particle 의 impact parameter – b(unknown)

  initial velocity v_0

  final velocity v_f

  electrostatic potential $\dfrac{1}{4\pi\varepsilon_0}\dfrac{zZe^2}{r}$

  표적 핵의 질량 >> α-입자의 질량, 따라서 표적핵의 반동(recoil) 무시 $\rightarrow$ 표적핵은 고정(원점), 좌표계 (r, ϕ), 산란각 θ



총에너지 보존 법칙

$$E=\tfrac{1}{2}mv_0^2=\tfrac{1}{2}mv_f^2=\tfrac{1}{2}m(\dot{r}^2+r^2\dot{\phi}^2)+\frac{zZe^2}{4\pi\varepsilon_0 r}$$

$v_f=v_0$: final asymptotic velocity = initial velocity

각운동량 보존 법칙 (← 中心力 작용)

$mr^2\dot{\phi}=mv_0 b=mv_f b'$; $v_f=v_0$ 이므로 $b'=b$

Let a parameter $2q\equiv$(정면 충돌 시의 최단 접근 거리)

$$=\frac{(zZe^2)/4\pi\varepsilon_0}{E}=\text{const}$$

$$\rightarrow \quad \dot{r}=\mp v_0\left(1-\frac{2q}{r}-\frac{b^2}{r^2}\right)^{1/2}$$ -: approaching, +: receding

$$\rightarrow \quad \frac{d\phi}{dr}=\mp\frac{b}{r^2}\left(1-\frac{2q}{r}-\frac{b^2}{r^2}\right)^{-1/2} \quad \leftarrow \quad \frac{d\phi}{dr}=\frac{\dot{\phi}}{\dot{r}}$$ instead of $\dot{\phi}$

$(r=\infty, \phi=0)\rightarrow$ approaching point A

(solution) $$\phi=\cos^{-1}\left[\frac{b}{\sqrt{b^2+q^2}}\left(1-\frac{2q}{r}-\frac{b^2}{r^2}\right)^{1/2}\right]-\cos^{-1}\left(\frac{b}{\sqrt{b^2+q^2}}\right)$$

closest approach : $r=r_A$, $\dot{r}_A=0 \quad\rightarrow\quad 1-\frac{2q}{r_A}-\frac{b^2}{r_A^2}=0$

$$\phi_A = \cos^{-1} 0 - \cos^{-1}\left(\frac{b}{\sqrt{b^2+q^2}}\right) = \frac{\pi}{2} - \cos^{-1}\left(\frac{b}{\sqrt{b^2+q^2}}\right)$$

symmetric trajectory about A :

$$\theta = \pi - 2\phi_A = 2\cos^{-1}\left(\frac{b}{\sqrt{b^2+q^2}}\right)$$

Let $\frac{b}{\sqrt{b^2+q^2}} = \cos\frac{\theta}{2}$, *then* $\frac{q}{\sqrt{b^2+q^2}} = \sqrt{1-\frac{b^2}{b^2+q^2}} = \sin\frac{\theta}{2}$.

$$\frac{b}{q} = \frac{\cos\frac{\theta}{2}}{\sin\frac{\theta}{2}} = \cot\frac{\theta}{2} \quad or \quad b = q\cot\frac{\theta}{2} \quad (b \text{ 와 } \theta\text{간의 관계})$$

impact parameter range (b, b+db) → area dσ → deflection (θ, θ-dθ)

dσ = 2πbdb

$$b = q\cot\frac{\theta}{2} \quad \rightarrow \quad db = -\frac{q}{2}\frac{d\theta}{\sin^2(\theta/2)}$$

$$d\sigma = 2\pi b db = \pi q^2 \frac{\cos(\theta/2)}{\sin^3(\theta/2)} d\theta = \frac{q^2}{4}\frac{d\Omega}{\sin^4(\theta/2)} \quad (\leftarrow d\Omega = 2\pi\sin\theta d\theta)$$

or $$\frac{d\sigma}{d\Omega} = \left(\frac{zZe^2}{4\pi\varepsilon_0}\right)^2 \frac{1}{16E^2}\frac{1}{\sin^4(\theta/2)}$$: Rutherford scattering cross section

