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VI. Series Expansions

VI.A Low-temperature expansions

Lattice models can also be studied by series expansions. Such expansions start with certain exactly solvable limits, and typically represent perturbations around such limits by graphs on the lattice. High temperature expansions are described in the next section. Here we describe the *low temperature* expansion for the Ising model with a Hamiltonian $-\beta\mathcal{H} = K \sum_{\langle i,j \rangle} \sigma_i \sigma_j$, on a d -dimensional hypercubic lattice. The ground state with $K = \beta J > 0$ is ferromagnetic, e.g. with $\sigma_i = +1$ for all spins. A series expansion for the partition function is obtained by including low energy excitations around this state. The lowest energy excitation is a single overturned spin. Any of N sites can be chosen for this excitation, which has an energy cost of $2K \times 2d$, with respect to the ground state. The next lowest energy excitation corresponds to a dimer of negative spins with energy cost of $2K \times (4d - 2)$, and a multiplicity of $N \times d$ (there are d possible orientations for the dimer). The first few terms in the expansion give

$$Z = 2e^{NdK} \left[1 + Ne^{-4dK} + dNe^{-4(2d-1)K} + \frac{N(N-2d-1)}{2}e^{-8dK} + \dots \right]. \quad (\text{VI.1})$$

The fourth term comes from flipping two disjoint single spins. The zeroth order term comes from the ground state, which has a two fold degeneracy. The overall factor of 2 is insignificant in the $N \rightarrow \infty$ limit, and

$$Z \simeq e^{NdK} \sum_{\text{droplets of } \ominus \text{ spins}} e^{-2K \times \text{boundary of droplet}}. \quad (\text{VI.2})$$

The free energy per site is obtained from the series,

$$\begin{aligned} -\beta f &= \frac{\ln Z}{N} = dK + \frac{1}{N} \ln \left[1 + Ne^{-4dK} + dNe^{-4(2d-1)K} + \frac{N(N-2d-1)}{2}e^{-8dK} + \dots \right] \\ &= dK + e^{-4dK} + de^{-4(2d-1)K} - \frac{(2d+1)}{2}e^{-8dK} + \dots. \end{aligned} \quad (\text{VI.3})$$

Note that there is an explicit cancellation of the term proportional to N^2 in the expansion for Z . Such higher N dependences result from *disconnected* diagrams with several disjoint

droplets. Extensivity of the free energy ensures that these terms are cancelled by products of connected graphs. The energy per site is then obtained from

$$\begin{aligned}\frac{E}{N} &= -\frac{\partial}{\partial \beta} \left(\frac{\ln Z}{N} \right) = -J \frac{\partial}{\partial K} \left(\frac{\ln Z}{N} \right) \\ &= -J \left[d - 4de^{-4dK} - 4d(2d-1)e^{-4(2d-1)K} + 4d(2d+1)e^{-8dK} + \dots \right],\end{aligned}\tag{VI.4}$$

and the heat capacity is proportional to

$$\begin{aligned}\frac{C}{Nk_B} &= \frac{1}{Nk_B} \frac{\partial E}{\partial T} = -\frac{K^2}{NJ} \frac{\partial E}{\partial K} \\ &= K^2 \left[16d^2e^{-4dK} + 16d(2d-1)^2e^{-4(2d-1)K} - 32d^2(2d+1)e^{-8dK} + \dots \right].\end{aligned}\tag{VI.5}$$

Can such series be used to extract the critical coupling K_c , and more importantly, the singularities associated with the disordering transition? Suppose that we have identified a number of terms in a series $C = \sum_{\ell=0}^{\infty} a_{\ell} u^{\ell}$. From the expected divergence of the heat capacity, we expect an asymptotic expansion of the form

$$C \simeq A \left(1 - \frac{u}{u_c} \right)^{-\alpha} = A \left[1 + \frac{\alpha}{u_c} u + \frac{\alpha(\alpha+1)}{2!u_c^2} u^2 + \dots + \frac{\alpha(\alpha+1)\dots(\alpha+\ell-1)}{\ell!u_c^{\ell}} u^{\ell} \dots \right].\tag{VI.6}$$

The above singular form is characterized by the three parameters A , u_c , and α . We can try to extract these parameters from the calculated coefficients in the series by requiring that they match at large ℓ , i.e. by fitting the ratio of successive terms to

$$\frac{a_{\ell}}{a_{\ell-1}} \simeq \left(\frac{\alpha + \ell - 1}{\ell u_c} \right) = u_c^{-1} \left(1 + \frac{\alpha - 1}{\ell} \right).\tag{VI.7}$$

