Chapter 7

Series expansion technique

Lecture-I

1. Introduction:

Determination of exact partition function for an interating system is always a difficult tusk as we have seen in the preveous chapter. In most of the cases it is not possible to obtain an analytic form of the partion fuction specially in higher diemnsion.

Exact power series expansion of thermodynamic functions is an important techniques to understand critical phenomena. The partition function here will be evaluated as a power series of an appropriate variable, exactly upto certain terms.Partition function is therefore an approximate partition function in this case. So there must be errors in estimating the critical exponents. But it will be much less than the experimental error or numerical error.For example, in the case of 2d Isingmodel $\beta_{exact} = 1/8$, from series expansion it is obtained as $\beta = 0.125 \ldots$ i.e. upto third decimal place it is exact.

The series expansion of the thermodynamic function can be made either in terms of temperatureor in terms of inverse temperature. In case of series expansion below the critical temperature, T<T_C,the expansion should be in terms of temperature and it is called low temperature expansion whereas in case of series expansion above the critical temperature,$T > T_C$, the expansion should be in terms of inverse of temperature and it is called high temperature expansion. The terms of the series, either high temperature or low temperature expansions, can be represented as different graphs on a lattice. The construction of a series is then boils down to counting the allowed graphs on a given lattice.

Obviously, the results obtained from the series expansion would be less erroneous if the order of the expansion is high. However, calculating higher order terms are also difficult. The work involved in calculating the last term is almost the same as that required to calculate all the preceding terms.

Though there is no rigorous reason that the series should be convergent, it is generally believed that in most of the cases the series converges and there exists a radius of convergence. The radius of convergence of a series is determined by the singularity that lies on nearest to the origin on the complex plane. If the singularity is on the positive real axis, it can be identified as the critical point and the associated critical exponents can be determined.

In most of the cases, the series behave in a sensible way and provide accurate results. The results obtained from series expansion agree well with those obtained from other numerical methods and exact calculations. The method is considered as one of the important techniques to determine critical properties of several systems.

2. High Temperature series expansion:

Let us consider the Spin -1/2 Ising model with zero external field. The Hamiltonian of the system is given by

$$\mathcal{H} = -J \sum_{<ij>} S_i S_j$$

where$S_i = \pm 1$, and $\langle \cdots \rangle$ represents nearest neighbor interaction.

The partition function can be obtained as

$$\mathbb{Z} = \sum_{\{S\}} \prod_{B_{ij}} e^{\beta J S_i S_j}$$

where the sum is over all possible states and the product is over all the nearest neighbor bonds.

Since $S_i S_j = \pm 1$, $e^{\beta J S_i S_j}$ is either $e^{\beta J}$ or $e^{-\beta J}$ and one may write a combined expression as

$$e^{\beta J S_i S_j} = \frac{1}{2}\left(e^{\beta J} + e^{-\beta J}\right) + \frac{1}{2} S_i S_j \left(e^{\beta J} - e^{-\beta J}\right) = \cosh(\beta J) + S_i S_j \sinh(\beta J)$$

or,

$$e^{\beta J S_i S_j} = \cosh(\beta J)(1 + v S_i S_j)$$

where $v = \tanh \beta J$.

The partition function then can be obtained as,

$$\mathbb{Z} = \sum_{\{S\}} \prod_{B_{ij}} \cosh(\beta J)(1 + v S_i S_j)$$

For a lattice with periodic boundary condition (pbc), the total number of bonds is given by $B = Nq/2$ where N is the total lattice site and q is the coordination number of the lattice. Thus, if there are$B$number of nearest neighbor bondsto present in the system, the partition function can be written as

$$\mathbb{Z} = \{\cosh(\beta J)\}^B \sum_{\{S\}} \prod_{B_{ij}} (1 + v S_i S_j) = \{\cosh(\beta J)\}^B \sum_{\{S\}} (1 + v S_i S_j)(1 + v S_k S_l) \cdots$$

or,

$$\mathbb{Z} = \{\cosh(\beta J)\}^B \sum_{\{S\}} \left(1 + v \sum_{B_{ij}} S_i S_j + v^2 \sum_{B_{ij} B_{kl}} S_i S_j S_k S_l + \cdots \right)$$

The coefficients associated with $v^n, n = 1,2,3,\cdots$ in the expansion represent different graphs on a lattice. It can be shown that only certain type of topology of graphs has non-vanishing contribution when it is summed over all possible states.

It can easily be noted that

$$\sum_{S_i=-1,,1} S_i = 0$$

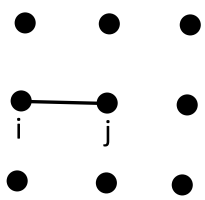
Also one has,

$$\sum_{S_i=-1,1} S_i{}^l = \begin{cases} 2 & \text{if } l \text{ is even} \\ 0 & \text{if } l \text{ is odd} \end{cases}$$

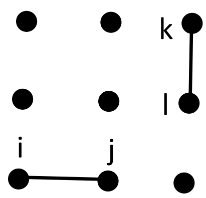
Since any even power of the spin variable S_i is one, it can be shown in general that,

$$\sum_{S_1=\pm1, S_2=\pm1, \cdots, S_N=\pm1} S_i^{n_i} S_j^{n_j} S_k^{n_k} \cdots = \begin{cases} 2^N \text{if all } n_i \text{ are even} \\ 0 \quad \text{otherwise} \end{cases}$$

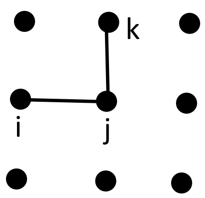
wherethe sum is over N spins. So in the product of several spins only those terms contribute where each spin appears in even number. These terms correspond to closed loops. Thus any graph with free ends is not allowed. Each closed graph then contributes to the partition function with the same weight,2^N. A few graphs on 2d square lattice is shown below. It can be seen that the configurations (a), (b), (c)and (e) contributes zero to the partition function whereas the closed loop configuration in (d) and (f) have finite contribution to the partition function.