Rutherford cross section : θ → 0, $(d\sigma/d\Omega)_R \rightarrow \infty$ (b→∞)

Real situation : b → large, potential (1/r) → (1/r)exp(-r/c)

Due to the electron screening of the nuclear charge

b_{max} ~ R (size of the atom)

$b > b_{max}$, potential ~ 0 little scattering

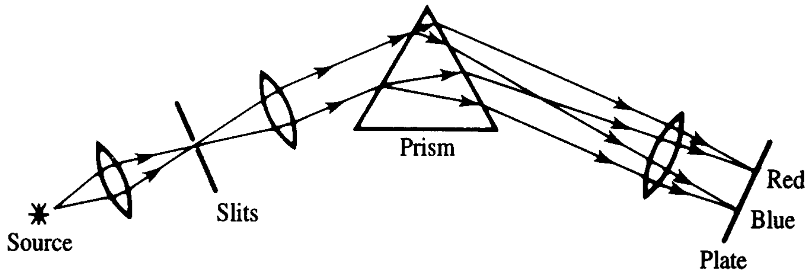
원자 구조 = 핵 + 궤도 전자 → 궤도 전자의 가속 및 에너지 방출 문제
표적의 반동을 고려하려면 CM계에서 위의 과정을 논의 → 결과식은 동일한 형태이되 $E = E_{cm} = \mu v^2/2$, θ = CM계에서의 산란각으로 취급하면 됨.

4. The Hydrogen Spectrum

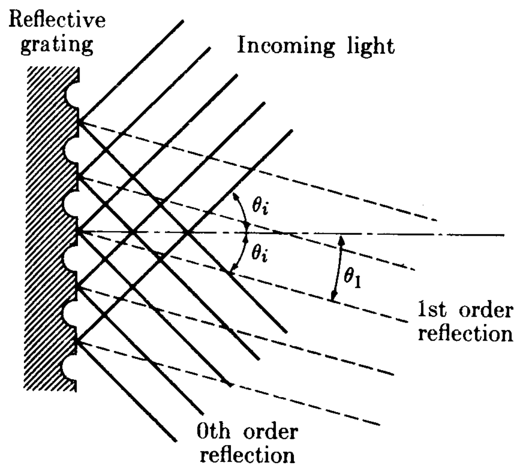
- Light spectrum = Distribution of intensity as a function of wavelength(or frequency)

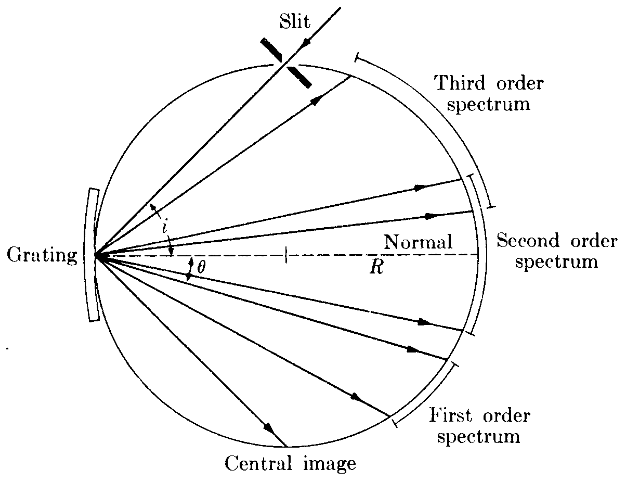
Optical spectrometer = light source(a discharge lamp) + dispersing device(a prism or a grating) + detection device(a simple screen or a photographic plate ora PM tube) + refining components(slits and lens etc.)

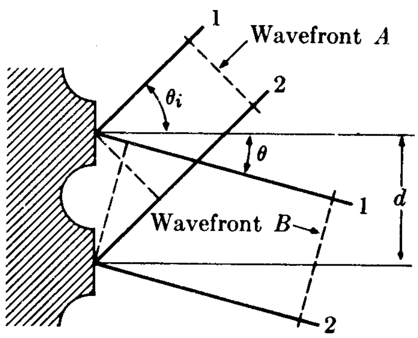
Prism spectrometer :



Grating spectrometer : transmission grating(fine grooves on a plane glass surface)
reflection grating(fine grooves on a polished metal mirror)







Reflection grating equation :

