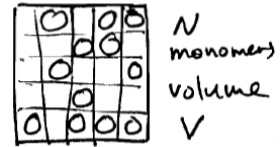


Problem Set # 8

Due: 10:30 am Friday 12/18

- [1] Obtain an expression for the radial position that corresponds to the maximum value of the radial distribution function for Ar at low pressures. Ar-Ar interactions can be approximated by the Lennard-Jones 12-6 potential with  $\epsilon/k_B = 120$  K,  $\sigma = 0.34$  nm.
- [2] Consider a system consisting of a colloidal particle of radius  $\sigma$  and charge  $Q=+20e$  ( $e$  is the charge of an electron) stationary in the center of a spherical cavity of radius  $R=5\sigma$ . Its counterions have negligible size and can be at any distance between  $\sigma$  and  $R$ . Estimate the counterion distribution function,  $g(r)$ , as a function of distance using a numerical solution of the Poisson-Boltzmann equations as described in the class notes. In particular, perform the calculations at conditions so that the Bjerrum length  $\xi = e^2/(4\pi\epsilon\epsilon_0k_B T)$  is (a)  $\xi = \sigma/5$  (b) the Bjerrum length is  $\xi = \sigma/50$  and (c)  $\xi = \sigma/2$ . Also obtain the total energy of the system for these three cases. Note that it is easier to work in reduced units, with length measured in units of  $\sigma$  and energy in units of  $e^2/4\pi\epsilon\epsilon_0\sigma$ .

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



- [4] The following problem uses the 2-dimensional Ising model applet that can be obtained from <http://stp.clarku.edu/simulations/ising/ising2d/index.html>.†

(a) Obtain the mean magnetization per spin,  $\langle M \rangle$ , for length  $L = 100$ , as a function of the field strength  $H$  at  $T=1.5$ ,  $T=3$ , and  $T=10$ . What is the key difference in behavior of  $\langle M \rangle$  versus  $H$  above and below the critical temperature?

(b) Obtain a mean-field expression for  $\langle M \rangle$  as a function  $H$  and compare simulation results of part (a) at  $T = 3$  and  $T = 10$  to the corresponding mean-field values. What is the reason for the deterioration of the quality of the mean-field predictions at the lower temperature and field strength?

(c) *Finite size scaling*. Compute the constant-volume specific heat at  $T = T_c \cong 2.269$  for  $L = 8, 16, 32$ , and  $64$ . Use as many Monte Carlo steps per spin as possible. Try both the Metropolis and Wolff updating algorithms and choose the algorithm that converges more quickly. Confirm that the specific heat diverges logarithmically with system size. Is this divergence consistent with the expectations of classical stability theory?

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† You may need to add the site <http://stp.clarku.edu/simulations/ising/ising2d/index.html> to your Java "Exception Site List" for the applet to run.