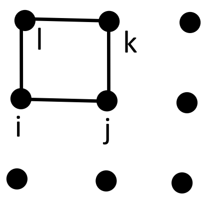
$(a)\ S_iS_j$



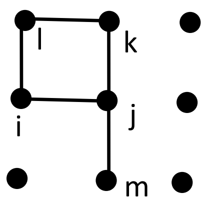
$(b)\ S_iS_jS_kS_l$



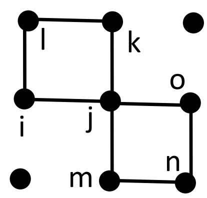
$(c)\ S_iS_j^2S_k$



$(d)\ S_i^2S_j^2S_k^2S_l^2$



$(e)\ S_i^2S_j^3S_mS_k^2S_l^2$



$(f)\ S_i^2S_j^4S_k^2S_l^2S_m^2S_n^2S_o^2$

So finding the contribution to the partition function of order v^n is thus reduced to the problem of counting the number of closed loops of n bonds than can be put on a given lattice. The total number of closed loops of a given number of bonds that can be formed on a given lattice is the sum of all different position and orientation of the loop. Two loops of a given number of bonds on a given lattice are considered to be different if they cannot be superimposed only by translation.

Therefore, the high temperature series expansion of the partition function can be given by

$$\mathbb{Z} = 2^N \{\cosh(\beta J)\}^B \sum_r n_r v^r$$

with $n_0 = 1$.

In the following high temperature series expansion of the partition function is performed for different lattices in one and two dimensions.

3. One dimensional spin 1/2Ising model

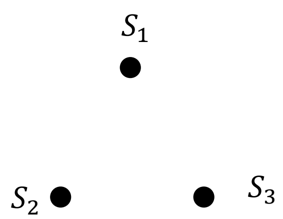
For simplicity, first consider 1d spin 1/2Ising chain of 3 spins with pbc.The total number of bonds is given by $N_B = \frac{N\times q}{2} = \frac{3\times 2}{2} = 3$. The partition function is the given by

$$\mathbb{Z} = \{\cosh(\beta J)\}^3 \left[\sum_{\{S\}} (1 + vS_1S_2)(1 + vS_2S_3)(1 + vS_3S_1)\right]$$

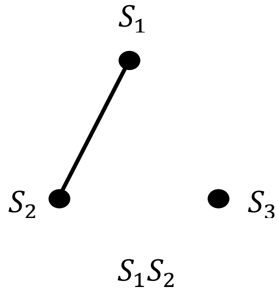
Or,

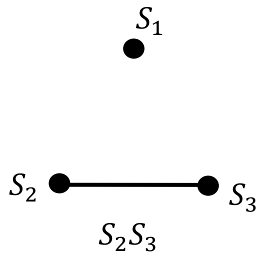
$$\frac{\mathbb{Z}}{\{\cosh(\beta J)\}^3} = \sum_{\{S\}} \{1 + v(S_1S_2 + S_2S_3 + S_3S_1) + v^2(S_1S_2S_2S_3 + S_2S_3S_3S_1 + S_3S_1S_1S_2) + v^3(S_1S_2S_2S_3S_3S_1)\}$$

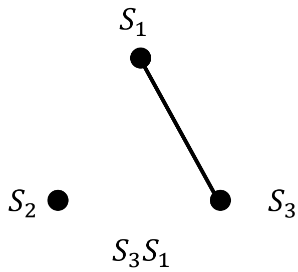
The coefficient to the v^0term corresponds to zero bonds and it can be represented by the following graph;



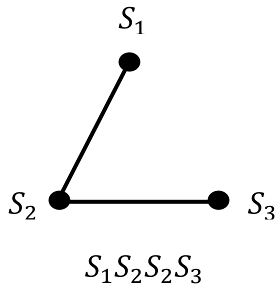
The coefficient to the v^1term corresponds to one bond and they can be represented by the following graphs:

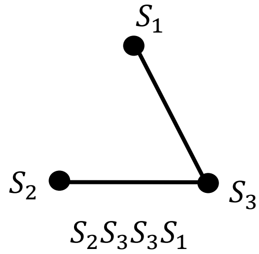


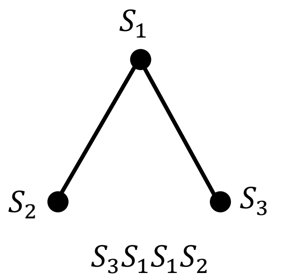




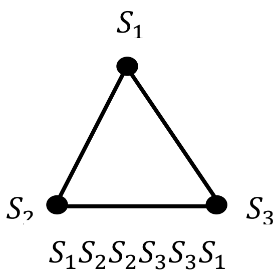
The coefficient to the v^2term corresponds to two bonds and they can be represented by the following graphs:







The coefficient to the v^3term corresponds tothree bonds and it can be represented by the following graph:



Now we take the summation over all states:

$$\sum_{\{S\}} S_1S_2 = S_2S_3 = S_3S_1 = 0$$

Also one has,

$$\sum_{\{S\}} S_1 S_2 S_2 S_3 = S_2 S_3 S_3 S_1 = S_3 S_1 S_1 S_2 = 0$$

But,

$$\sum_{\{S\}} S_1 S_2 S_2 S_3 S_3 S_1 = 2^3$$

the only surviving term. It should be noted here thatin case of all even power spins, the spin configuration corresponds a close loop and their contribution added to the partition function. If the spins do n ot form a closed loop configuration, they will not contribute to the partition function.

Hence, the partition function (for 3 spins) becomes

$$Z_3 = \{\cosh(\beta J)\}^3(8 + 8v^3) = 2^3(\cosh^3(\beta J) + \sinh^3(\beta J))$$

The result can be generalized for $1d$ chain of Ising$N$ spin with pbc as

$$Z_N = 2^N[\cosh^N(\beta J) + \sinh^N(\beta J)]$$

It can be checked that it is the same partition function that was obtained by the Transfer Matrix method in the previous chapter.

Since the ordering temperature in 1d Ising model is $T_c = 0$, the high temperature series expansion is expected to be convergent at all finite temperatures.

Lecture-II

3. Two-dimensional Ising Model:

Let us consider a square lattice of size $L \times L$ in 2 dimensions. The total number of spins present in the system is then $N = L^2$. If there is pbc in both the directions, the number of nearest neighbor bond in the lattice is given by

$$B = \frac{N \times q}{2}$$

where q is the coordination number of the lattice. Since for a square lattice $q = 4$, the number of bonds should be $B = 2N$.

