[lex176] Exchange integral

The two-electron wave functions written in the form,

$$\Psi_{\rm S}(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{\sqrt{2}}\Big[\phi_a(\mathbf{r}_1)\phi_b(\mathbf{r}_2) + \phi_a(\mathbf{r}_2)\phi_b(\mathbf{r}_1)\Big]\chi_{\rm S},$$
$$\Psi_{\rm T}(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{\sqrt{2}}\Big[\phi_a(\mathbf{r}_1)\phi_b(\mathbf{r}_2) - \phi_a(\mathbf{r}_2)\phi_b(\mathbf{r}_1)\Big]\chi_{\rm T},$$

have symmetric/antisymmetric spatial parts and antisymmetric/symmetric spin parts, respectively, as described in [lln23]. $\chi_{\rm S}$ and $\chi_{\rm T}$ are spin singlet/triplet states. Both wave functions are antisymmetric overall as is required for fermions. The interaction Hamiltonian $\mathcal{H}$ contains kinetic energy and Coulomb repulsion but no significant interaction between electron spins. The energies of the singlet and triplet states in first-order perturbation theory become,

$$E_{\rm S} = \int d\mathbf{r}_1 d\mathbf{r}_2 \Psi^*_{\rm S}(\mathbf{r}_1,\mathbf{r}_2)\mathcal{H}\Psi_{\rm S}(\mathbf{r}_1,\mathbf{r}_2), \quad E_{\rm T} = \int d\mathbf{r}_1 d\mathbf{r}_2 \Psi^*_{\rm T}(\mathbf{r}_1,\mathbf{r}_2)\mathcal{H}\Psi_{\rm T}(\mathbf{r}_1,\mathbf{r}_2).$$

Show that the level spacing between singlet and triplet states is determined by the exchange integral defined as follows:

$$2J \doteq E_{\rm S} - E_{\rm T} = 2\int d\mathbf{r}_1 d\mathbf{r}_2 \phi^*_a(\mathbf{r}_1)\phi^*_b(\mathbf{r}_2)\mathcal{H}\phi_a(\mathbf{r}_2)\phi_b(\mathbf{r}_1).$$

Solution: