

•  $\alpha$ 粒子散射实验:

$$\text{偏转角公式: } \cot \frac{\theta}{2} = \frac{2b}{a}, a = \frac{zZe^2}{4\pi\epsilon_0 E}$$

$$\text{轨道最小距离: } r_m = \frac{1}{2} a (1 + \csc \frac{\theta}{2})$$

$$\text{微分散射界面: } \frac{d\sigma(\theta)}{d\Omega} = \frac{1}{16} a^2 \frac{1}{\sin^4(\theta/2)}$$

$$\text{• 玻尔理论: } \begin{cases} r_n = \frac{m_e n^2}{\mu Z} a_0 \\ E_n = \frac{\mu Z^2}{m_e n^2} E_1, E_1 = -\frac{1}{2} m_e c^2 \alpha^2 \\ L_n = n\hbar \end{cases}$$

$$\text{• 里德伯公式: } \tilde{\nu} = R \left( \frac{1}{m^2} - \frac{1}{n^2} \right), R_A = R_\infty \frac{1}{1+m_e/M}, E = -\frac{hcR}{n^2}$$

$$\text{• 德布罗意波, } \lambda = \frac{h}{p} \approx \frac{h}{\sqrt{2mT}}$$

$$\text{• 斜入射布拉格条件: } 2d \sin \theta = n\lambda$$

$$\text{• 不确定关系: } \Delta x \cdot \Delta p_x \geq \frac{\hbar}{2}, \Delta x \cdot \Delta p_x \approx \hbar, \Delta E \cdot \Delta t \geq \frac{\hbar}{2}, \Gamma \cdot \tau = \hbar$$

$$\text{• } \psi(\mathbf{r}, t) = \psi_0 e^{i(\mathbf{p}\cdot\mathbf{r} - Et)/\hbar} \Rightarrow \text{定态薛定谔方程: } \left( -\frac{\hbar^2}{2m} \nabla^2 + V \right) \psi = E\psi$$

$$\text{• 单电子原子: } n^{2s+1} L_j$$

$$\text{磁矩: } \boldsymbol{\mu}_s = -g_s \frac{\mu_B}{\hbar} \mathbf{S}, \boldsymbol{\mu}_l = -g_l \frac{\mu_B}{\hbar} \mathbf{L}, \mathbf{J} = \mathbf{L} + \mathbf{S}$$

$$\text{精细结构: 自旋-轨道耦合能 } \Delta E_{nl} = \begin{cases} 0, l = 0 \\ -E_n \frac{\alpha^2 Z^2}{n^2} \frac{n[j(j+1) - l(l+1) - s(s+1)]}{2l(l+1/2)(l+1)}, l \neq 0 \end{cases}, \text{相}$$

$$\text{对论性修正 } \Delta E = \frac{1}{2} m_e c^2 \frac{\alpha^4 Z^4}{n^4} \left( \frac{3}{4} - \frac{n}{j+1/2} \right)$$

兰姆移位:  $g_s = 2(1 + a)$ ,  $j = 1/2$  移位最大,  $j > 1/2$  移位很小, 可忽略;

$n$ 越大, 兰姆移位越小。

$$\text{超精细相互作用: } \Delta E = \frac{a}{2} [F(F+1) - J(J+1) - I(I+1)]$$

$$\text{塞曼效应: 弱磁场时, } \mu_j = g_j \sqrt{j(j+1)} \mu_B, g_j = 1 + \frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)}, \tilde{\nu} =$$

$\tilde{\nu}_0 + (m_2 g_2 - m_1 g_1) \mathcal{L}$ 。强磁场时,  $\mu_z = (g_j m_j + g_s m_s) \mu_B, \tilde{\nu} = \tilde{\nu}_0 + \Delta m_l \mathcal{L}$ 。塞曼

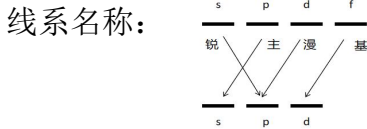
分裂的各谱线都是偏振的。

电偶极跃迁:  $\Delta l = \pm 1, \Delta j = 0, \pm 1, \Delta m_s = 0, \Delta m_l = 0, \pm 1$ 。

