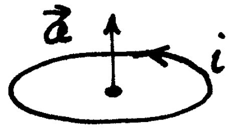
(Lecture 10) Intrinsic Spin of Electron

1. Magnetic Moment of Atom



- Magnetic moment of plane current loop :

  current i, area vector $\vec{a}$ $\rightarrow$

  magnetic moment $\vec{\mu} = i\vec{a}$

$\leftarrow$ particle charge q, circular orbit radius r, velocity v, frequency $v/2\pi r$:

$$i = \frac{qv}{2\pi r}, \qquad \mu = |\vec{\mu}| = \frac{qv}{2\pi r} \cdot \pi r^2 = \frac{1}{2} qvr$$

$$\therefore \quad \vec{\mu} = \frac{1}{2} q\, \vec{r} \times \vec{v} = \frac{q}{2m} \vec{r} \times \vec{p} = \frac{q}{2m} \vec{L} \qquad (1)$$

i.e. $\vec{\mu}$ is proportional to $\vec{L}$ classically.

$\mu/L = q/(2m)$: classical gyromagnetic ratio

$-e/(2m_e)$: electron's classical gyromagnetic ratio

$\vec{\mu}$ 가 자장과 기울어져서 존재할 때, 실제 측정되는 양 :

μ_z (z-component of μ) and L_z (z-component of L)

$\rightarrow$ gyromagnetic ratio $\gamma = \mu_z / L_z$

- Quantized magnetic moment :

$\vec{L} \rightarrow \hat{L}$, $\vec{\mu} \rightarrow \hat{\mu}$ (operator) 로서 양자 상태에 관련.

$\mu_z = -\frac{e}{2m_e} L_z$ depends on the eigenstate of L_z.

$\rightarrow$ For $L_z = m\hbar$ state, $\mu_z = (-\frac{e\hbar}{2m_e})m$ for the electronic state.

여기서 $(-\frac{e\hbar}{2m_e})$는 electronic magnetic moment 를 표시하기에 좋은 단위

$\rightarrow$ $\mu_B \equiv (-\frac{e\hbar}{2m_e})$: Bohr magneton (B.m.)

만약 gyromagnetic ratio 가 알려져 있다면, μ_z의 측정은 m의 측정과 동등. 양자론적으로는 점전하, 점질량 대신 전하 및 질량이 파동함수로 주어지는 분포를 하게 되나, 두 분포(Charge density, mass density distribution)가 동일하면 (1)식이 성립. 일치하지 않는 보다 복잡한 분포에 대해서는

$\mu_z = g\mu_B m$, g : g-factor

전자의 orbital motion 에 의한 magnetic moment : $g = 1$

- Magnetic moment in a magnetic field :

energy $E = -\vec{\mu} \cdot \vec{B}$

torque $\vec{\tau} = \vec{\mu} \times \vec{B}$ (if $\vec{\mu}, \vec{B}$ are parallel, $\vec{\tau} = 0$).

force in inhomogeneous magnetic field $\vec{F} = (\vec{\mu} \cdot \vec{\nabla})\vec{B}$

Torque in magnetic field $\vec{B}$:

$$\vec{\tau} = \frac{d\vec{L}}{dt} = \vec{\mu} \times \vec{B} = -\frac{eg}{2m_e}\vec{L} \times \vec{B} \quad (\vec{\tau} \perp \vec{L})$$

torque 에 의해 angular momentum 은 크기는 일정하되 방향만 바뀜.

