# Section A. Quantum Mechanics

1. **Two Hydrogen Atoms**

   Consider two hydrogen atoms with their nuclei held at fixed positions such that the displacement $\vec{R}$ between them is large compared to the ground-state size of the atoms. Treat the Coulomb interaction as instantaneous (no retardation), neglect nuclear spins and nuclear motion, and neglect any contribution of the electron spins to the energy (no spin-orbit interactions). The appropriate basis set for discussing the energetics of this system is spanned by states of the type $\psi^{(1)}_{n\ell m}(\vec{r}_1)\psi^{(2)}_{n'\ell' m'}(\vec{r}_2)$ where each electron is in a single-atom eigenstate about its nucleus. Take the $z$ axis to lie along the displacement $\vec{R}$ between the two nuclei. Under these conditions, the dominant interaction between the two atoms comes from the electric dipole-dipole interaction:

$$U_{dipole}(\vec{R}) = \frac{1}{4\pi\epsilon_0 R^3}\left[\vec{d}^{(1)}\cdot\vec{d}^{(2)} - 3d_z^{(1)}d_z^{(2)}\right]$$

   where $\vec{d}^{(n)}$ is the dipole operator for the electron bound to nucleus $n$. The ground state energy of this pair of atoms depends on $R$ at large $R$ as

$$E_0(r) = E_0(\infty) + A_0 R^{-\delta_0} + \ldots\ .$$

   The two electrons can of course be in either a state of total spin $S = 0$ or $S = 1$; in what follows, let the two electrons always have total spin $S = 0$.

   (a) Write down the leading approximation to the ground state wave function in the limit of large $R$ (i.e. explain how you would calculate $E_0(\infty)$).

   (b) Explain what physics determines the exponent $\delta_0$ governing the R-dependence of the correction to the ground state energy. Give the value of $\delta_0$.

   (c) Give an order of magnitude estimate for the constant $A_0$ and give a general argument for its sign.

   (d) The energy of the lowest energy electronic *excited* eigenstate of this pair of atoms depends on $R$ at large $R$ as

$$E_1(R) = E_1(\infty) + A_1 R^{-\delta_1} + \ldots\ .$$

   What is the exponent $\delta_1$? Give an order of magnitude estimate of $A_1$. What is the sign of $A_1$? What is the full wavefunction of this excited eigenstate at leading order in large $R$?