Physics 5456 – Problem set 3

H_2^+ ion: overlap, Coulomb, exchange integrals

In this problem, you will compute the overlap, Coulomb, and exchange integrals appearing in the analysis of the hydrogen molecular ion.

Let

$$r_{1,2} \;=\; |\vec{r} - \vec{R}_{1,2}| \;=\; \sqrt{\rho^2 \;+\; (z \mp R/2)^2}$$

denote the distance between the electron and the two nuclei, in cylindrical coordinates oriented so that both nuclei lie along the z axis, equidistant from the origin. Define the elliptical coordinates

$$\xi \;=\; (r_1 + r_2)/R, \quad \eta \;=\; (r_2 - r_1)/R$$

1. Show that $1 \leq \xi < \infty$, $-1 \leq \eta \leq 1$.
2. Show that the Jacobian for converting $d\rho dz$ to $d\xi d\eta$ is given by

$$\frac{R^3}{8\rho}\left(\xi^2 \;-\; \eta^2\right)$$

   For the next parts, use the hydrogen ground state wavefunction

$$\varphi(\vec{r}) \;=\; \left(\pi a^3\right)^{-1/2} e^{-r/a}$$

   where a is the Bohr radius.

3. Compute the overlap integral $S(R) = \langle\varphi_1|\varphi_2\rangle$.
4. Compute the direct Coulomb integral $D(R) = e^2\langle\varphi_1|r_2^{-1}|\varphi_1\rangle$.
5. Compute the exchange Coulomb integral $X(R) = e^2\langle\varphi_1|r_2^{-1}|\varphi_2\rangle$.