3.1 High temperature series expansion

The high temperature series of the partition function is given by

$$\mathbb{Z} = 2^N \{\cosh(\beta J)\}^B \sum_r n_r v^r$$

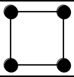
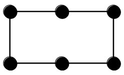
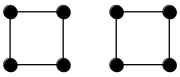
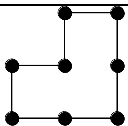
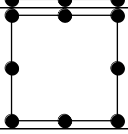
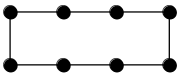
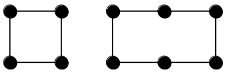
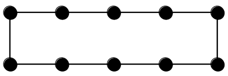
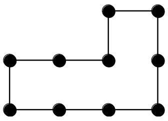
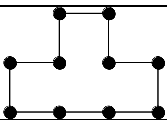
with $n_0 = 1$ and each n_r represents closed graphs with r spins. Since the minimum number of spins required to form a closed graph on a square lattice is 4, the first surviving term in the series must be v^4. At the same time, higher order closed graphs can be formed only by even number of spins. The partition function then can be written as

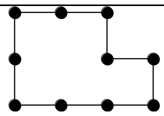
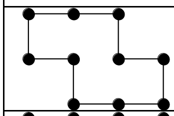
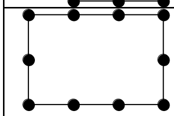
$$\mathbb{Z} = 2^N \{\cosh(\beta J)\}^{2N} (1 + n_4 v^4 + n_6 v^6 + n_8 v^8 + n_{10} v^{10} + O(v^{12}))$$

Now one needs to count the closed graphs of different number of spins. Below, a list of the coefficients n_r and the corresponding closed graphs with different possibilities is given. It is found that $n_4 = N$, $n_6 = 2N$, $n_8 = N(N+9)/2$ and $n_{10} = 2N(N+6)$. The partition function is then given by

$$\mathbb{Z} = 2^N \{\cosh(\beta J)\}^{2N} \left\{1 + Nv^4 + 2Nv^6 + \frac{1}{2}N(N+9)v^8 + 2N(N+6)v^{10} + \cdots\right\}$$

This could be noted that the partition function is exact uptov^{10}. Higher order graphs are not only complicated but also have many different possibilities of constructing a closed graph with higher number of spins. Such counting are usually made using a computer.

Order	Graphs	Possibilities	Count	Totaln_r
v^4		Can be placed at N different positions.	N	$n_4 = N$
v^6		Two orientations and each can be placed at N different positions.	$2N$	$n_6 = 2N$
v^8		As one of the blocks is placed, the other block cannot be placed on and around the first block at five different positions and the two blocks are identical.	$\frac{N(N-5)}{2}$	$n_8 = \frac{N(N+9)}{2}$
		Four reflections and each can be placed at N different positions.	$4N$	
		Can be placed at N different positions.	N	
		Two orientations and each can be placed at N different positions.	$2N$	
v^{10}		As the longer block is placed, the other block cannot be placed on and around the first block at eight positions and the longer block has two possible orientations.	$2N(N-8)$	$n_{10} = 2N(N+6)$
		Tow orientations and each can be placed at N different positions.	$2N$	
		Two orientations, four reflections for each orientation at N different positions.	$8N$	
		Four reflections and N different positions.	$4N$	

		Two orientations, four reflections for each orientation at N different positions.	$8N$	
		Four reflections and N different positions.	$4N$	
		Two orientations and each can be placed at N different positions.	$2N$	

Since the partition function is known, one may construct the free energy, $F = -k_B T \ln Z$, series. It can be given as

$$F = -Nk_B T \ln 2 - 2Nk_B T \ln \cosh(\beta J) - k_B T \ln\left(1 + Nv^4 + 2Nv^6 + \frac{1}{2}N(N+9)v^8 + 2N(N+6)v^{10} + \cdots\right)$$

Since,tanh $\beta J = v$, one has $\cosh \beta J = (1 - v^2)^{-1/2}$. The free energy is then given by

$$F = -Nk_B T \ln 2 + Nk_B T \ln(1 - v^2) - k_B T \ln\left(1 + Nv^4 + 2Nv^6 + \frac{1}{2}N(N+9)v^8 + 2N(N+6)v^{10} + \cdots\right)$$

In the limit $v \to 0$, the logarithms in the free energy can also be expanded in power series as

$$F = -Nk_B T \ln 2 + Nk_B T\left(-v^2 - \frac{v^4}{2} - \frac{v^6}{3} - \frac{v^8}{4} - \frac{v^{10}}{5} - \cdots\right) - k_B T\left(Nv^4 + 2Nv^6 + \frac{1}{2}N\,(N+9)v^8 + 2N(N+6)v^{10} + \cdots\right)$$

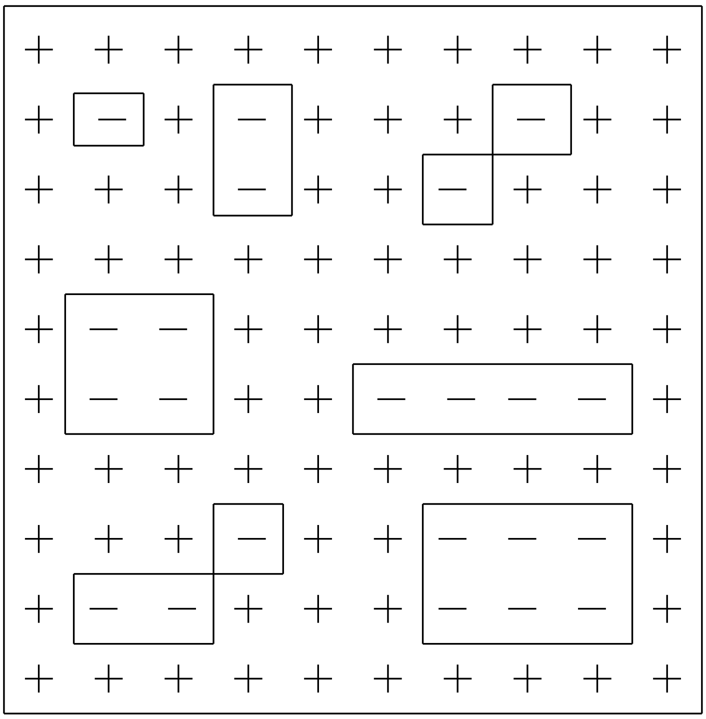
Since free energy is extensive, higher order terms in N are dropped and the free energy series can be obtained as

$$F = -Nk_B T\left\{\ln 2 + v^2 + \frac{3}{2}v^4 + \frac{7}{3}v^6 + \frac{19}{4}v^8 + \frac{61}{5}v^{10} + \cdots\right\}$$

Taking derivative of the above free energy with respect to temperature, the specific heat series can also be obtained.