Thus a plot of $a_{\ell}/a_{\ell-1}$ versus $1/\ell$ should be a straight line with intercept u_c^{-1} , and slope $u_c^{-1}(\alpha - 1)$. Note, however, that adding a finite sum $\sum_{\ell=0}^{\ell_m} d_{\ell} u^{\ell}$ does not change the asymptotic singular form, but essentially renders the first ℓ_m terms useless in determining α and u_c^{-1} . There is thus no a priori guarantee that such a fitting procedure will succeed with a finite number of coefficients. In practice, this procedure works very well and very good estimates of critical exponents in $d = 3$ (e.g. $\alpha = 0.105 \pm 0.007$) are obtained in this way by including a rather large number of terms.

The three terms calculated for the heat capacity in eq.(VI.5) have different signs, unlike those of eq.(VI.6). As this continues at higher orders in e^{-K} , the ratio fitting procedure described above cannot be used directly. The alternation of signs usually signifies singularities in the *complex* $z = e^{-K}$ plane, closer to the origin than the critical point of

interest at real $z_c = e^{-K_c}$. If it is possible to construct a mapping $u(z)$ on the complex plane such that the spurious singularities are pushed further away than $u_c = u(z_c)$, then the ratio method can be used. In the case of low temperature series, the choice of $u = \tanh K$ achieves this goal. (As we shall demonstrate shortly, $\tanh K$ is also the natural variable for the high temperature expansion.) Quite sophisticated methods, such as *Padé approximants*, have been developed for analyzing the singular behavior of series.

Low temperature expansions can be similarly constructed for other *discrete* spin systems, such as the Potts model. For *continuous* spins, the low energy excitations are Goldstone modes, and the perturbation series cannot be represented in terms of lattice graphs. The low temperature description in this case starts with the Gaussian treatment of the Goldstone modes. Further terms in the series involve interactions between such modes, and a corresponding calculation will be performed later on.

VI.B High-temperature Expansions

High temperature expansions work equally well for discrete and continuous spin systems. The basic idea is to start with *independent* spins, and expand the partition function in powers of $\beta = (k_B T)^{-1}$, i.e.

$$Z = \text{tr} \left(e^{-\beta \mathcal{H}} \right) = \text{tr} \left[1 - \beta \mathcal{H} + \frac{\beta^2 \mathcal{H}^2}{2} - \dots \right], \quad (\text{VI.8})$$

and

$$\frac{\ln Z}{N} = \frac{\ln Z_0}{N} - \beta \frac{\langle \mathcal{H} \rangle_0}{N} + \frac{\beta^2}{2} \frac{\langle \mathcal{H}^2 \rangle_0 - \langle \mathcal{H} \rangle_0^2}{N} - \dots. \quad (\text{VI.9})$$

The averages $\langle \rangle_0$ are calculated over non-interacting spins. For the Ising model, it is more convenient to organize the expansion in powers of $\tanh K$ as follows. Since $(\sigma_i \sigma_j)^2 = 1$, the Boltzmann factor for each bond can be written as

$$e^{K \sigma_i \sigma_j} = \frac{e^K + e^{-K}}{2} + \frac{e^K - e^{-K}}{2} \sigma_i \sigma_j = \cosh K (1 + t \sigma_i \sigma_j), \quad (\text{VI.10})$$

where $t \equiv \tanh K$ is a good high temperature expansion parameter. Applying this transformation to each bond of the lattice results in

$$Z = \sum_{\{\sigma_i\}} e^{K \sum_{\langle i,j \rangle} \sigma_i \sigma_j} = (\cosh K)^{\text{number of bonds}} \sum_{\{\sigma_i\}} \prod_{\langle i,j \rangle} (1 + t \sigma_i \sigma_j). \quad (\text{VI.11})$$

