Chapter 11

Phase Transition and Low Temperature Physics

6. Ising Model

Theory of second order phase transition is quite complicated, specially when a three-dimensional system is considered and all interactions are included. Ising considered that each spin interacts with the nearest neighbours only, and $\in_{i,i'}$ can be taken as the average value $\in$.

One-dimensional Ising model

In one-dimensional Ising model, we account for one dimensional chain of N spins (atoms). Further, we assume that each spin interacts with the nearest neighbours (Ising approximation). Thus, in the one-dimensional case, each spin is interacting with its two nearest neighbours only. For one-dimensional configuration specified by $\{\sigma_1, \sigma_2, \ldots . \sigma_N\}$, energies of the levels are

$$E = -\in \sum_{i=1}^{N} \sigma_i \sigma_i + 1$$

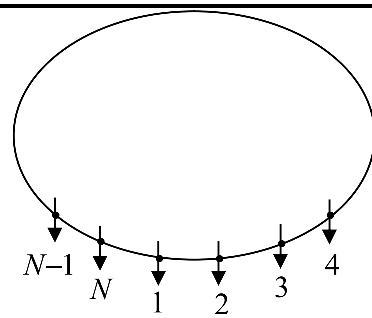
where $\in$ is the average energy of interaction between the two adjacent spins. In order to maintain continuity of the crystal, it is convenient to arrange the chain in the form of a ring so that $\sigma_{N+1} = \sigma_1$ (Figure 7). The partition function is

$$Z=\sum_{\sigma_1\pm1}\sum_{\sigma_2\pm1}....\sum_{\sigma_N\pm1}\exp\left(\beta\in\sum_{i=1}^{N}\sigma_i\sigma_{i+1}\right)$$

$$=\sum_{\sigma_1\pm1}\sum_{\sigma_2\pm1}....\sum_{\sigma_N\pm1}\prod_{i=1}^{N}\left(\cos\beta\in+\sigma_i\sigma_{i+1}\sinh\beta\in\right)$$

where $\beta=(1/kT)$ and we have used

$$\exp(c\sigma\sigma')=\cosh c+\sigma\sigma'\sinh c$$



N Ising spins arranged in a ring so that $\sigma_{N+1}=\sigma_1$

as $\sigma\sigma'$ can be either +1 or –1. Expansion of right side of equation gives

$$Z=2^N\left[(\cosh\beta\in)^N+(\sinh\beta\in)^N\right]$$

For $\beta\in=\in/kT\neq\infty(T\neq0)$, we have $\cosh\beta\in>\sinh\beta\in$. Thus, for $N>>1$, we have

$$(\cosh\beta\in)^N>>(\sinh\beta\in)^N$$

(i) The Helmholtz free energy is

$$F=-kT\ln Z=-NkT\ln(2\cosh\beta\in)=-NkT\ln\left(2\cosh\frac{\in}{kT}\right)$$

(ii) Total energy of the system is

$$U=\frac{\partial(F/T)}{\partial(1/T)}=-Nk\frac{\partial}{\partial(1/T)}\left\{\ln\left[2\cosh\left(\frac{\in}{kT}\right)\right]\right\}$$

$$=-Nk\frac{2\sinh(\in/kT)}{2\cosh(\in/kT)}\frac{\in}{k}=-N\in\tanh\left(\frac{\in}{kT}\right)$$

The specific heat at constant volume c_V is

$$c_V=\left[\frac{\partial U}{\partial T}\right]_V=-N\in\sec h^2\left(\frac{\in}{kT}\right)\left(-\frac{\in}{kT^2}\right)=\frac{N\in^2}{kT^2}\sec h^2\left(\frac{\in}{kT}\right)$$

It shows that c_V varies with T smoothly and there is no transition temperature. Thus, one-dimensional Ising model cannot explain the ferromagnetic behaviour of a metal.