3.2 Low temperature expansion:

The ground state of the spin 1/2 Ising model consists of eitherall spins up or all spins down, with total energy $E_0 = -JN$, if there are N spins in the system. At a small finite temperature, the dominant contribution to the partition function is from states where few spins are flipped relative to their ground state configuration. Flipping a single spin in the ground state creates q unlike nearest-neighbor pairs on a lattice with coordination number q. It is shown in the figure below on a square lattice for which $q = 4$. The flipped spins are shown by $(-)$sign and theunflipped spins are shown by $(+)$ sign. The cluster of flipped spins is represented by a closed graph.The perimeter length of a closed graph represents the number of unlike bonds associated with the cluster of flipped spins. It could be seen that for a single flipped spin, the perimeter of the closed graph is four unitand there are four unlike bonds. Therefore, flipping a single spin costs $2Jq$ energy on a lattice of coordination number q.



Let us denote the bond between two nearest neighbor up-spins by $(++)$, the bond between two nearest neighbor down-spins by $(--)$, the bond between two nearest neighbor unlike spins is denoted by $(+-)$. If at a given small finite temperature, there are N_{++} up spin-up spin bonds, N_{--} down spin-down spin bonds, and $N_{\pm-}$ unlike bonds are present in the system, the total numbers of bonds is given by

$$B = N_{++} + N_{--} + N_{\pm-} = 2N$$

The Hamiltonian of the system then can be written as

$$\mathcal{H} = -J(N_{++} + N_{--} - N_{\pm-}) = -J(2N - 2N_{\pm-}) = -2JN + 2JN_{\pm-}$$

The total unlike bonds $N_{\pm-}$ is the sum of unlike bonds associated with all possible flipped spin clusters present in the system at a given temperature below T_c.

The low temperature partition function is obtained as a series in terms of the Boltzmann factor$u = e^{-2J/k_BT}$ since as $T \to 0$, $u \to 0$. The partition function then can be written as

$$Z = e^{\frac{2JN}{k_BT}} \sum_r m_r\, e^{-\frac{2Jr}{k_BT}} = e^{\frac{2JN}{k_BT}} \sum_r m_r\, u^r$$

where $m_0 = 1$ andm_r is the number of distinct ways in which flipped spin clusters are so arranged that yield $r$unlike bonds. Since on the square lattice, a single spin flip causes 4 unlike bonds, 2 nearest neighbor spins flip cause 6 unlike bonds and so on, the first surviving term in the series will be u^4 and all subsequent powers of u would have even powers. Thus the low temperature partition function can be written as

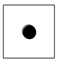
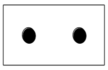
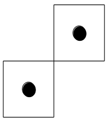
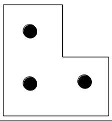
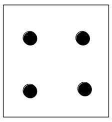
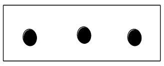
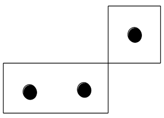
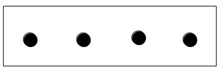
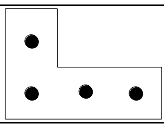
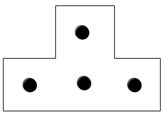
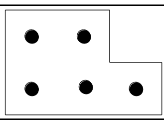
$$Z = e^{\frac{2JN}{k_BT}}[1 + m_4u^4 + m_6u^6 + m_8u^8 + m_{10}u^{10} + O(u^{12})]$$

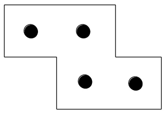
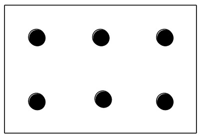
Each term in the expansion is then associated with a closed graph that separates the down spin region from the up spin region. The determination of low temperature partition function then reduces to counting of distinct closed graphs of perimeter r,the number of unlike bonds, that can be drawn on a given lattice. A list of the coefficients m_r and the corresponding closed graphs of different possibilities with r unlike bonds those can be drawn on the square lattice are given below. It is found that $m_4 = N$, $m_6 = 2N$, $m_8 = N(N+9)/2$ and $m_{10} = 2N(N+6)$. The partition function is then given by

$$Z = e^{2KN}\left[1 + Nu^4 + 2Nu^6 + \frac{1}{2}N(N+9)u^8 + 2N(N+6)u^{10} + \cdots\right]$$

where $K = \frac{J}{k_BT}$.

It can be noted that the partition functions obtain as high temperature series and low temperature series are exact upto certain terms. Though both the expansions are valid at all temperature, the high temperature expansion is useful for $T > T_c$ and the low temperature expansion is useful for $< T_c$ .It can also be noted that the coefficient of u^r in the low temperature expansion is exactly equal to that of v^r of high temperature expansion.

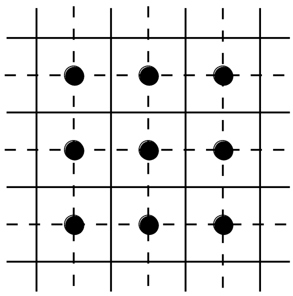
Order	Graphs	Possibilities	Count	Total m_r
u^4		Can be placed at N different positions.	N	$m_4 = N$
u^6		Two orientations and each can be placed at N different positions.	$2N$	$n_6 = 2N$
u^8		As one of the spins is placed, the other spin cannot be placed on and around it at five different positions and the two spins are identical.	$\frac{N(N-5)}{2}$	$m_8 = \frac{N(N+9)}{2}$
		Four reflections and each can be placed at N different positions.	$4N$	
		Can be placed at N different positions.	N	
		Two orientations and each can be placed at N different positions.	$2N$	
u^{10}		As the two spins cluster is placed, the other spin cannot be placed on and around it at eight positions and the cluster has two possible orientations.	$2N(N-8)$	$m_{10} = 2N(N+6)$
		Two orientations and each can be placed at N different positions.	$2N$	
		Two orientations, four reflections for each orientation at N different positions.	$8N$	
		Four reflections and N different positions.	$4N$	
		Two orientations, four reflections for each orientation at N different positions.	$8N$	

