Problem Set 1
Physics 520

Fall 2005
L. Sander
9/8/05 due 9/15/05

1. Calculate the van der Waals' interaction between two H atoms in their ground state. Use the Hamiltonian for the two the single atoms as a reference:

$$\mathcal{H} = \Sigma_{i=1,2}\, p_i^2/2m - e^2/|\mathbf{r_i} - \mathbf{R_i}|$$

and the rest as a perturbation:

$$\delta\mathcal{H} = -e^2/|\mathbf{r_1}-\mathbf{R_2}| - e^2/|\mathbf{r_2}-\mathbf{R_1}| + e^2/|\mathbf{r_1}-\mathbf{r_2}| + e^2/|\mathbf{R_1}-\mathbf{R_2}|$$

See Ashcroft and Mermin, Schiff, *Quantum Mechanics*. Assume that $r_i << d$, where d is the distance between the nuclei. Consider only the first excited state of H in your perturbation theory; do not use the trick in Schiff's book which involves using an approximate summation over all states.

2. a.) He is a liquid sufficiently near T=0. Explain why. (Hint: estimate the zero point kinetic energy due to the localization of He atoms in a cell of size σ =2.56 Angstrom. The energy parameter is $\varepsilon = 1.4 \times 10^{-15}$ ergs.). b.) H_2 is a solid. However, H_2 is lighter and has bigger zero point fluctuations. Explain.

3. Argon has $\varepsilon = 1.7 \times 10^{-14}$ ergs and σ= 3.4 Angstrom. Find the equilibrium distance between atoms and the binding energy per atom for (hypothetical) simple cubic Ar.

4. a.) When spheres are as closely packed as possible they form either a fcc lattice or a hcp crystal. Prove that when spheres are packed they fill the following percentages of the available volume (the packing fraction).

simple cubic	52%
body-centered cubic	68%
fcc	74%

b.) Find the c/a ratio such that hcp is close-packed. What is the packing fraction?

5. Show that no two dimensional Bravais lattice can have a 5 or 7-fold axis of rotation, i.e., no axis such that a rotation by $2\pi/5$ or $2\pi/7$ leaves that lattice invariant. See AM p. 129 for a hint.