J99Q.1—Hydrogen Molecule

Problem

Consider two hydrogen atoms with their nucleii separated by a fixed distance $R > 2r_b$ where r_b is the Bohr radius

a) In terms of the electronic wavefunctions on the separate atoms write an approximate two electron wavefunction for the ground state, including spin and orbital degrees of freedom.

b) There are terms in the hamiltonian of the molecule which are absent in two separate atoms. Write an expression for these perturbations. Using perturbation theory find an expression for the lowest order nonvanishing energy difference between the singlet and triplet states. (The result may be left in terms of an integral.)

c) For large separation between the hydrogen molecules, the perturbation can be treated in a dipole approximation. Find an expression for the effective interaction energy and in particular find its *dependence on the separation* R in the limit $R \gg 2r_b$.