PHYS 225: Applications of Modern Physics **Marie Lopez del Puerto**

HW #3

1. **(Kasap 1.3) The covalent bond** Consider the H_2 molecule in a simple way as two touching H atoms, as depicted in the figure. Does this arrangement have a lower energy than two separated H atoms? Suppose that electrons totally correlate their motions so that they move to avoid each other as in the snapshot in the figure. The radius r_0 of the hydrogen atom is 0.0529 nm. The electrostatic potential energy of two charges Q_1 and Q_2 separated by a distance r is given by $Q_1Q_2/(4\pi\varepsilon_0 r)$. Using the virial theorem consider the following:

    a. Calculate the total electrostatic potential energy *PE* of all the charges when they are arranged as shown in the figure. In evaluating the *PE* of the whole collection of charges you must consider all pairs of charges and, at the same time, avoid double counting of interactions between the same pair of charges. The total *PE* is the sum of the following: electron 1 interacting with the proton at a distance r_0 on the left, proton at r_0 on the right, and electron 2 at a distance $2r_0$, plus electron 2 interacting with a proton at r_0 and another proton at $3r_0$, plus two protons, separated by $2r_0$, interacting with each other. Is this configuration energetically favorable?

    b. Given that in the isolated H atom the *PE* is 2 x (-13.6 eV), calculate the change in *PE* in going from two isolated H atoms to the H_2 molecule. Using the virial theorem, find the change in the total energy and hence the covalent bond energy. How does this compare with the experimental value of 4.51 eV?