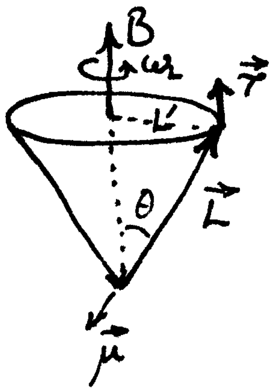
→ Larmor precession

angular frequency of precession

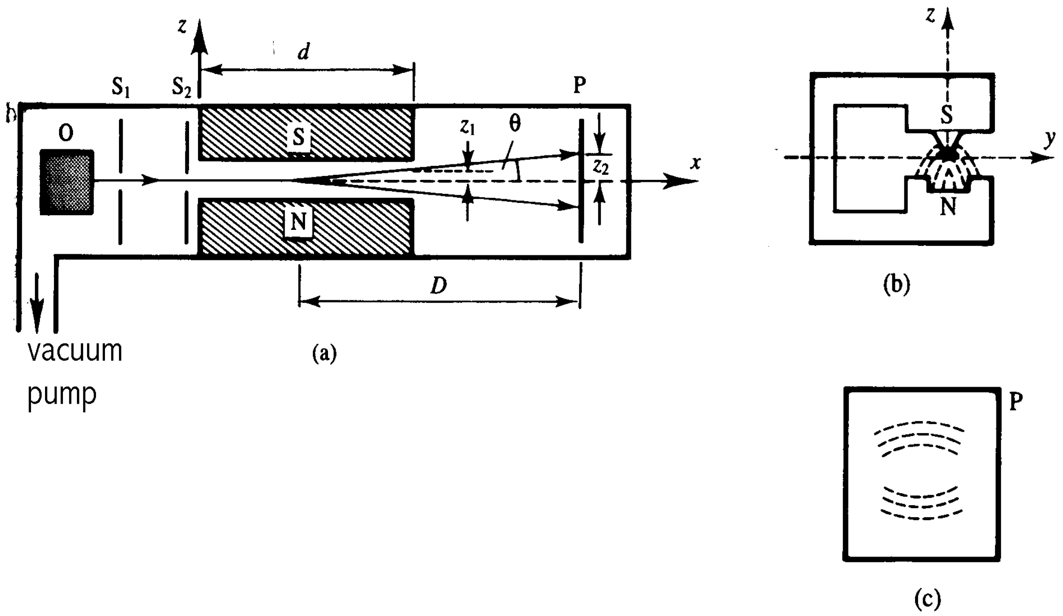
$$\Omega_L = \frac{d\phi}{dt} = \frac{dL/L'}{dt}$$

$$= \frac{dL/dt}{L\sin\theta} = \frac{egBL\sin\theta}{2m_e L\sin\theta}$$

$$= \frac{eg}{2m_e}B = \gamma B$$



2. The Stern-Gerlach Experiment



- Quantization of μ_z = quantization of angular momentum (space quantization)
  Neutral silver (^{47}Ag) atoms into inhomogeneous magnet (1921, 1922)
  → spatial split of atomic beam into two groups

$$F_z = \mu_z \frac{\partial B_z}{\partial z}$$

magnet 통과 시간 Δt 라면 z-방향 separation

$$\Delta z = \frac{1}{2} \cdot \frac{F_z}{m} (\Delta t)^2$$

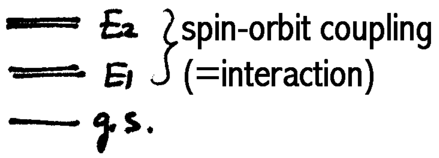
자장 내에서 $\vec{\mu}$가 자장에 대해 임의의 방향을 가질 수 있다면, μ_z는 $\pm(\mu_z)_{max}$ 내에서 연속적인 값을 가지게 되며, 따라서 Δz 분포도 연속적.
(Stern-Gerlach experiment by using atomic hydrogen beam (1927))

[실험 결과] Beam split into two → two possible values for μ_z
ground state hydrogen atom 의 경우 L = 0(s-state), m=0.
Ag 의 경우에는 여러 전자 각각의 orbital angular momentum 합산
→ L quantum number = 정수 → magnetic substate 의 갯수=(2L+1)=odd

3. Intrinsic Spin of the Electron

- 수소 원자의 energy level : Bohr and Sommerfeld work
  The excited states are energy degenerated
  → 여러 종류의 l-state 들이 동일한 energy level

i) High resolution spectrometer 로 조사하면 실제로 excited level 들은 doublet
→ fine structure



ii) 수소 원자의 Stern-Gerlach 실험 결과 : quantization of spin angular momentum

iii) anomalous Zeeman effect : not 3 lines in magnetic field

→ Intrinsic spin of electron (←$\hbar$ /2) 제안 : Uhlenbeck and Goudsmit (1925)
→ Relativistic wave equation for electron : P.A.M. Dirac (1928)
1) 수소 원자의 fine structure 설명
2) 전자의 spin 설명
3) positron 의 이론적 예측 토대

