Quantum Mechanics 2

Problem set 9

1. Show that the He_2^{3+} (that is, 2 Helium atoms in a molecule, ionized 3 times) does not exist.

2. Work out the VDW forces due to dipole-dipole interaction between two hydrogen atoms, one in the ground state, and one in the first excited state. Unlike what we did in class last week, perform the full calculation for the proportionality constant(s). Is the interaction attractive or repulsive? Is the interaction stronger or weaker than the ground state case?

3. Prove
$$\int \frac{d\Omega_1 d\Omega_2}{|\vec{r}_1 - \vec{r}_2|} = \frac{(4\pi)^2}{r_>}$$
where $r_> = \max\{r_1, r_2\}$ (we used this result last week in the Helium atom calculations)

4. Calculate explicitly the integral
$$S(R) = \int d^3x \psi_A(\vec{x})\psi_B(\vec{x})$$
which we used for the H_2^+ molecule, and where $\psi_{A,B}(\vec{x})$ are the Hydrogen ground-state wave functions of an electron orbiting a proton at $\vec{X}_A$ or $\vec{X}_B$ respectively.

5. We introduced two methods for calculating the ground state energy of molecules: the molecular orbitals method and the Heitler-London method.

   (a) Discuss the shortcomings of the two methods, and the advantage of the Heitler-London method over the molecular orbitals method (you may use the examples we worked out in class to illustrate your reasoning).

   (b) For the H_2^+ molecule one can do better, even with the shortcomings you discussed above, by introducing an effective charge to the protons, and minimize the energy with respect to this parameter in addition to the nuclei separation. Derive the function that needs to be minimized explicitly (perform the integrations). Don't try the minimization itself. you may use
   $$\int d^3x \psi_A H \psi_B = \left(E_1 + \frac{e^2}{R}\right) S(R) - \int d^3x \psi_A \psi_B \frac{e^2}{\left|\vec{x} - \vec{X}_B\right|}$$
   (which is true when *not* accounting for the effective charge).