

## EXACT ONE-DIMENSIONAL ISING MODEL

The one-dimensional Ising model consists of a chain of  $N$  spins, each spin interacting only with its two nearest neighbors. The simple Ising problem in one dimension can be solved directly in several ways.

**First** the chain is considered as open ended and the Hamiltonian in the form:

$$H = -J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} \quad J > 0$$

The partition function is given by

$$Z_N = \sum_{\{\sigma_i = \pm 1\}} e^{K \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1}} \quad (7.5.1)$$

where  $K = \beta J$ . The exponential can be factored as a product of terms of the form  $e^{K \sigma_i \sigma_{i+1}}$ , each of which can be written as (Note that:  $(\sigma_i \sigma_{i+1})$  can only be +1 or -1,  $\cosh(\pm x) = x$  and  $\sinh(\pm x) = \pm x$ )

$$e^{K \sigma_i \sigma_{i+1}} = \cosh(K \sigma_i \sigma_{i+1}) + \sinh(K \sigma_i \sigma_{i+1}) = \cosh(K) + \sigma_i \sigma_{i+1} \sinh(K) \quad *$$

$$= (1 + \sigma_i \sigma_{i+1} y) \cosh(K)$$
(7.5.2)

where  $y = \tanh(K)$ .

Here we have used:

$$* e^{c \sigma \sigma'} = \begin{cases} e^c & \sigma \sigma' = 1 \\ e^{-c} & \sigma \sigma' = -1 \end{cases} = \cosh(c) + \sigma \sigma' \sinh(c)$$

which holds because can only +1 or -1.

The partition function (7.5.1) then becomes

$$Z_N = \cosh^{N-1} K \sum_{\{\sigma_i = \pm 1\}} \prod_{i=1}^{N-1} (1 + \sigma_i \sigma_{i+1} y)$$

$$= (\cosh K)^{N-1} \sum_{\{\sigma_i = \pm 1\}} (1 + \sigma_1 \sigma_2 y)(1 + \sigma_2 \sigma_3 y) \cdots (1 + \sigma_{N-1} \sigma_N y). \quad (7.5.3)$$

Summation over  $\sigma_1 = \pm 1$  gives  $(1 + \sigma_2 y)(\cdots) + (1 - \sigma_2 y)(\cdots)$ , where  $(\cdots)$  represents

$$\prod_{i=2}^{N-1} (1 + \sigma_i \sigma_{i+1} y),$$

and the indicated summation yields  $2(\cdots)$ . Next, summation over  $\sigma_2 = \pm 1$  gives another factor 2 and a product of  $N - 3$  terms. Continued summations finally produce the result

$$Z_N = \{2 \cosh(K)\}^{N-1} \quad (7.5.4)$$

### Average energy and the specific heat:

In the thermodynamic limit, the free energy per spin is given by:

$$f = -k_B T \lim_{N \rightarrow \infty} \frac{1}{N} \ln Z_N = -k_B T \ln \{2 \cosh(K)\},$$

$$U = \langle E \rangle = \lim_{N \rightarrow \infty} \left[ -\frac{1}{N} \frac{\partial \ln Z_N}{\partial \beta} \right] = -J \tanh(K)$$
(7.5.5)

and the heat capacity  $C$  is

$$C = \frac{\partial \langle E \rangle}{\partial T} = k_B K^2 \cosh^2(K)$$
(7.5.6)

The energy and heat capacity are smoothly varying, always finite functions of temperature, exhibiting no phase transition. Thus the molecular-mean-field- approximation is incorrect, no matter how plausible, for a one-dimensional system, and its validity in n-dimensions then is immediately to be doubted.