		Four reflections and N different positions.	$4N$	
		Two orientations and each can be placed at N different positions.	$2N$	

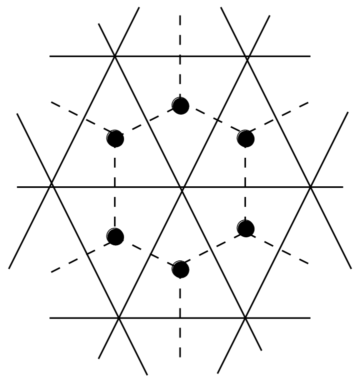
Lecture-III

3.3 Duality transformation and Determination of T_c:

Though the coefficients of high and low temperature expansions are equal, an important relationship between them can be obtained by constructing dual lattice. The dual lattice of a given lattice can be constructed by drawing right bisectors of all the bonds in the lattice. The points of intersections of these bisectors become the lattice sites of the dual lattice. The construction of dual lattice is demonstrated in for the square and triangular lattice in the figure below in which the solid line represent the original lattice and the dotted lines represent the dual lattice.



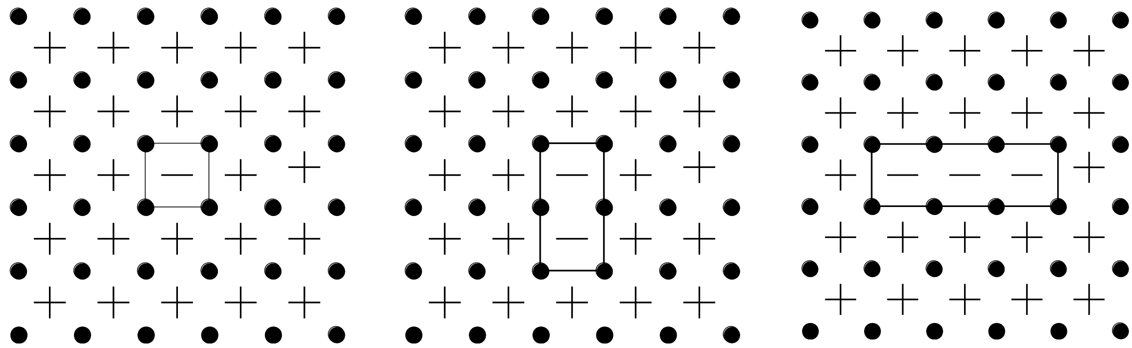
(a) Dual lattice of the square lattice is a square lattice.



(b)) Dual lattice of the triangular lattice is a honeycomb lattice and vice versa.

The dual lattice is not necessarily of the same structure of the original lattice. The dual lattice of a square lattice is a square lattice whereas the dual lattice of the triangular lattice is a honeycomb lattice and vice versa.However, the number of lattice sites N multiplied by the coordination number q is always equal to the number of dual lattice sites N_D multiplied by the coordination number of the dual lattice q_D, i.e.; $qN = q_D N_D$.

Let us now consider the closed graphs on the square lattice and on its dual lattice. We demonstrate this considering three different closed graph configurations in the figure below in which the solid circles represent the square lattice and the plus and minus signs represent the dual lattice of the original lattice. In Fig.(a), we have considered a closed graph of four spins. The dual lattice point inside the closed graph is represented by a minus sign whereas as all other dual lattice points are represented by plus signs. It can easily be checked that there are four unlike bonds associated with the closed graph of perimeter length four. In Fig.(b) and (c) it is demonstrated for the closed graphs of six and eight interacting spins. The same closed graphs are associated with six and eight unlike bonds respectively. Therefore, if a closed graph of r bonds is drawn on a given lattice and its dual lattice is constructed by placing spins of one sign inside the graph and spins of opposite signs outside the graph, the same closed graph will represent a configuration with r unlike bond on the dual lattice. Conversely, one may start with the dual lattice and construct the original lattice (dual of the dual lattice). In that case, the closed graph of perimeter r representing a configuration of r unlike bonds will also represent a closed graph configuration of r spins on the original lattice. Thus one has, $n_r = m_r^D$ and $m_r = n_r^D$ where D stands for dual lattice.



(a) A closed graph of four spins on the original lattice represents a configuration of four unlike spins on the dual lattice.

(b) A closed graph of six spins on the original lattice represents a configuration of six unlike spins on the dual lattice.

(c) A closed graph of eight spins on the original lattice represents a configuration of eight unlike spins on the dual lattice.

Defining $K = \frac{J}{k_B T}$, the low temperature (LT) and the high temperature (HT) partition functions can be written as

$$Z_{LT} = e^{2KN} \sum_r m_r u^r$$

and

$$Z_{HT} = 2^N \{\cosh(K)\}^B \sum_r n_r v^r$$

where$u = e^{-2K}$, $v = \tanh K$ and $m_0 = n_0 = 1$.

Say, there exists a temperature T^* $(K^* = \frac{J}{k_B T^*})$, such that

$$v^* = u \qquad \text{or} \tanh K^* = e^{-2K}$$

Since $n_r = m_r^D$and $m_r = n_r^D$, the low temperature partition function can be written as

$$Z_{LT}(N,T) = e^{2KN} \sum_r n_r^D (v^*)^r$$

On the other hand, the high temperature partition function calculated on the dual lattice at temperature T^* is given by

$$Z_{HT}^D(N,T^*) = 2^{N_D} \{\cosh(K^*)\}^{B_D} \sum_r n_r^D (v^*)^r$$

Comparing the two equations above, one has

$$Z_{LT}(N,T) = 2^{-N_D}\{\cosh(K^*)\}^{-B_D} e^{2KN} Z_{HT}^D(N,T^*)$$

This is known as duality transformation.