- Intrinsic spin angular momentum

  magnitude $S^2 = \hbar^2 s(s+1)$, s = 1/2 = spin angular momentum quantum number

  z-component $S_z = \hbar m_s$, m_s = -1/2 or +1/2

  g-factor for electron spin g = 2

  cf. g-factor for orbital angular momentum g=1

4. Commutator Relations

Quantum Mechanical commutator : operator $\hat{Q}_1$, $\hat{Q}_2$ 에 대해

$$[\hat{Q}_1, \hat{Q}_2] \equiv \hat{Q}_1 \hat{Q}_2 - \hat{Q}_2 \hat{Q}_1 .$$

$[\hat{Q}_1, \hat{Q}_2] = 0$: $\hat{Q}_1$, $\hat{Q}_2$ 는 commute (교환적, 交換的)

$[\hat{Q}_1, \hat{Q}_2] \neq 0$: $\hat{Q}_1$, $\hat{Q}_2$ 는 non-commute (비교환적, 非交換的)

$[\hat{Q}_1, \hat{Q}_2] = 0 \quad \leftrightarrow \quad \hat{Q}_1$, $\hat{Q}_2$ 는 (simultaneous) eigenfunction 을 공유(共有)

e.g. $[\hat{L}^2, \hat{L}_z] = 0$: $Y_{lm}(\theta, \phi)$

$[\hat{L}^2, \hat{H}] = 0$: $R_{nl}(r) Y_{lm}(\theta, \phi)$

↑ Hamiltonian operator for central force problem

- Non-commutable operators :

  $$[\hat{L}_x, \hat{L}_y] = \hat{L}_x \hat{L}_y - \hat{L}_y \hat{L}_x = \hbar^2 \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) = i\hbar \hat{L}_z \quad \text{and}$$

  $[\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x$, $[\hat{L}_z, \hat{L}_x] = i\hbar \hat{L}_y$ (cyclic relation)

  Also, $[\hat{x}_i, \hat{x}_j] = 0$, $[\hat{p}_i, \hat{p}_j] = 0$, $[\hat{x}_i, \hat{p}_j] = i\hbar \delta_{ij}$

  Proof is straightforward by noting that

  $\hat{x}_1 = x, \quad \hat{x}_2 = y, \quad \hat{x}_3 = z$

  $$\hat{p}_1 = \hat{p}_x = -i\hbar \frac{\partial}{\partial x}, \quad \hat{p}_2 = \hat{p}_y = -i\hbar \frac{\partial}{\partial y}, \quad \hat{p}_3 = \hat{p}_z = -i\hbar \frac{\partial}{\partial z}$$

- Spin operators based on commutation rules

Define the spin operators satisfying the similar commutator relations with those for the orbital angular momentum operators.

$$[\hat{S}_x, \hat{S}_y] = i\hbar \hat{S}_z \qquad \text{etc.}$$

이를 만족하는 가장 간단한 요소들 : Pauli's spin matrices

$$\sigma_x\ (or\ \sigma_1) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y\ (or\ \sigma_2) = \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix}, \quad \sigma_z\ (or\ \sigma_3) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\hat{S}_x = \frac{\hbar}{2}\sigma_x, \quad \hat{S}_y = \frac{\hbar}{2}\sigma_y, \quad \hat{S}_z = \frac{\hbar}{2}\sigma_z \quad or \quad \hat{\mathrm{S}} = \frac{\hbar}{2}\sigma$$