This limitation of one-dimensional Ising model can be understood in the following manner. A linear chain can be easily broken at any point, and each break destroys the long-range order and increases the energy by $2\in$. A break in the chain can be at any one of the N sites. The gain in the entropy is $(k\ln N)$ and therefore, the change in free energy is $(2\in-kT\ln N)$. If N is sufficiently large, even for low values of T, this change is always negative. Thus, the free energy is still negative and hence it has no singularity, which provides a phase transition phenomenon.

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↑ Break

Figure: Long chain order in a linear chain; a single break destroys the long range order shown in the lower line.

Renormalization

Kadanoff considered that near the critical point, the spins act together in the large blocks and therefore, he introduced a concept of 'block spin transformation' for Thing ferromagnets. This concept provided a facility to work with the average spins of the large blocks instead of individual spins. Now, starting from the Ising Hamiltonian, we can describe the system in terms of an effective Hamiltonian involving only the block spins. The operation of coarse graining followed by rescaling is known as the 'renormalization group' (RG) transformation. Let us consider a system of N spins at temperature T in the absence of external magnetic field. The spins will be denoted as σ_i. Each spin can point either up $(\sigma_i = 1)$ or down $(\sigma_i = -1)$. The Hamiltonian H of the Thing ferromagnet is

$$H = -\in \sum_{ij} \sigma_i \sigma_j$$

where $\in > 0$ is the exchange interaction. The canonical partition function Z is

$$Z = \sum e^{-\beta H}$$

where $\beta = 1/kT, H$ the Hamiltonian and the Σ in equation (10.37) stands for summation over all possible combinations $\sigma_1 = \pm 1, \sigma_2 = \pm 1$, etc. We define g as the negative dimensionless free energy per spin,

$$g = -\frac{F}{NkT} = \frac{1}{N} \ln Z \qquad F = -kT \ln Z$$

where F is the Helmholtz free energy and Z the partition function of the system. For convenience, the negative sign is included such that g s usually positive.

One-dimensional Ising chain

In order to understand the process of normalization, let us consider a simple example of one dimensional Ising chain having N spins (left side of figure). Define $K = \beta \in$, the canonical partition function $Z(K, N)$ of N - spin system is

$$Z(K,N) = \sum_{1}^{N} e^{K(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_4 + \sigma_4\sigma_5 + ...)}$$

$\sigma_1\ \sigma_2\ \sigma_3\ \sigma_4\ \sigma_5\ \sigma_6\ \sigma_7\ \ldots. \rightarrow \sigma_1\ \sigma_3\ \sigma_5\ \sigma_7\ \ldots.$

Removal of half of the spins from one dimensional Ising chain.

Hence, the summation is over N spins $\sigma_1 = \pm 1, \sigma_2 = \pm 1, \sigma_3 = \pm 1$, etc. In the Renormalization Group theory, we remove half of the spins (right side of Figure). This process is known as the 'decimation process'. For decimation process, we group the exponentials on the right side of equation (10.39) in pairs and thus we have

$$Z = (K, N) = \sum_{1}^{N}\left[e^{K(\sigma_1\sigma_2+\sigma_2\sigma_3)}\right]\left[e^{K(\sigma_3\sigma_4+\sigma_4\sigma_5)}\right]\left[e^{K(\sigma_5\sigma_6+\sigma_6\sigma_7)}\right]\ldots.$$

Now, we note that σ_2 appears only in the first square bracket, σ_4 appears in the second square bracket, σ_6 appears in the third square bracket, and so on. For the first square bracket, we remove σ_2 by summing over $\sigma_2 = 1$ and $\sigma_2 = -1$; for the second square bracket, we remove $\sigma_4 = -1$ by summing over $\sigma_4 = 1$ and $\sigma_4 = -1$; and so on. Thus, we have

$$Z(K, N) = \sum_{1,3,5\ldots}\left[e^{K(\sigma_1+\sigma_3)} + e^{-K(\sigma_1+\sigma_3)}\right]\left[e^{K(\sigma_3+\sigma_5)} + e^{-K(\sigma_3+\sigma_5)}\right]$$

$$\left[e^{K(\sigma_5+\sigma_7)} + e^{-K(\sigma_5+\sigma_7)}\right]\ldots.$$