磁共振现象:  $h\nu = g_j \mu_B B$

• 碱金属原子

轨道贯穿效应:  $E_{nl} = -\frac{1}{2} \mu \alpha^2 c^2 \frac{1}{n^{*2}}, n^* = n/Z_{nl}^* = n - \Delta_{nl}$



相对论效应修正:  $\Delta E_{nl} = \begin{cases} 0, l = 0 \\ \frac{1}{2} \mu c^2 \frac{\alpha^4 Z_{fs}^{*4}}{n^3} \frac{j(j+1) - l(l+1) - s(s+1)}{2l(l+1/2)(l+1)}, l \neq 0 \end{cases}$

• 多电子原子

泡利原理: 原子中不能有两个电子具有完全相同的四个量子数。

基态原子核外电子排布: 按照  $n + l$  值增大的次序填充, 当  $n + l$  值相同时, 按照  $n$  增大的次序填充。

简并度: 非等效  $G = \prod_{i=1}^n 2(2l_i + 1)$ , 等效  $G = C_{2(2l+1)}^v$

拉波特定则: 要求  $\Delta \sum l_i = \pm 1$

LS 耦合:  $^{2S+1}L_J$

朗德间隔定则:  $\Delta E_J - \Delta E_{J-1} = \xi(L, S) J \hbar^2$

洪特定则: 基态原子拥有可行的最大  $S, L$ , 半满以下  $J$  最小, 以上  $J$  最大

塞曼效应:  $\mu_J = -g_J \frac{\mu_B}{\hbar} J, g_J = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}, \Delta E = M_J g_J \mu_B B$

电偶极跃迁:  $\begin{cases} \Delta S = 0, \Delta L = 0, \pm 1 \\ \Delta J = 0, \pm 1, J = 0 \rightarrow J = 0 \text{ 除外} \\ \Delta M_J = 0, \pm 1, \Delta J = 0 \text{ 时}, M_J = 0 \rightarrow M_J = 0 \text{ 除外} \end{cases}$

jj 耦合下:  $(j_1, \dots, j_v)_J$

电偶极跃迁:  $\begin{cases} \Delta j = 0, \pm 1 \\ \Delta J = 0, \pm 1, J = 0 \rightarrow J = 0 \text{ 除外} \\ \Delta M_J = 0, \pm 1, \Delta J = 0 \text{ 时}, M_J = 0 \rightarrow M_J = 0 \text{ 除外} \end{cases}$

• X 射线特征谱:  $\tilde{\nu}_{n,\alpha} = R(Z - \Delta_{n\alpha})^2 \left( \frac{1}{n^2} - \frac{1}{(n+\alpha)^2} \right)$

• 双原子分子:  $^{2S+1}\Lambda_{\Lambda+\Sigma}, \lambda = |m_l|, \Lambda = |M_L|, M_L = \sum m_{li}, \Sigma = M_S, \Omega = |\Lambda + \Sigma|$

转动:  $E_r = \frac{\hbar^2}{2I} J(J+1), I = \mu R_0^2, \tilde{\nu}_J = 2BJ, \Delta J = \pm 1, \Delta M_J = 0, \pm 1$ , 它是等间隔

的。二阶修正产生离心畸变, 即间距缩小。

振动:  $E_v = (v + \frac{1}{2})h\nu_0, \nu_0 = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}}, \Delta v = \pm 1$ , 须考虑高次势能修正,  $E_v =$

$h\nu_0(v + \frac{1}{2}) - hv_0\eta(v + \frac{1}{2})^2, \Delta v = \pm 1, \pm 2, \dots$

电子振动转动光谱选择定则  $\left\{ \begin{array}{l} \Delta \Lambda = 0, \pm 1 \\ \Delta S = 0 \\ \Delta v = 0, \pm 1, \dots \\ \Delta J = 0, \pm 1 (0 \leftarrow 0 \text{ 除外}) \end{array} \right. \circ$

• 拉曼散射:

