

(4)

$$\text{Now } \vec{L} \cdot \vec{S} = L_z S_z + \frac{1}{2} (L^+ S^- + L^- S^+)$$

where

$$\left. \begin{array}{l} L_z \\ L^+ = L_x + i L_y \\ L^- = L_x - i L_y \end{array} \right\} \text{generates on } \phi_n(\vec{r})$$

and

$$\left. \begin{array}{l} S_z \\ S^+ = S_x + i S_y \\ S^- = S_x - i S_y \end{array} \right\} \text{generates on } \alpha \times \beta$$

with $S_z |\alpha\rangle = \frac{1}{2} |\alpha\rangle, \quad S_z |\beta\rangle = -\frac{1}{2} |\beta\rangle$
 $S^+ |\beta\rangle = \alpha, \quad S^+ |\alpha\rangle = 0$
 $S^- |\beta\rangle = 0, \quad S^- |\alpha\rangle = \beta$

so that

$$\langle \alpha | S_z | \alpha \rangle = \frac{1}{2}, \quad \langle \beta | S_z | \beta \rangle = -\frac{1}{2}$$

$$\langle \alpha | S^+ | \beta \rangle = 1, \quad \langle \beta | S^- | \alpha \rangle = 1$$

others zero

$$\begin{aligned} \frac{C_n' S}{C_n \alpha} &= -\lambda \frac{\iint \phi_n^*(\vec{r}) \alpha^* (\hat{L}_z \hat{S}_z) \phi_o(\vec{r}) \alpha d\vec{r}_S d\vec{r}}{E_n - E_o} \\ &\quad - \frac{1}{2} \lambda \frac{\iint \phi_n^*(\vec{r}) \beta^* (L^+ S^-) \phi_o(\vec{r}) \alpha d\vec{r}_S d\vec{r}}{E_n - E_o} \\ &= -\frac{\lambda}{2} \left[\frac{\iint \phi_n^*(\vec{r}) \hat{L}_z \phi_o(\vec{r}) d\vec{r}}{E_n - E_o} + \frac{\iint \phi_n^*(\vec{r}) L^+ \phi_o(\vec{r}) d\vec{r}}{E_n - E_o} \right] \end{aligned}$$

. $\int \alpha^* d\vec{r}_S \quad (1)$. $\int \beta^* d\vec{r}_S \quad (2)$

(5)

$$C_n^\beta = -\lambda \frac{\iint \phi_n^*(\vec{r}) \beta^* (\hat{L}_z \hat{S}_z) \phi_o(\vec{r}) \beta d\vec{r} d\vec{r}_o}{E_n - E_o}$$

$$-\frac{\lambda}{2} \frac{\iint \phi_n^*(\vec{r}) \alpha^* (\hat{L}^- \hat{S}^+) \phi_o(\vec{r}) \beta d\vec{r} d\vec{r}_o}{E_n - E_o}$$

$$= -\frac{\lambda}{2} \left[\frac{\iint \phi_n^*(\vec{r}) \hat{L}_z \phi_o(\vec{r}) d\vec{r}}{E_n - E_o} + \frac{\iint \phi_n^*(\vec{r}) \hat{L}^- \phi_o(\vec{r}) d\vec{r}}{E_n - E_o} \right]$$

Therefore

$$|+\rangle = \phi_o(\vec{r}) \cdot \alpha - \sum_n' \frac{\lambda}{2} \left(\frac{1}{E_n - E_o} \right) \left[\int \phi_n^*(\vec{r}) \hat{L}_z \phi_o(\vec{r}) d\vec{r} + \int \phi_n^*(\vec{r}) \hat{L}^+ \phi_o(\vec{r}) d\vec{r} \right] \phi_n(\vec{r})$$

and

$$|- \rangle = \phi_o(\vec{r}) \beta - \sum_n' \frac{\lambda}{2} \left(\frac{1}{E_n - E_o} \right) \left[\int \phi_n^*(\vec{r}) \hat{L}_z \phi_o(\vec{r}) d\vec{r} + \int \phi_n^*(\vec{r}) \hat{L}^- \phi_o(\vec{r}) d\vec{r} \right] \phi_n(\vec{r})$$

Zeeman Energy

$$\langle + | g_s \beta \vec{S} \cdot \vec{H} + g_L \beta \vec{L} \cdot \vec{H} | + \rangle$$

$$= \int \left(\phi_o^*(\vec{r}) \alpha^* + \sum_n' C_n^* \psi_n^*(\vec{r}, \vec{r}_o) \right) \left(g_s \beta \vec{S} \cdot \vec{H} + g_L \beta \vec{L} \cdot \vec{H} \right) \left(\phi_o(\vec{r}) \alpha + \sum_n' C_n \psi_n(\vec{r}, \vec{r}_o) \right) d\vec{r}$$

$$= \int \phi_o^*(\vec{r}) \alpha^* (g_s \beta \vec{S} \cdot \vec{H}) \phi_o(\vec{r}) \alpha d\vec{r} + \int \psi_o^*(\vec{r}, \vec{r}_o) (g_L \beta \vec{L} \cdot \vec{H}) \sum_n' C_n \psi_n(\vec{r}, \vec{r}_o) d\vec{r}$$