Phys 4050 Assignment 2

1. Quantum Solid. In a quantum solid the dominant repulsive energy is the zero point energy of the atoms. Consider a crude one dimensional model of crystalline He^4 with each He atom confined to a line segment of length L. In the ground state the wavefunction within each segment is taken as a half wavelength of a free particle. Find the zero point kinetic energy per particle.

2. Cohesive energy of bcc and fcc neon. Using the Lennard-Jones potential, calculate the ratio of the cohesive energies of neon in the bcc and fcc structures. The lattice sums for the bcc structures are:

$$\sum_j{}' p_{ij}^{-12} = 9.11418$$

$$\sum_j{}' p_{ij}^{-6} = 12.2533$$

3. Solid molecular hydrogen. For H_2, one finds from measurements on the gas that the Lennard-Jones parameters are $\varepsilon = 50 \times 10^{-16}$ erg and $\sigma = 2.96$ Angstrom. Find the cohesive energy in kJ per mole of H_2; do the calculation for an fcc structure. Treat each H_2 molecules as a sphere. The observed value of the cohesive energy is 0.751 kJ/mol, much less than we calculated, so that quantum corrections must be very important.