From simple matrix multiplication or Hermitian and unitary property,

$$\sigma_1^2 = \sigma_2^2 = \sigma_3^2 = 1 \ \text{(unit matrix)}$$

$$\sigma_i\dagger = \sigma_i \quad \text{and} \quad \sigma_i\dagger = \sigma_i^{-1}$$

$$\sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}$$

$$[\sigma_i, \sigma_j] = \sigma_i\ \sigma_j - \sigma_j\ \sigma_i = 2i\varepsilon_{ijk}\sigma_k, \qquad \varepsilon_{ijk} : \text{Levi-Civita symbol}$$

$$\sigma_x^2 + \sigma_y^2 + \sigma_z^2 = 1 + 1 + 1 = 3 \cdot 1 = 3\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$ 이므로

$$\hat{S}^2 = \frac{\hbar^2}{4}(\sigma_x^2 + \sigma_y^2 + \sigma_z^2) = \frac{3\hbar^2}{4} \cdot 1$$

Spin wave function :

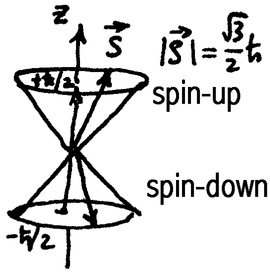
amplitude for spin-up ($m_s = +1/2$ or $S_z = +\hbar/2$) state = a (let)

amplitude for spin-down ($m_s = -1/2$ or $S_z = -\hbar/2$) state = b

전체 상태는 column vector 로 표현 가능 :

$$|\chi\rangle = \chi = \begin{pmatrix} a \\ b \end{pmatrix} \quad \rightarrow \quad \langle\chi|\chi\rangle = \chi\dagger\chi = |a|^2 + |b|^2 = 1 \quad : \text{normalization}$$

Pure spin state ($\hat{S}_z$ eigenstate) :



$$|\alpha\rangle = \alpha = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\beta\rangle = \beta = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

α = pure spin-up state ($m_s = +1/2$ 일 확률이 1)

β = pure spin-down state ($m_s = -1/2$ 일 확률이 1)

왜냐하면 $\hat{S}_z\alpha$ or $\hat{S}_z|\alpha\rangle = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}|\alpha\rangle$

이며 $\hat{S}_z\beta$ or $\hat{S}_z|\beta\rangle = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = -\frac{\hbar}{2}|\beta\rangle$.

5. Total Angular Momentum

- Addition of two angular momenta : $\vec{J} = \vec{L}_1 + \vec{L}_2$ *or* $\vec{L} + \vec{S}$

  Quantum Mechanics : $\hat{J} = \hat{L} + \hat{S}$ operator

  strict expression : $\hat{J} = \hat{L} \otimes \hat{1} + \hat{1} \otimes \hat{S}$

  where the identity operators have the dimension of the spin and the orbital angular momentum operator's, respectively.

  Total angular momentum : commutation rule

  $$[\hat{J}_i, \hat{J}_j] = i\hbar\varepsilon_{ijk}\hat{J}_k$$

  quantum numbers j, m_j :

  $$-j \le m_j \le j\,, \quad |l - s| \le j \le l + s$$

  전자의 경우 $s = 1/2$ 이므로, $|l - \frac{1}{2}| \le j \le l + \frac{1}{2}$

  Spectroscopic notation : quantum numbers $(n, l, j) \rightarrow nl_j$

  e.g. $3d_{5/2}$: $n = 3$, $l = 2$, $j = 5/2$

  Many electron atoms : quantum numbers $(S, L, J) \rightarrow {}^{2S+1}L_J$

  S : total spin angular momentum q. number

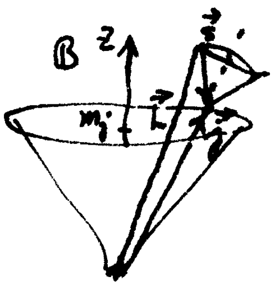
  L : total orbital angular momentum q. number

  J : total angular momentum q. number

  associated quantum numbers M_L, M_S, M_J all good?

