ChE 210B: Homework 4. Due February 3, 2005.

Problem 1. Consider the Ising model in two dimensions on a square lattice (the lattice is a chess board type structure, and spins occupy the squares that chess pieces could occupy)

$$E(x) = -\sum_{<i,j>} J s_i s_j \tag{1}$$

where $x \equiv \{s_1 \ldots s_N\}$ and $s_i \in \{-1, 1\}$. The sum over $< i, j >$ denotes a sum over each pair of nearest neighbor spins, and each spin has four nearest neighbors. There is an energy $-J$ for each pair of neighboring spins in the same state. Unlike the model in the first homework, there is no external field.

Here, we study a Monte Carlo algorithm that flips multiple spins at each step. At each step, pick a spin s_i. Then consider each spin on a nearest neighbor site of s_i in the same state. With probability $P_{add} = 1 - e^{-\beta 2J}$, add a neighboring spin in the same state to the "cluster". For each additional spin added to the cluster, repeat this procedure. This procedure terminates when either there are no neighboring spins of the cluster in the same state or we pick not to include all neighboring spins of the same state with probability $1 - P_{add} = e^{-\beta 2J}$. This constitutes a trial move $t(x, y)$. The transition probability is $t(x, y)A(x, y)$, where $A(x, y)$ is the probability of accepting a move from y to x, and accepting a move implies flipping each spin in the cluster. Developing an expression for $t(x, y)$ and determine the $A(x, y)$ such that the detailed balance condition

$$\frac{t(x, y)A(x, y)}{t(y, x)A(y, x)} = \frac{\sigma(x)}{\sigma(y)} \tag{2}$$

holds. This is the Wolff algorithm, and it is extremely efficient at sampling the equilibrium distribution of the Ising model near its critical temperature.

Problem 2. Develop an expression for $\langle U(r^N) \rangle$ in terms of particle density functions $\rho_N^{(n)}(\mathbf{r}_1 \ldots \mathbf{r}_n)$ for homogeneous system with an isotropic potential

$$U(r^N) = \sum_{i<j=1}^{N} u(|\mathbf{r}_i - \mathbf{r}_j|) + \sum_{i<j<k=1}^{N} u^{(3)}(|\mathbf{r}_i - \mathbf{r}_j|, |\mathbf{r}_j - \mathbf{r}_k|) \tag{3}$$

Problem 3. The structure factor defined in class is

$$S(\mathbf{k}) = \left\langle \sum_{i,j=1}^{N} e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \right\rangle. \tag{4}$$

For a homogeneous, isotropic fluid, show that

$$\frac{S(k)}{N} = 1 + 4\pi\rho \int_0^\infty \frac{\sin(kr)}{kr} g(r) r^2 dr. \tag{5}$$