$d(\sin\theta_i - \sin\theta) = n\lambda$ (n : integer)

Zero-order reflection (mirror reflection)

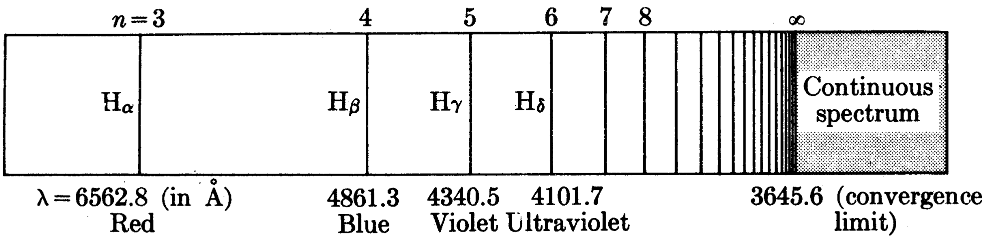
$\theta_i = \theta$

Typically, d ~ 10^{-4} cm, λ ~ 10^{-5} cm

- Empirical formulas :

  Balmer formula of hydrogen spectrum

$$\lambda(\text{Å}) = \frac{3645.6n^2}{n^2 - 4} \quad , \qquad n = 3,4,\ldots$$



Rydberg formula for heavier elements

$$\bar{\nu} = \frac{1}{\lambda} = A - \frac{R}{(n+\alpha)^2}$$

$\bar{\nu}$: wave number = 1/λ 또는 reduced wave number k/2π

R : Rydberg constant $1.09737\times10^7\ \text{m}^{-1}$

A, α : adjusting constants to the particular element, part of the spectrum or spectral series

Ritz formula :

$$\bar{\nu} = \frac{1}{\lambda} = \frac{R}{(m+\beta)^2} - \frac{R}{(n+\alpha)^2}$$

if α=β=0, m=2, this is reduced to the Balmer formula

Paschen's hydrogen lines in the infrared region :

α=β=0, m=3, n=4,5,6, …

$$\rightarrow \quad \bar{\nu} = R\left(\frac{1}{m^2} - \frac{1}{n^2}\right) \quad , \qquad m \neq n$$

5. The Bohr Model

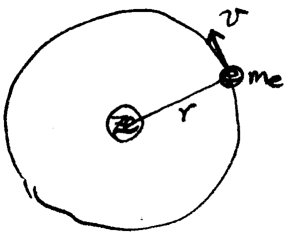
The accurate empirical formula for hydrogen spectrum

$$\bar{\nu} = R\left(\frac{1}{m^2} - \frac{1}{n^2}\right)$$

1913 년, Danish physicist Niels Bohr

일종의 planetary model 을 수소 원자에 대해 제안.

단일 행성의 태양계	단일 전자의 수소
중력(만유인력)에 의한 행성 운동	전자기력에 의한 전자 운동
$F = G\dfrac{MM'}{r^2}$	$F = \dfrac{1}{4\pi\varepsilon_0}\dfrac{qq'}{r^2}$
elliptic orbit	circular orbit(가정)



centre of the orbit ≈ location(centre) of the nucleus

$$F = \frac{1}{4\pi\varepsilon_0}\frac{Ze\cdot e}{r^2} = m_e a = \frac{m_e v^2}{r}$$

or $$v^2 = \frac{Ze^2}{4\pi\varepsilon_0 m_e r}$$

No further limitation on v and r in classical physics.

♣ Bohr's postulate : angular momenta = n(h/2π) or nħ

$$m_e vr = n\hbar, \qquad \hbar = h/2\pi, \qquad n = 1,2,3,\cdots$$

$$\rightarrow \quad r = r_n = \frac{\varepsilon_0 h^2 n^2}{\pi m_e Z e^2} = 0.529\frac{n^2}{Z}(A^\circ) \quad or \quad a_0\frac{n^2}{Z}$$

where a_0 = Bohr radius (radius of the first orbit in hydrogen)

$$= \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2} = 0.529\times 10^{-10}\ \text{m}$$

$$v_n = \frac{n\hbar}{m_e r} = \frac{Z}{(m_e a_0/\hbar)}\frac{1}{n} = \frac{v_1}{n}$$

