Statistical Physics - Tutorial II

Amir Bar

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In this tutorial we shall see how the Ising model can be used to model interacting gasses, and to probe the liquide-gas transition. This follows Huang, Statistical Mechanics (2nd edition 1987) Ch. 14.2.

1 Ising model reminder

The Ising model is defined over an undirected graph $G = (V, E)$ where on each site $i \in V$ there is a spin $s_i = \pm 1$, and the energy is

$$H_I = -J \sum_{(i,j)\in E} s_i s_j - h \sum s_i. \tag{1}$$

The order parameter is the average magnetization $M = \frac{1}{v} \sum s_i$, where $v = |V|$ is the volume.. For any lattice in dimension higher than 1 there is a first order phase transition at $h = 0$ and $T < T_c$ between an up ferromagnetic state in which $M > 0$ and a down state in which $M < 0$. This first order line is terminated at $T = T_c$ in a second order phase transition. For $T > T_c$, there is no phase transition at $h = 0$, but instead there is a smooth crossover from $M > 0$ to $M < 0$. This phenomelogy is similar to that of the liquid-gas transition. Is there a deeper connection between the two? In the next section we shall see such connection.

2 Lattice gas

The particles of a real interacting gas live in real space. However, in order to have a model which is similar to the Ising model we must assume particles that occupy a lattice (or more generally a graph). We make several additional simplifying assumptions: we assume that in each lattice site there is at most a single particle, so that for each site there is an occupation variable $n_i = 0, 1$. Clearly, a mapping between a spin and an occupation variable can be made as follows

$$s_i = 2n_i - 1 \qquad ; \qquad n_i = \frac{s_i + 1}{2}. \tag{2}$$

In addition it is assumed that the interactions between particles are nonvanishing only when the two particles are nearest-neighbors, that is the Hamiltonian is

$$\tilde{H}_{LG} = -\epsilon \sum_{(i,j)\in E} n_i n_j. \tag{3}$$

Notice also that the kinetic energy was ignored. The similarity between Eq.(1) and (3) is already quite apparent. Using the mapping (2) we get

$$\tilde{H}_{LG} = -\frac{\epsilon}{4} \sum_{(i,j)\in E} s_i s_j - \frac{\epsilon\zeta}{2} \sum s_i + const.$$

ζ is the number of nearest neighbors (we assume a regular graph, like a square lattice, in which all sites have the same number of nearest neighbors). From this we see the correspondance $\epsilon = 4J$. What about the magnetic field? In the Ising model the magnetic field is coupled to the magnetization

$$M = \frac{1}{v}\sum s_i = \frac{1}{v}\sum (2n_i - 1) = 2\rho - 1, \tag{4}$$

where $\rho \equiv \frac{N}{v} = \frac{1}{v}\sum n_i$ is the density of particles. Hence the magnetic field corresponds to a chemical potential that is coupled to the number of particles. More formally, the partition function is

$$Q(N) = \sum_{\{n_i\}}{}' e^{-\beta \tilde{H}_{LG}},$$

where $\sum'$ is a constrained sum over $\{n_i\}$ such that $\sum n_i = N$. The grand partition function is

$$\mathcal{L}(\mu) = \sum_{n_1 \ldots n_v} e^{-\beta \tilde{H}_{LG}} e^{\beta\mu \sum n_i} \equiv \sum_{n_1 \ldots n_v} e^{-\beta H_{LG}},$$

with

$$H_{LG} = -\frac{\epsilon}{4}\sum_{(i,j)\in E} s_i s_j - \left(\mu + \frac{\epsilon\zeta}{2}\right)\sum s_i + const. \tag{5}$$

Hence under the mapping

$$\epsilon = 4J, \tag{6}$$
$$h = (\mu + 2J\zeta), \tag{7}$$

there is equivalence between the Ising Hamiltonian and the lattice gas Hamiltonian.

3 Phase diagram

The order parameter for the lattice gas is the density ρ. The translation of the Ising phenomenology for the lattice gas is the following: For $T > T_c$ there is no phase transition. For $T < T_c$, there is a phase transition at $\mu = \mu_c \equiv -2J\zeta$ between a high density phase $\rho > \frac{1}{2}$ and a low density phase $\rho < \frac{1}{2}$. At $T = T_c$ there is a second order phase transition.

While for a magnetic system it is natural to work in the constant magnetic field ensemble, which corresponds to the grand canonical ensemble in the lattcie gas, for the latter a natural ensemble is the constant total density ensemble. In this ensemble the total density is fixed, and hence any density is possible. However, below the critical temperature, $T < T_c$, there is a region of densities which cannot be obtained in the grand canonical ensemble (corresponding to a magnetization between $M(T, h \to 0_+)$ and $M(T, h \to 0_-)$). What happens if the density is set to such value? The answer is that there is a **phase separation**: the system decomposes into a region of high density and a region of low density.