  $\rightarrow$ depends on the coupling scheme

- Coupling of two angular momenta : $\vec{L}$ *and* $\vec{S}$



i) In weak magnetic field or no magnetic field :

  coupling of $\vec{L}$ *and* $\vec{S}$ is strong

  $\rightarrow$ good quantum numbers are L, S, J, M_J

  $\vec{L}$ *and* $\vec{S}$ precession around $\vec{J}$

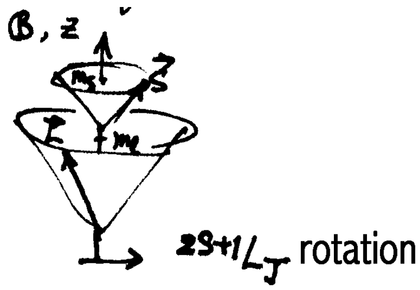
→ jj-coupling in heavy elements

ii) In strong magnetic field :

coupling of $\vec{L}$ *and* $\vec{S}$ is destroyed

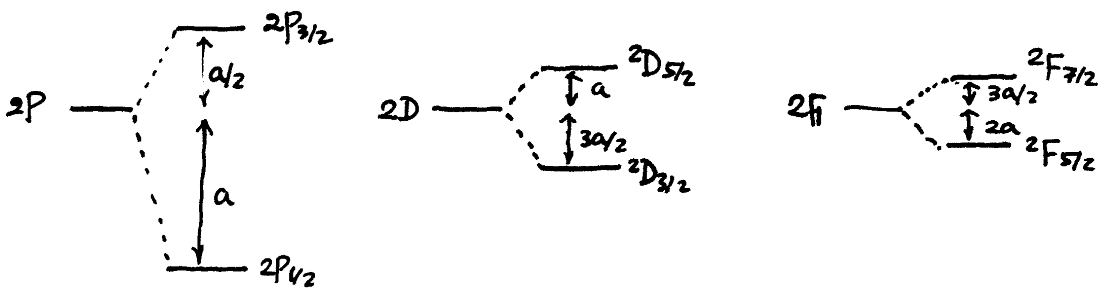
→ independent precession of $\vec{L}$ *and* $\vec{S}$

→ good quantum numbers are L, S, M_L, M_S



6. Fine Structure of Atomic Hydrogen

s-state를 제외하고는 doublet : e.g. H_α, D_α fine structure



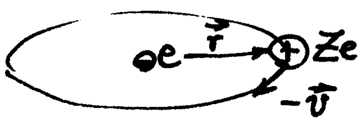
- Dominant effect : spin-orbit interaction (fine structure)

  electron's orbital motion → produce magnetic field $\vec{B}$

  electron's spin → produce magnetic moment $\mu_z = \pm\mu_B$

  ⟶ energy shift $\Delta E = -\vec{\mu}\cdot\vec{B}$

Electron's coordinate system :



$$\vec{B} = \frac{\mu_0}{4\pi}\cdot\frac{i\,d\vec{l}\times\vec{r}}{r^3}$$

$$= \frac{1}{4\pi\varepsilon_0 c^2}\cdot\frac{Ze}{m_e}\cdot\frac{\vec{L}}{r^3}$$

$$\left(i\,d\vec{l} = -Ze\vec{v},\quad \mu_0 = \frac{1}{\varepsilon_0 c^2},\quad \vec{L} = \vec{r}\times(m_e\vec{v})\right)$$

$$\rightarrow\quad \Delta E = -\vec{\mu}\cdot\vec{B} = \frac{Ze^2}{8\pi\varepsilon_0 c^2}\cdot\frac{\hbar^2}{m_e^2}\cdot\frac{1}{r^3}\cdot(\vec{l}\cdot\vec{s})\quad \vec{L} = \hbar\vec{l},\ \vec{S} = \hbar\vec{s}$$

$\vec{l}$ // $\vec{s}$ $\rightarrow$ $j = l + 1/2$, $\Delta E > 0$ ($\leftarrow \vec{l}\cdot\vec{s} > 0$)

$\vec{l}$ // -$\vec{s}$ $\rightarrow$ $j = l - 1/2$, $\Delta E < 0$ ($\leftarrow \vec{l}\cdot\vec{s} < 0$)

Wave mechanical treatment for electron : no definite position $\rightarrow$ no definite r

probabilistic amplitude for position r $\rightarrow$ average by wave function

$$\left\langle \frac{1}{r^3} \right\rangle = \left(\frac{Z}{na_0}\right)^3 \cdot \frac{1}{l(l+\frac{1}{2})(l+1)}$$