Since the square lattice is self dual, there must not be any distinction between Z_{LT} and Z_{HT}^D. Moreover, for the square lattice $q = q_D = 4$ and following $N_D = qN/q_D$, one has $N_D = N$ and $B_D = \frac{q_D N_D}{2} = 2N$. Therefore,

$$Z(N,T) = 2^{-N}\{\cosh(K^*)\}^{-2N} e^{2KN} Z(N,T^*)$$

Or,

$$Z(N,T) = 2^{-N}\{\cosh^2(K^*) e^{-2K}\}^{-N} Z(N,T^*)$$

Since $\tanh K^* = e^{-2K}$,

$$Z(N,T) = 2^{-N}\{\cosh^2(K^*)\tanh(K^*)\}^{-N} Z(N,T^*)$$

Or,

$$Z(N,T) = \{2\sinh(K^*)\cosh(K^*)\}^{-N} Z(N,T^*)$$

The duality transformation on the square lattice then is given by

$$Z(N,T) = \sinh(2K^*)^{-N} Z(N,T^*)$$

At $T = T^* = T_C$

$$Z(N,T_C) = \sinh(2K_C)^{-N} Z(N,T_C)$$

Thus one has,

$$\sinh 2K_C = 1$$

The solution to this equation is given by,

$$K_C \approx 0.4407 \quad \text{or} \frac{k_B T_C}{J} \approx 2.269117$$

The result may be compared with exact result given by $\frac{k_B T_c}{J} = 2.269185$. The series expansion result is found to be exact upto 4th decimal place.

For the other lattices like triangular or honeycomb, the situation is not straight forward as discussed above for the square lattice which is self dual. If a lattice is not self-dual, the equation representing the duality transformation becomes complicated and one needs apply other tricks.

Lecture-IV

4. Extrapolation methods of a series:

Physical quantities obtained as a series always have finite number of terms. However, the singular behavior of a physical quantity is associated with the infinite series. One therefore needs to obtain information about the limiting behavior of a thermodynamic function from the knowledge of the first few coefficients in the expansion of the function in a series. In fact, without extrapolation we do not achieve anything. For example, the susceptibility $\chi \to \infty$as $T \to T_C$. However, a susceptibility series with a few terms in it will always be finite except at $T \to 0$ limit.

On the other hand, the radius of convergence of a power series is determined by the singularity nearest to the origin in the complex plane. If the singularity lies on the positive real axis corresponding to a physical singularity it can be identified as the critical point. Since most of the thermodynamic functionsare finite for all temperature $T > T_C$ and become singular as $T \to T_C$, determination of radius of convergence would be useful in locating the critical point.In doing so, we are assuming that there is no non-physical singularity in the complex plane closer to the origin than the physical singularity.

4.1 Ratio method: First we describe here how to determine the radius of convergence by ratio test. The radius of convergence r_c of a series is defined as

$$\frac{1}{r_c} = \lim_{n\to\infty} \frac{a_n}{a_{n-1}}$$

wherea_n is the coefficient of the nth term in the series and it is assumed that the above limit exists.

In the critical regime $t = (T - T_C)/T_C \to 0$, a thermodynamic quantity is given by

$$Y \approx t^{-\lambda} = \left(\frac{T - T_C}{T_C}\right)^{-\lambda} = \left(\frac{T}{T_C}\right)^{-\lambda} \left(1 - \frac{T_C}{T}\right)^{-\lambda}$$

Let us define $y = \beta J = \frac{J}{k_B T}$ and$y_c = \beta_C J = \frac{J}{k_B T_C}$, then one has $\frac{y}{y_C} = \frac{T_C}{T}$ and Y can be expressed as

$$Y \approx \left(\frac{y}{y_C}\right)^{\lambda} \left(1 - \frac{y}{y_C}\right)^{-\lambda}$$

Since for a high temperature series, $y/y_C = T_C/T < 1$, it can expanded in a power series as

$$Y \approx \left(\frac{y}{y_C}\right)^{\lambda}\left[1+\lambda\left(\frac{y}{y_C}\right)+\frac{\lambda(\lambda+1)}{2!}\left(\frac{y}{y_C}\right)^2+\cdots+\frac{\lambda(\lambda+1)\ldots(\lambda+n-1)}{n!}\left(\frac{y}{y_C}\right)^n+\cdots\right]$$

Or,

$$Y = \sum_{n=0}^{\infty} a_n y^{n+\lambda}$$

where

$$a_n = \frac{\lambda(\lambda+1)\ldots(\lambda+n-1)}{n!\ {y_C}^{n+\lambda}}$$

Then the ratio of two successive coefficients is given by

$$\frac{a_n}{a_{n-1}} = \frac{\lambda(\lambda+1)\ldots(\lambda+n-1)}{n!\ {y_C}^{n+\lambda}}\cdot\frac{(n-1)!\ {y_C}^{n+\lambda-1}}{\lambda(\lambda+1)\ldots(\lambda+n-2)} = \frac{\lambda+n-1}{ny_C}$$

Or

$$\frac{a_n}{a_{n-1}} = \frac{\lambda-1}{y_C}\cdot\frac{1}{n}+\frac{1}{y_C}$$

Therefore in the asymptotic $n \to \infty$ limit, the above equation will represent an equation of a straight line when plotted against $1/n$ with an intercept $1/y_C$ and slope $(\lambda-1)/y_C$. Note that, $\lim_{n\to\infty} a_n/a_{n-1} = 1/y_C$. Thus the radius of convergence corresponds to the singularity. In the figure below, a typical variation of a_n/a_{n-1} against $1/n$ is shown.

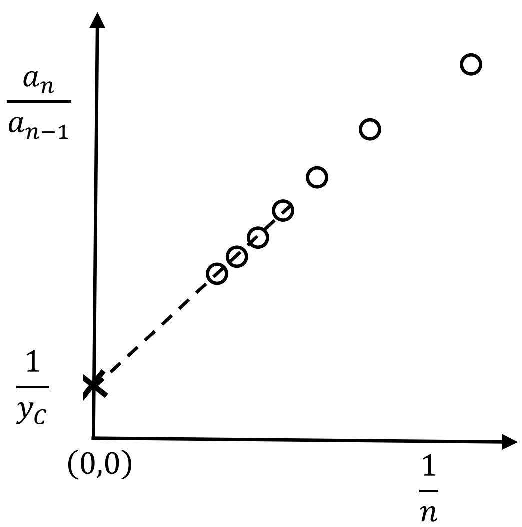


Figure: Plot of a_n/a_{n-1} against $1/n$.

