

1. Show in detail that Eq.(4.50) follows from Eq.(4.47).

Eq.(4.50) is

$$E_{ab,LS}^{(1)} = \eta^2 \sum_{m's\mu's} \begin{array}{c} \downarrow l_a m_a \\ \text{---} LM_L \\ \downarrow l_b m_b \end{array} \begin{array}{c} \downarrow 1/2\mu_a \\ \text{---} SM_S \\ \downarrow 1/2\mu_b \end{array} \begin{array}{c} \downarrow l_a m'_a \\ \text{---} LM_L \\ \downarrow l_b m'_b \end{array} \begin{array}{c} \downarrow 1/2\mu'_a \\ \text{---} SM_S \\ \downarrow 1/2\mu'_b \end{array} \left[ g_{a'b'ab} \delta_{\mu'_a \mu_a} \delta_{\mu'_b \mu_b} - g_{a'b'ba} \delta_{\mu'_a \mu_b} \delta_{\mu'_b \mu_a} - (\delta_{a'a} \delta_{b'b} - \delta_{a'b} \delta_{b'a})(U_{aa} + U_{bb}) \right].$$

where

$$g_{abcd} = \sum_k \begin{array}{c} \downarrow l_a m_a \\ \text{---} k \\ \downarrow l_c m_c \end{array} \begin{array}{c} \downarrow l_b m_b \\ \text{---} k \\ \downarrow l_d m_d \end{array} + X_k(abcd).$$

The sums over  $\mu$ 's associated with  $\delta_{\mu'_a \mu_a} \delta_{\mu'_b \mu_b}$  gives

$$\begin{array}{c} \downarrow 1/2\mu_a \\ \text{---} SM_S \\ \downarrow 1/2\mu_b \end{array} \begin{array}{c} \downarrow 1/2\mu_a \\ \text{---} SM_S \\ \downarrow 1/2\mu_b \end{array} = \begin{array}{c} \downarrow 1/2 \\ \text{---} SM_S \\ \downarrow 1/2 \end{array} \bigcirc \begin{array}{c} \downarrow 1/2 \\ \text{---} SM_S \\ \downarrow 1/2 \end{array} = 1$$

Similarly, the sums over  $\mu$ 's associated with  $\delta_{\mu'_a \mu_b} \delta_{\mu'_b \mu_a}$  gives

$$\begin{array}{c} \downarrow 1/2\mu_a \\ \text{---} SM_S \\ \downarrow 1/2\mu_b \end{array} \begin{array}{c} \downarrow 1/2\mu_b \\ \text{---} SM_S \\ \downarrow 1/2\mu_a \end{array} = \begin{array}{c} \downarrow 1/2 \\ \text{---} SM_S \\ \downarrow 1/2 \end{array} \bigcirc \begin{array}{c} \downarrow 1/2 \\ \text{---} SM_S \\ \downarrow 1/2 \end{array} = (-1)^{1/2+1/2+S} = (-1)^{1+S}$$

The sum over  $m$ 's associated with the first two-body term can be rotated into the following form where a sum over  $M_L$  has been done and the factor  $[L]$  correspondingly dropped.

$$\begin{array}{c} \downarrow l_a \\ \text{---} L \\ \downarrow l_b \end{array} \begin{array}{c} \downarrow l_b \\ \text{---} k \\ \downarrow l_a \end{array} + \begin{array}{c} \downarrow l_b \\ \text{---} L \\ \downarrow l_a \end{array} \begin{array}{c} \downarrow l_a \\ \text{---} k \\ \downarrow l_b \end{array} = (-1)^{l_a+l_b+L+k} \left\{ \begin{array}{ccc} l_a & l_b & L \\ l_b & l_a & k \end{array} \right\}$$

Similarly, the sum over  $m$ 's associated with the second two-body term can be put in the form

$$\begin{array}{c} \downarrow l_a \\ \text{---} L \\ \downarrow l_b \end{array} \begin{array}{c} \downarrow l_b \\ \text{---} k \\ \downarrow l_a \end{array} + \begin{array}{c} \downarrow l_b \\ \text{---} L \\ \downarrow l_a \end{array} \begin{array}{c} \downarrow l_a \\ \text{---} k \\ \downarrow l_b \end{array} = (-1)^{l_a+l_b+k} \left\{ \begin{array}{ccc} l_a & l_b & L \\ l_a & l_b & k \end{array} \right\}$$

Finally, the sums over  $m$  associated with the one-body terms can be treated precisely as the sums over  $\mu$  above, leading to the following result for the one-body part

$$-\eta^2 (1 + (-1)^{L+S} \delta_{ab}) (U_{aa} + U_{bb}) = -U_{aa} - U_{bb}$$

Putting all of the above together, leads to the following expression for the first-order energy:

$$E_{ab,LS}^{(1)} = \eta^2 \sum_k \left[ (-1)^{L+k+l_a+l_b} \begin{Bmatrix} l_a & l_b & L \\ l_b & l_a & k \end{Bmatrix} X_k(abab) \right. \\ \left. + (-1)^{S+k+l_a+l_b} \begin{Bmatrix} l_a & l_b & L \\ l_a & l_b & k \end{Bmatrix} X_k(abba) \right] - U_{aa} - U_{bb}.$$