(l, s, j) state 에 대해

$$\vec{j}\cdot\vec{j} = (\vec{l}+\vec{s})\cdot(\vec{l}+\vec{s}) = \vec{l}\cdot\vec{l} + \vec{s}\cdot\vec{s} + 2\vec{l}\cdot\vec{s}$$

$$\vec{j}\cdot\vec{j} = j(j+1), \quad \vec{l}\cdot\vec{l} = l(l+1), \quad \vec{s}\cdot\vec{s} = s(s+1)$$

$$\therefore\ \vec{l}\cdot\vec{s} = \frac{1}{2}\left[\vec{j}\cdot\vec{j} - \vec{l}\cdot\vec{l} - \vec{s}\cdot\vec{s}\right] = \frac{1}{2}\left[j(j+1) - l(l+1) - \frac{3}{4}\right] = \begin{cases} l/2, & j = l + \frac{1}{2} \\ -(l+1)/2, & j = l - \frac{1}{2} \end{cases}$$

$a_0 = \dfrac{4\pi\varepsilon_0\hbar^2}{m_e c^2}$ 을 대입하고, $R = \dfrac{m_e e^4}{8\varepsilon_0^2 h^3 c}$, $\alpha = \dfrac{e^2}{4\pi\varepsilon_0 \hbar c} = \dfrac{1}{137}$ 로서 표시.

$$\rightarrow \quad \Delta E = hcR\alpha^2 Z^4 \cdot \frac{\vec{l}\cdot\vec{s}}{n^3 l(l+\frac{1}{2})(l+1)} = hc\cdot a(\vec{l}\cdot\vec{s}) \quad : \quad \alpha^2\text{-order}$$

cf. $hcR = \dfrac{m_e e^4}{8\varepsilon_0^2 h^2} = 13.6\ eV$

$a \equiv \dfrac{R\alpha^2 Z^4}{n^3 l(l+\frac{1}{2})(l+1)}$: const for a given (n, l) state, decreasing for higher (n, l)

state

$(\vec{l}\cdot\vec{s}) = \begin{cases} 1/2 \\ -1 \end{cases}$ for p-state, $\begin{cases} 1 \\ -3/2 \end{cases}$ for d-state etc.

- Relativistic correction : Heisenberg (1926)

$$\Delta E_r = -\frac{hcR\alpha^2 Z^4}{n^3}\left(\frac{1}{l+\frac{1}{2}} - \frac{3}{4n}\right)$$

- Total correction : Sommerfeld-Dirac result

$$\Delta E = \Delta E_{ls} + \Delta E_r = -\frac{hcR\alpha^2 Z^4}{n^3}\left(\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\right) \quad : \quad (n, j) \text{ dependent only}$$

- Further refinements : QED (vacuum polarization) effect and Hyperfine interaction
- Hydrogen-like Atom Levels
  He^+ (or He II) spectrum observation :

Balmer series

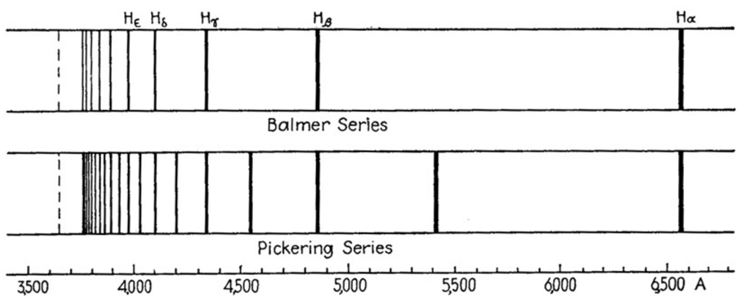


FIG. 1.14.—Comparison of the Balmer series of hydrogen and the Pickering series.