For N_b bonds on the lattice, the above product generates 2^{N_b} terms, which can be represented diagrammatically by drawing a line connecting sites i and j for each factor of $t\sigma_i\sigma_j$. Note that there can at most be one such line for each lattice bond, which is either empty or occupied. This is a major simplification, resulting from the use of t , rather than K , as the expansion parameter. Each site now obtains a factor of $\sigma_i^{p_i}$, where p_i is the number of occupied bonds emanating from i . Summing over the two possible values $\sigma_i = \pm 1$, gives a factor of 2 if p_i is even, and 0 if p_i is odd. Thus, the only graphs that survive the sum have an even number of lines passing through each site. The resulting graphs are collections of closed paths on the lattice, and

$$Z = 2^N \times (\cosh K)^{N_b} \sum_{\text{All closed graphs}} t^{\text{number of bonds in the graph}}. \quad (\text{VI.12})$$

For a d -dimensional hypercubic lattice, the smallest closed graph is a square of 4 bonds which has $d(d-1)/2$ possible orientations. As the next graph has 6 bonds,

$$Z = 2^N (\cosh K)^{dN} \left[1 + \frac{d(d-1)N}{2} t^4 + d(d-1)(2d-3) t^6 + \dots \right], \quad (\text{VI.13})$$

and

$$\frac{\ln Z}{N} = \ln 2 + d \ln \cosh K + \frac{d(d-1)}{2} t^4 + \dots. \quad (\text{VI.14})$$

In the following sections, we shall employ high temperature expansions not as a numerical tool, but to establish the following: (a) Exact solution of the Ising model in $d = 1$. (b) The duality relating models at low and high temperatures. (c) The validity of the Gaussian model in high dimensions. (d) Exact solution of the Ising model in $d = 2$.

VI.C Exact Solution of the One Dimensional Ising Model

The graphical method provides a rapid way of solving the Ising model at zero field in $d = 1$. We can compare and contrast the solutions on chains with open and closed (periodic) boundary conditions.

1. *An open chain* of N sites has $N_b = N - 1$ bonds. It is impossible to draw any closed graphs on such a lattice, and hence

$$Z = 2^N \cosh K^{N-1} \times 1, \implies \frac{\ln Z}{N} = \ln[2 \cosh K] - \frac{\ln[\cosh K]}{N}. \quad (\text{VI.15})$$

The same method can also be used to calculate the correlation function $\langle \sigma_m \sigma_n \rangle$, since

$$\langle \sigma_m \sigma_n \rangle = \frac{1}{Z} \sum_{\{\sigma_i\}} e^{K \sum_{\langle i,j \rangle} \sigma_i \sigma_j} \sigma_m \sigma_n = \frac{2^N (\cosh K)^{N-1}}{Z} \sum_{\{\sigma_i\}} \sigma_m \sigma_n \prod_{\langle i,j \rangle} (1 + t \sigma_i \sigma_j). \quad (\text{VI.16})$$

The terms in the numerator involve an additional factor of $\sigma_m \sigma_n$. To get a finite value after summing over $\sigma_m = \pm 1$ and $\sigma_n = \pm 1$, we have to examine graphs with an odd number of bonds emanating from these *external* sites. The only such graph for the open chain is one that directly connects these two sites, and results in

$$\langle \sigma_m \sigma_n \rangle = t^{|m-n|} = e^{-|m-n|/\xi}, \quad \text{with} \quad \xi = -\frac{1}{\ln \tanh K}. \quad (\text{VI.17})$$

These results are in agreement with the RG conclusions of sec.V.B; the correlation length diverges as e^{2K} for $K \rightarrow \infty$, and there is no power law modifying the exponential decay of correlations.

2. A *closed chain* has the same number of sites and bonds, N . It is now possible to draw a closed graph that circles the whole chain, and

$$\begin{aligned} Z &= (2 \cosh K)^N [1 + t^N] = 2^N (\cosh K^N + \sinh K^N), \\ \implies \quad \frac{\ln Z}{N} &= \ln(2 \cosh K) + \frac{\ln [1 + t^N]}{N}. \end{aligned} \quad (\text{VI.18})$$

The difference between the free energies of closed and open chains vanishes in the thermodynamic limit. The correction to the extensive free energy, $N \ln(2 \cosh K)$, is of the order of $1/N$ for the open chain, and can be regarded as the surface free energy. There is no such correction for the closed chain, which has no boundaries; there is instead an exponential term t^N . The correlation function can again be calculated from eq.(VI.16). There are two paths connecting the points m and n , and

$$\langle \sigma_m \sigma_n \rangle = \frac{t^{|m-n|} + t^{N-|m-n|}}{1 + t^N}. \quad (\text{VI.19})$$

Note that the final answer is symmetric with respect to the two ways of measuring the distance between the two sites m and n .