However, for finite series, finite number of terms in the series, not only there will be deviation from the above equation due to correction to scaling but also the plot will terminate far away form $1/n = 0$. One then needs to extrapolate the ratio a_n/a_{n-1}upto$1/n = 0$. In order to do so one may define a linear extrapolantr_n as

$$r_n = n\frac{a_n}{a_{n-1}} - (n-1)\frac{a_{n-1}}{a_{n-2}}$$

Since $\frac{a_n}{a_{n-1}} = \frac{\lambda-1}{y_C}\cdot\frac{1}{n} + \frac{1}{y_C}$, the ratio $\frac{a_{n-1}}{a_{n-2}}$ is then given by

$$\frac{a_{n-1}}{a_{n-2}} = \frac{\lambda-1}{y_C}\cdot\frac{1}{n-1} + \frac{1}{y_C}$$

Therefore,

$$r_n = n\left(\frac{\lambda-1}{y_C}\cdot\frac{1}{n} + \frac{1}{y_C}\right) - (n-1)\left(\frac{\lambda-1}{y_C}\cdot\frac{1}{n-1} + \frac{1}{y_C}\right)$$
$$= n\left(\frac{1}{y_C}\right) - (n-1)\left(\frac{1}{y_C}\right) = \frac{1}{y_C}$$

It is then expected that r_n will converge to $1/y_C$than a_n/a_{n-1}.

The exponent λ can be determined as

$$\lambda_n = 1 + n\left(\frac{a_n}{a_{n-1}}y_C - 1\right)$$

Example: The susceptibility series for the spin-1/2 Ising model is given by

$$\tilde{\chi} = k_B T\chi = 1 + 4v + 12v^2 + 36v^3 + 100v^4 + 276v^5 + \cdots$$

where$v = \tanh\beta J$ and $\beta = 1/k_B T$.The singularity of the reduced susceptibility is given by $\tilde{\chi}\sim(T - T_C)^{-\gamma}$. One needs to determine $T_C$and γ. The linear extrapolantr_n and the exponent γ_n are calculated and listed in the table below.

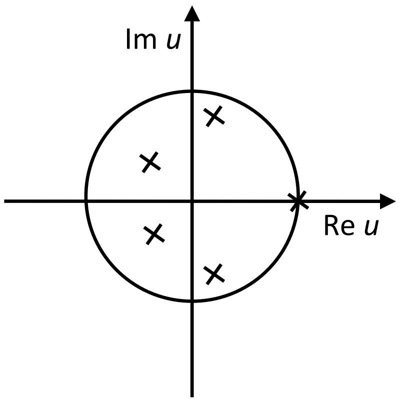
n	$\boldsymbol{r_n}$	$\boldsymbol{\gamma_n}$
3	3	1.7265
4	2.1111	1.6007
5	2.6889	1.7140

Since $r_n = 1/v_C$ and $v_C = \tanh\beta_C J \approx \beta_C J$. Therefore, $k_B T_C/J \approx 2.6889$ whereasthe exact value is 2.269185. The exact value of γ is 1.75. From this small series it is already obtained as 1.714.

4.2Pade' Approximation: In most of the cases the ratios of the successive coefficients appear not to be regular. It may happen for the following reasons: (i) the series is not long enough, (ii) the series of a_n/a_{n-1} against $1/n$ is not smooth but that of other quantities such as $(a_n/a_{n-1})^{1/2}$or $a_n^{1/n}$, etc. are found to be smooth, (iii) the singularity closest to the origin in the complex plane is not the physical singularity about which the information are required. The third reason most often appears in the case of low temperature series for magnetization of the Ising model. The magnetization series of the Ising model for the FCC lattice is given by

$$m = 1 - 2u^6 - 24u^{11} + 26u^{12} - \cdots$$

where $u = e^{-4J/k_B T}$. For this series, the singularity closest to the origin of the complex u-plane is not the physical singularity $u_c = e^{-4J/k_B T_c}$ that lies on the positive real axis. The radius of convergence determined by a singularity on the positive real axis demands that all the coefficients of the series must be positive. The above series has mixed signs for its coefficients and hence, it is not expected that the physical singularity would be on the positive real axis. The singularities of this series are distributed all over the complex u-plane and it is roughly sketched in the following figure where the circle of convergence is determined by a complex conjugate pair of non-physical singularities that are close to the origin.



For such cases, the method of Pade approximants is found to be very useful.

Consider a function Q of x is given by

$$Q(x) = \sum_{l=0}^{\infty} a_l x^l$$

The Pade approximants $P_D^N(x)$to the function $Q$is the ratio of two polynomials of order N and D respectively and is given by

$$P_D{}^N(x) = \frac{n_0 + n_1 x + \cdots + n_N x^N}{1 + d_1 x + \cdots + d_D x^D}.$$

There are N+D+1 undetermined coefficients. If only L+1 terms in the series of $Q$are known,
$P_D^N(x)$is uniquely determined if $N + D \leq L$. To determinen_is and d_is one needs to solve$L$ simultaneous equations obtained from

$$(□_0 + □_1□ + \cdots + □_□□^□) \times (1 + □_1□ + \cdots + □_□□^□) = (□_0 + □_1□ + \cdots + □_□□^□)$$

Or,

$$□_0 = □_0, \qquad □_1 = □_0□_1 + □_1, \qquad □_2 = □_0□_2 + □_1□_1 + □_2, \qquad \cdots$$

The motivation for doing such a procedure is that one can easily obtain the singularity and the critical exponent of a thermodynamic quantity which has a power law singularity. For example, if the singularity of the function $□(□)$ is given by

$$□(□) = \sum_{□=0}^{\infty} □_□□^□ \sim (□ - □_□)^{-□}$$

where$□_□$ corresponds to the singularity and $□$ is the critical exponent.

Then logarithm of $□(□)$ is given by

$$\log □(□) \sim \log\{(□ - □_□)^{-□}\} = -□ \log(□ - □_□)$$

and its derivative should go as

$$□ \log □ = \frac{□}{□□}(\log □(□)) \sim \frac{-□}{□ - □_□}$$

where the singularity corresponds to the simple pole of the function $□ \log □$and the residue corresponds to the exponent. Therefore one needs to construct the series of the logarithmic derivative of the physical quantity of interest. The series for $□ \log □$is given by

$$□ \log □ = \frac{\sum_{□=1}^{□} □□_□□^{□-1}}{\sum_{□=0}^{□} □_□□^□}$$

If the original series is known upto$□ + 1$ terms, the $□ \log □$ series can be obtained upto $□$ terms using the above relation. Different Pade' approximants for the $□ \log □$ series can be constructed. One of the roots of the denominator series of the Pade' approximants should correspond to the physical singularity $□_□$ and the residue of the approximants will be the exponent.