Pickering series (1897) : ζ-Puppis star spectrum → new hydrogen? → actually He^+

Bohr's explanation (1913) :

H, He^+, Li^{2+}, Be^{3+} : single electron atoms with Z = 1,2,3,4

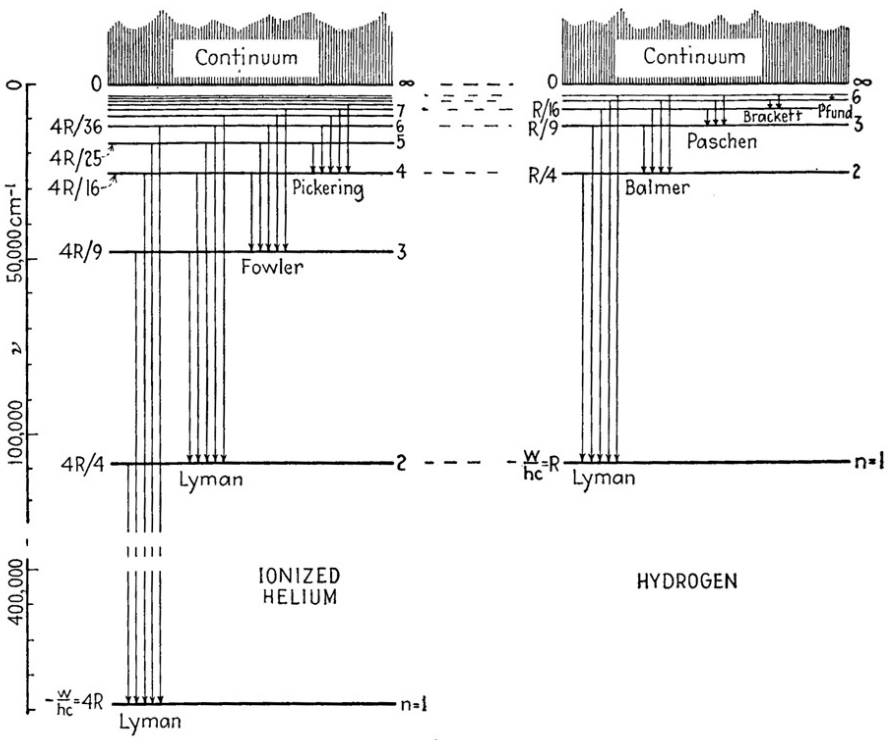


FIG. 2.8.—Energy level diagrams of hydrogen and ionized helium.

Energy levels

$$E_n = -hcR \cdot \frac{Z^2}{n^2} = -13.598 \cdot \frac{Z^2}{n^2} \quad eV\ .$$

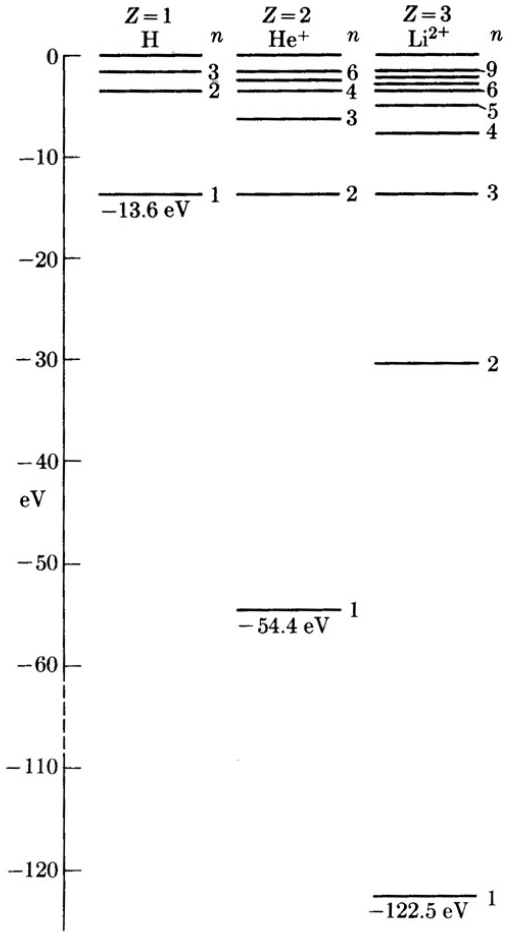


Figure 23.4 Some energy levels of H, He$^+$ and Li^{2+}.

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