Lattice gas

Consider the lattice gas defined by the Hamiltonian

$$H = v_0 \sum_{\langle ij \rangle} t_i t_j$$

on a lattice with periodic boundary conditions. The notation $\langle ij \rangle$ means that the sum is restricted to terms where i and j are neighboring sites. t_i is 1 when a particle occupies site i and 0 otherwise. The total number of particles is $N = \sum_i t_i$. v_0 is a positive constant with units of energy.

1. Exact solution for small systems

In this subproblem consider the above lattice gas on the smallest two dimensional lattice, a 2×2-lattice, with periodic boundary conditions.

a) Find expressions for $\langle E \rangle$ (E is the energy) and $\langle N \rangle$ as functions of $\mu, v_0, \beta = 1/(k_B T)$ in the grand canonical ensemble. (hint: write down all possible configurations).

b) Make a plot of $\langle N \rangle$ vs. μ/v_0 for $\beta v_0 = 1$.

c) Which value of μ/v_0 gives $\langle N \rangle = 2$ for $\beta v_0 = 1$? what is $\langle N \rangle$ and $\langle E \rangle$ for $\beta v_0 = 1$ and $\mu/v_0 = 4.48388$?

2. Transfer matrix solution of the 1d lattice gas

In this subproblem the lattice is one-dimensional with periodic boundary conditions, i.e. a ring with L sites.

a) Write down the transfer matrix for the lattice gas in the grand canonical ensemble (include a chemical potential term $-\mu N$), and find its eigenvalues.

b) Find an expression for the grand potential per site using transfer matrices in the limit $L \to \infty$.

c) Use the answer in b) to find expressions (for $L \to \infty$) for the average number of particles per site $\langle N \rangle / L$ as functions of v_0, β and μ. Do not worry if your answer does not look "pretty". You only need to carry out the calculation so far that you can make a graph of the result, to be used in problem 3.

3. Monte Carlo simulation

a) Make a Monte Carlo program for the lattice gas in the grand canonical ensemble (use for instance the Metropolis algorithm, see chapter 7 in Yeomans). Check that the Monte Carlo program reproduces the values you found in problem 1. Make a table which compares your Monte Carlo results for $\langle N \rangle$ and $\langle E \rangle$ to your results in problem 1.

b) Make plots of $\langle N \rangle / L$ as a function of μ / v_0 for a high temperature $\beta v_0 = 1$ and a low temperature $\beta v_0 = 10$ for an $L = 100$ site ring using your Monte Carlo code. On the same plot superimpose your $L \to \infty$ transfer matrix results from problem 2.

c) Now consider a 10×10-lattice with periodic boundary conditions. Set the chemical potential to $\mu = 2v_0$. Calculate the heat capacity per site of the system at constant μ and system size at different temperatures using your Monte Carlo code. Make a plot. Is there any indication of a phase transition in this system as the temperature is varied? If so, give a rough estimate of the critical temperature.