An important constant frequently met in the quantum electrodynamics:

Fine structure constant

$$\alpha = \frac{v_1}{c} = \frac{\hbar}{m_e c a_0} = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{\hbar c} = \frac{1}{137.04}$$

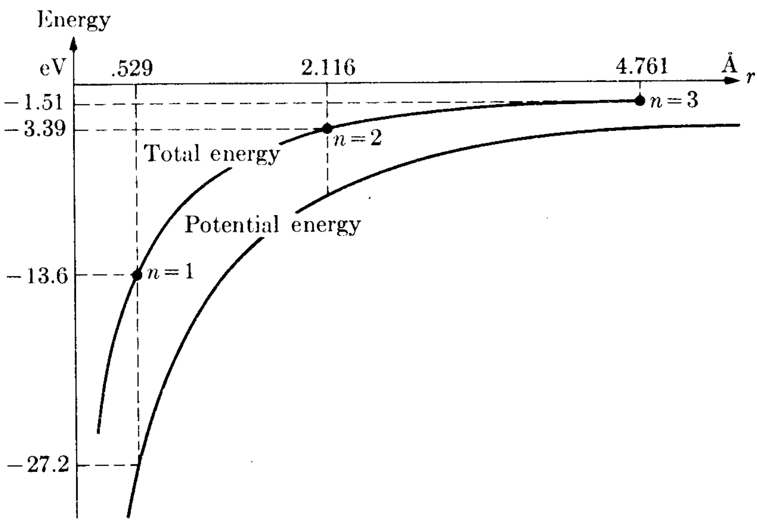
Potential energy (of electron) $E_p = -\dfrac{Ze^2}{4\pi\varepsilon_0 r}$

Kinetic energy $E_k = \frac{1}{2}m_e v^2 = \dfrac{Ze^2}{8\pi\varepsilon_0 r}$

Total energy

$$E = E_k + E_p = -\frac{Ze^2}{8\pi\varepsilon_0 r} = -\frac{Ze^2}{8\pi\varepsilon_0}\frac{\pi m_e Z e^2}{\varepsilon_0 h^2 n^2} = -\frac{m_e Z^2 e^4}{8\varepsilon_0^2 h^2 n^2} = -\frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{2a_0}\frac{1}{n^2}$$

n = 1,2,3,… : principal quantum number (주양자수 主量子數)



$$E = E_n = -\frac{13.6}{n^2} \quad (eV),$$

$-E_n$: binding energy of the n-th orbit electron

One problem) 하전 입자의 가속 → radiation 발생 (고전전자기학)

Larmor's formula : $\dfrac{dE}{dt} = \dfrac{q^2 a^2}{6\pi\varepsilon_0 c^3}$, a : acceleration

→ orbital energy loss by radiation → fall down to the nucleus

♣ Bohr's second postulate on radiation :

궤도 상의 전자는 radiation energy 를 방출하지 않음. Radiation 은 높은 에너지 준위에서 낮은 에너지 준위로 천이(transition)할 때, 그 에너지 차이 만큼이 radiation quantum hν 로 방출됨.

Bohr's formula $h\nu = E_{n2} - E_{n1} \quad (n_2 > n_1)$

$$\nu = \frac{m_e Z^2 e^4}{8\varepsilon_0^2 h^3}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) \quad or \quad \bar{\nu} = \frac{1}{\lambda} = \frac{\nu}{c} = \frac{m_e Z^2 e^4}{8\varepsilon_0^2 h^3 c}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

where the coefficient is the Rydberg constant,

$$R = \frac{m_e e^4}{8\varepsilon_0^2 h^3 c} = 1.0973731\times10^7 \text{ m}^{-1} \equiv R_\infty \quad (M=\infty).$$

Finite nuclear mass → electron and nucleus orbit around the CM

CM 계에서의 계산 → $R = \dfrac{R_\infty}{1 + (m_e / M)}$

A slight variation from element to element

Identification of various spectral series :

