PROBLEM SET 9

1. Obtain equations for (a) the pressure and (b) the chemical potential for a system of non-interacting lattice monomers valid at all volume fractions, φ (= N/V). You may want to use virtual MC simulations in your derivation.

2. The following problem utilizes the LJ Molecular Dynamics simulation applet found in http://www.ccr.buffalo.edu/etomica/app/modules/sites/Ljmd/. The applet computes thermodynamic and structural properties for the 2-dimensional Lennard-Jones system.

(a) Obtain the pressure versus density curves (isotherms) at T=0.3, 0.5 and 0.7 and estimate the location of the vapor-liquid critical point.

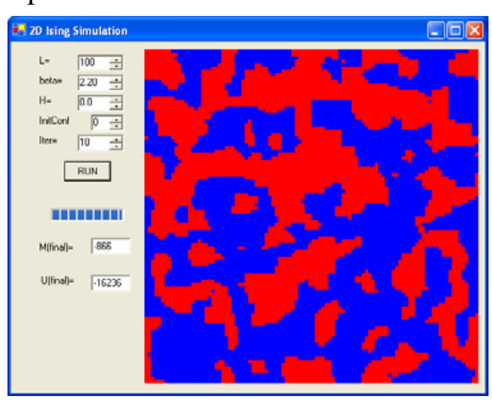
(b) Obtain the radial distribution functions for T=0.3, ρ=0.9; T = 0.5, ρ=0.6; T=0.7, ρ=0.1 and comment on their features.

(c) T=0.3 is below the triple point, so there is equilibrium between solid and gas phases. Estimate the density of the equilibrium solid phase at this temperature.

3. The following problem uses the 2-dimensional Ising model in http://poros.princeton.edu/ChE503/Ising2D.exe . You will need to save this to a temporary directory and run it on your PC (only runs under Windows, sorry). The only non-obvious input parameter is "InitConf," which can be set to 1 for random initial configuration, 0 for using the final configuration of the previous run and 2 for a two-phase system.

(a) Obtain the mean magnetization per spin M as a function of the field strength H at various fixed temperatures both above and below Tc. What key difference in behavior do you observe above and below the critical temperature?

(b) Perform a mean-field calculation for the expected value of the mean magnetization per spin as a function of field strength at high temperatures. Do results from the code quantitatively support this calculation?



(c) At zero field, H=0 one can observe "spinodal decomposition" after a rapid quench from $T_i > T_c$ to $T_f < T_c$ - see example to the right. How does the size of domains vary with observation time and quench depth? Perform this by qualitatively comparing the results of quenches at different T_f for corresponding observation times.