Mapping between the Lattice Gas and the Ising Model

Grand partition function for a fluid model:

$$\Xi(T, V, \mu) = \sum_{N=0}^{\infty} e^{\beta \mu N} Z_N(T, V) = \sum_{N=0}^{\infty} \left( \frac{e^{\beta \mu}}{N^d} \right)^N Q_N(T, V)$$

$$Q_N(T, V) = \frac{1}{N!} \int d^N \mathbf{r} \exp \left(-\beta U_N(\mathbf{r}_1, \ldots, \mathbf{r}_N)\right)$$

Approximate the integrals by sums by dividing space up into a periodic lattice $\left\{ \mathbf{R} \right\}$

$$Q_N(T, V) = \frac{v^N}{N!} \sum_{\mathbf{R}_1} \ldots \sum_{\mathbf{R}_N} \exp \left(-\beta U_N(\mathbf{R}_1, \ldots, \mathbf{R}_N)\right) = \frac{v^N}{N!} \sum_{\mathbf{R}_1} \ldots \sum_{\mathbf{R}_N} \exp \left(-\frac{1}{2} \sum_{\mathbf{R} \neq \mathbf{R}'} \beta \phi (\mathbf{R} - \mathbf{R}')\right)$$

where $v$ is the volume of a unit cell in the lattice. This volume is chosen small enough so that there is no chance that two particles will occupy the same cell at the same time. This requires for the potential to diverge if two particles approach each other. Then the grand partition function is

$$\Xi(T, V, \mu) = \sum_{N=0}^{\infty} \frac{v^N}{N!} \exp \left(\beta \mu N\right) \exp \left(-\frac{1}{2} \sum_{\mathbf{R} \neq \mathbf{R}'} \beta \phi (\mathbf{R} - \mathbf{R}')\right)$$

If there are $N_s$ sites on the lattice then there are $\frac{N_s!}{(N - N_s)!}$ terms in the sum over the positions. Since $\sum_{N=0}^{\infty} \frac{N_s!}{N! (N_s - N)!} = 2^{N_s}$, we can count each term in $\Xi$ by summing over the $2^{N_s}$ possible configurations of the occupancies ($n=0,1$) of the lattice sites. The grand partition can then be written in terms of a sum over all possible occupancies of the lattice sites.

$$\Xi(T, V, \mu) = \sum_{\{n(R) = 0,1\}} \exp \left(\beta \mu \sum_{\mathbf{R}} n(\mathbf{R}) - \frac{1}{2} \sum_{\mathbf{R} \neq \mathbf{R}'} \phi (\mathbf{R} - \mathbf{R}') n(\mathbf{R}) n(\mathbf{R}')\right)$$

where $\beta \mu = \beta \mu + \ln \left(\frac{v}{N^d} \right)$. This describes a set of interacting particles moving around a lattice connected to a reservoir of particles. This is called the lattice-gas model. We can map this onto an Ising model, a magnetic model of spins that interact with each other and with an applied magnetic field. The Ising model consists of spins on a lattice that have values $\pm 1$. The interaction with an applied field is of the form $-g \mu_b H \sum_{j=1}^{N} s_j$ and the interaction between pairs of spins on different lattice sites is of the form $-J_{ij} s_i s_j$. If the exchange energy $J_{ij}$ is positive the energy favors alignment, both $+1$ or both $-1$. This is called a ferromagnetic interaction. If the exchange energy $J_{ij}$ is negative the energy
favors antialignment, one +1 and the other -1. This is called an antiferromagnetic interaction. The partition function for the Ising model is then

\[ Z_N(T,H) = \sum_{\{s_i = \pm 1\}_{i=1}^N} \exp \left( \frac{1}{2} \sum_{i \neq j} K_{ij}s_is_j + h \sum_{j=1}^N s_j \right) \]

where \( K_{ij} = \frac{J_{ij}}{k_BT} \) is the coupling between spins and \( h = \frac{g\mu_B H}{k_BT} \) is the interaction of the spins with the applied magnetic field. By using the identification \( s_i = 2n(R_i) - 1 \) we can map the lattice gas model onto the Ising model. Up (\( s=+1 \)) is equivalent to occupied (\( n=1 \)) while down (\( s=-1 \)) is equivalent to empty (\( n=0 \)). Up to constant terms the mapping is

\[ K_{ij} = -\frac{\beta \varphi(R_{ij})}{4} \quad \text{and} \quad h = \frac{\beta \bar{\mu}}{2} - \frac{1}{4} \sum_{R_{ij}=0} \beta \varphi(R) \]

An attractive (negative) piece of the pair potential corresponds to ferromagnetic interaction. A repulsive (positive) piece of the pair potential corresponds to an antiferromagnetic interaction. A chemical potential in excess of the net interaction with all of the neighbors results in a positive field which will tend to lead to an average spin greater than zero (positively magnetized). A large chemical potential (high density) corresponds to a large positive net spin (large positive magnetization). Large negative chemical potential (low density) corresponds to a large negative net spin (large negative magnetization).