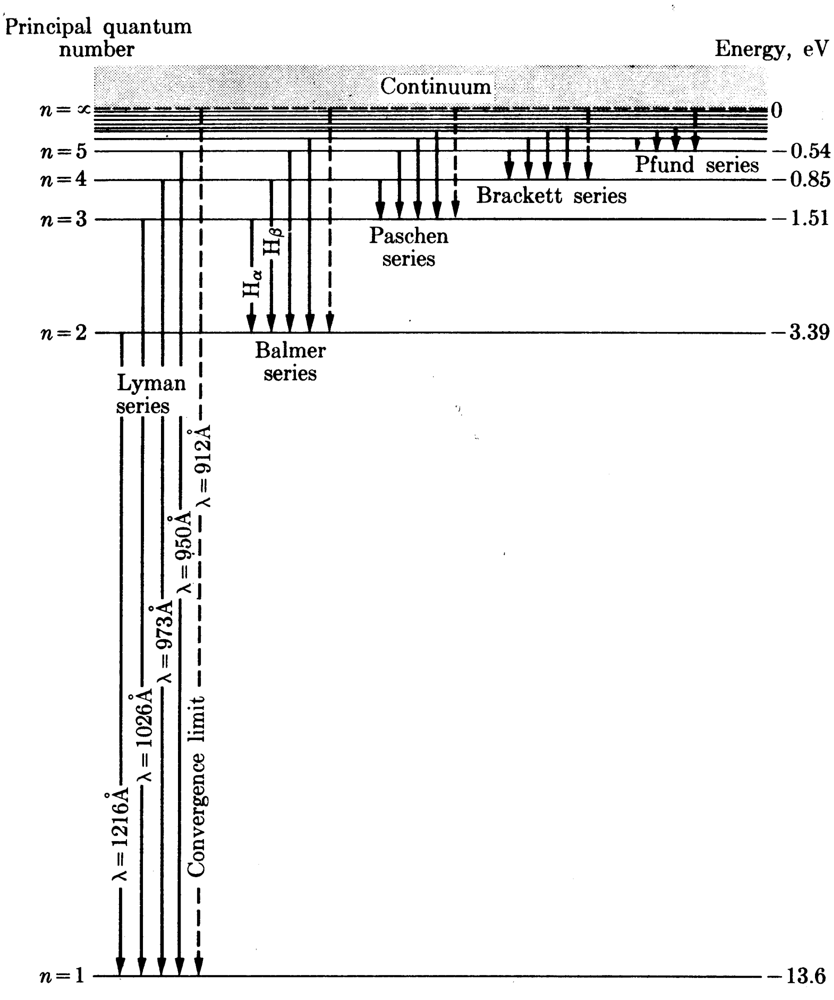
$n_1 = 2$: Balmer series (1884) visible light

$n_1 = 3$: Paschen series (1908) infrared(IR)

$n_1 = 1$: Lyman series (1916) far ultraviolet(UV)

$n_1 = 4$: Brackett series (1922) infrared

$n_1 = 5$: Pfund series (1924) infrared



6. Criticism and later development

M. Planck : quantization of radiation(electromagnetic field)

↔ energy exchange between heated body and the surrounding EM field

N. Bohr : quantization of angular momentum and
quantization of energy levels in atoms

(문제점)

1. 수소 원자의 fine spectrum : 고분해능 분광계로 측정하면 n=2,3,… 등의 line 들이 분리되어 있음 (doublet)
   → Sommerfeld's elliptic orbit treatment & relativistic correction
   (r, θ) 두 개의 운동 자유도
   → radial and azimuthal quantum numbers n_r, n_θ
   Old quantization rules $\oint p_q dq = n_q h, \quad q = r \;\; or \;\; \theta$
   → Uhlenbeck and Goudsmit : electron spin 제의 (1925) ←1/2
   → 1928, P. A. M. Dirac 의 전자 상대양자론
2. One electron model :
   두 개 이상의 전자가 존재할 때 central force 조건은 충족 불능.
   → 파동역학(量子力學)의 방법론.
   He 이상의 원자번호에 대해서는 수학적으로 여전히 해석적 해가 난해. → Hartree-Fock approach
3. Quantum Jump :
   하나의 에너지 준위에서 다른 에너지 준위로의 transition 이 quantum jump 로 발생. → Sommerfeld 의 old quantization condition 으로 quantum jump 에 selection rule 이 존재함을 발견하나 설명은 난이함.
   → Wave mechanics (또는 양자역학 Quantum Mechanics)로서 해결.

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