Example: Consider the high temperature reduced susceptibility series for the spin ½ Ising model on the triangular lattice

$$\tilde{\chi} = k_B T \chi = 1 + 6v + 30v^2 + 138v^3 + 606v^4 + \cdots$$

where $v = \tanh \beta J$. First we need to construct the $\frac{d}{dv} \ln \tilde{\chi}$ series and it is given by

$$\frac{d}{dv} \ln \tilde{\chi} = \frac{6 + 60v + 414v^2 + 2424v^3 + \cdots}{1 + 6v + 30v^2 + 138v^3 + \cdots}$$

Since for high temperature v is small, therefore the denominator can be expanded in a power series as

$$(1 - x)^{-1} = 1 + x + x^2 + x^3 + \cdots$$

and can be multiplied with the numerator. Keeping terms upto v^3, the final series can be obtained as

$$\frac{d}{dv} \ln \tilde{\chi} = 6 + 24v + 90v^2 + 336v^3 + \cdots$$

Since $\tilde{\chi} \sim (v - v_c)^{-\gamma}$, then it is expected that

$$\frac{d}{dv} \ln \tilde{\chi} \approx \frac{-\gamma}{v - v_c}$$

Now we construct the Pade approximant

$$P^2_1(v) = \frac{a_0 + a_1 v + a_2 v^2}{1 + b_1 v} = 6 + 24v + 90v^2 + 336v^3$$

Therefore,

$$a_0 + a_1 v + a_2 v^2 = (1 + b_1 v)\left(6 + 24v + 90v^2 + 336v^3\right)$$

and one has,

$$336 + 90b_1 = 0 \quad \text{or } b_1 = -\frac{336}{90}$$

$$a_0 = 6, \qquad a_1 = 24 + 6b_1 = 1.6, \qquad \text{and } a_2 = 90 + 24b_1 = 0.4$$

Then,

$$P^2_1(v) = \frac{6 + 1.6v + 0.4v^2}{1 - \frac{336}{90}v} = \frac{6 + 1.6v + 0.4v^2}{\frac{336}{90}\left(\frac{90}{336} - v\right)} = \frac{-\left(\frac{90}{336}\right)\left(6 + 1.6v + 0.4v^2\right)}{v - \frac{90}{336}}$$

Therefore $v_c = \tanh \beta_c J \approx \beta_c J = 90/336$ or $k_B T_c/J = 336/90 \approx 3.733$. For triangular lattice, the best known value for $k_B T_c/J$ is 3.64098. The exponent γ is given by

$$\gamma = \left(\frac{90}{336}\right)\left(6 + 1.6v_c + 0.4v_c^2\right) \approx 1.729$$

whereas the exact value of γ is $7/4 = 1.75$. Note that we have considered a series upto only cubic term. A series having higher order terms provide more accurate result.

Problems

Problem 1. The reduced susceptibility series for Isingferromagnet on triangular lattice is given by

$$\tilde{\chi} = 1 + 6v + 30v^2 + 138v^3 + 606v^4 + 2586v^5 + 10818v^6 + 44574v^7 + 181542v^8 + 732678v^9 + 2935218v^{10} + \cdots$$

where $v = \tanh \beta J$. Since $\tilde{\chi} \sim (v - v_c)^{-\gamma}$, using ratio method determine the critical temperature and the exponent γ.

The series is finite but the singularity is associated with the infinite series. We need to extrapolate this finite series up to infinity.

Problem2. The per spin spontaneous magnetization m of the spin-1/2 Ising model on the square lattice is given by

$$m = 1 - 2z^2 - 8z^3 - 34z^4 - 152z^5 - 714z^6 - \cdots$$

where $z = e^{-4J/k_B T}$. Since $m \sim (z_c - z)^{\beta}$, using ratio method determine the critical temperature and the exponent β. Compare with the exact values $z_c = 3 - 2\sqrt{2}$ and $\beta = 1/8$.

Problem3. The reduced susceptibility series for Isingferromagnet on simple cubic lattice is given by

$$\tilde{\chi} = 1 + 6v + 30v^2 + 150v^3 + 726v^4 + 33510v^5 + \cdots$$

where $v = \tanh \beta J$. Show that the logarithmic derivative series $D \ln \tilde{\chi}$ is given by

$$D \ln \tilde{\chi} = 6 + 24v + 126v^2 + 528v^3 + 2646v^4 + \cdots$$

Calculating the Pade approximant P_1^2 estimate the critical temperature and the exponent γ. The known values are $k_B T_c/J \approx 4.5833$ and $\gamma = 5/4$.

[Solution:

$$\square \ln \widetilde{\square} = \frac{6 + 60\square + 450\square^2 + 2904\square^3 + 1755\square^4 + \cdots}{1 + 6\square + 30\square^2 + 150\square^3 + 726\square^4 + 33510\square^5 + \cdots}$$

$$= 6 + 24\square + 126\square^2 + 528\square^3 + 2646\square^4 + \cdots$$

Construct:

$$\square_1^2(\square) = \frac{\square_0 + \square_1\square + \square_2\square^2}{1 + \square_1\square} = 6 + 24\square + 126\square^2 + 528\square^3$$

and solve for $\square_1, \square_0, \square_1,$ & $\square_2$.

References

[1] R. K. Pathria and P. D. Beale, *Statistical Mechanics*, (Elsevier, London, 2011).

[2] D. Dhar, *Graphical Enueration Techniques: Series Expansiona and Animal Problems*, in Computational Statistical Physics, edited by S. B. Santra and P. Ray, (Hindustan Book Agency, New Delhi, 2011).

[3] S. Kumar, *Graphical Enueration Techniques: Application to Polymers*, in Computational Statistical Physics, edited by S. B. Santra and P. Ray, (Hindustan Book Agency, New Delhi, 2011).

[4] J. M. Yeomans, *Statistical Mechanics of Phase Transitions*, (Oxford University Press, New York, 1994).

[5] H. E. Stanley, *Introduction to Phase Transitions and Critical Phenomena*, (Oxford University Press, New York, 1987).

[6] C. Domb and M. S. Green, *Phase Transitions and Critical Phenomena*, Vol.3, (Academic press, New York, 1974).