Another direct technique for the open, one-dimensional chain makes use of a change in variables  $\eta_i = \sigma_i \sigma_{i+1} = \begin{cases} 1 & \text{if } \sigma_i = \sigma_{i+1} \\ -1 & \text{if } \sigma_i = -\sigma_{i+1} \end{cases}$ ,  $1 \leq i \leq N-1$ , where it may be seen from Eq. (7.5.1) or (7.5.3) that  $Z_N$  is independent of  $\eta_i$ . For the open chain, the  $\eta$ 's are independent, and  $Z_N$  can be written as

$$Z_N = \sum_{\{\eta_i = \pm 1\}} e^{K \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1}} = \left( \sum_{\eta_1 = \pm 1} e^{K \eta_1} \right) \left( \sum_{\eta_2 = \pm 1} e^{K \eta_2} \right) \dots$$

$$= \{2 \cosh(K)\}^{N-1}$$

where each sum on a  $\eta_i$  yields a factor  $2 \cosh(K)$ , and the final result is the product of  $N-1$  such independent factors, in agreement with Eq. (7.5.4). For closed chains in one dimension and for Ising lattices of higher dimension, no such simple technique will work because the  $\eta$ 's are no longer independent.

**Second** When the chain is closed, with  $S_1 = S_{N+1}$ :

For the open ended chain, the Hamiltonian has the form:

$$H = -J \sum_{i=1}^N S_i S_{i+1} \quad J > 0$$

The partition function is given by

$$Z_N = \sum_{\{S_i = \pm 1\}} e^{K \sum_{i=1}^N S_i S_{i+1}}$$

When the chain is closed, with  $S_1 = S_{N+1}$ , direct evaluation of  $Z_N$  becomes slightly more difficult, but other procedures are often simpler for the closed chain than for the open one. For the closed chain,  $Z_N$  becomes:

$$Z_N = \{ \cosh(K) \}^N \sum_{\{S\}} \prod_{i=1}^N (1 + y S_i S_{i+1})$$

where  $K = \beta J$  and  $y = \tanh(K)$ . We work out the product and sort terms in powers of  $y$  :

$$Z_N = \{ \cosh(K) \}^N \sum_{\{S\}} \{ 1 + y (S_1 S_2 + S_2 S_3 + \dots + S_N S_1) + y^2 (S_1 S_2 S_2 S_3 + \dots) + \dots + y^N (S_1 S_2 S_2 \dots S_N S_N S_1) \}$$

The terms, linear in  $y$  contain products of two different (neighboring) spins, like  $S_i S_{i+1}$ . The sum over all spin configurations of this product vanish,  $\sum_{S_i \text{ or } S_{i+1}} (S_i S_{i+1}) = 0$ , because there are two configurations with parallel spins ( $S_i S_{i+1} = 1$ ) and two with antiparallel spins ( $S_i S_{i+1} = -1$ ). Thus, the term linear in  $y$  vanishes after summation over all spin configurations. For the same reason also the sum over all spin configurations, which appear at the term proportional to  $y^2$ , vanish. In order for a term to be different from zero, all the spins in the product must appear twice (then,  $\sum_{S_i} S_i^2 = 2$ ). This condition is fulfilled only in the last term, which after summation over all spin configurations gives  $2^N y^N$ . Therefore the partition function of the Ising model of a linear chain of  $N$  spins is:

$$Z_N = \{ 2 \cosh(K) \}^{N-1} [ 1 + y^N ]$$

a result that differs from that of  $Z_N = \{ 2 \cosh(K) \}^{N-1}$  for open chain. In the limit of very large  $N$ , however, the  $y^N$  contribution becomes vanishingly small, since  $y = \tanh K < 1$  for all finite  $J$  and  $\beta$ .

**Note that:**

i-  $\sum_{\{S\}} 1 = 2,$

ii-  $\sum_{S_i} S_i S_{i+1} = (1 + -1) S_{i+1} = 0,$

iii-  $\sum_{S_i \text{ or } S_{i+1}} (S_i S_{i+1}) = \underbrace{\uparrow\uparrow}_{+1} + \underbrace{\uparrow\downarrow}_{-1} + \underbrace{\downarrow\uparrow}_{-1} + \underbrace{\downarrow\downarrow}_{+1} = 1 - 1 - 1 + 1 = 0$

iv-  $\sum_{\{S\}_i} (S_i S_{i+1} S_j S_{j+1}) = \uparrow\uparrow\uparrow\uparrow + \uparrow\uparrow\uparrow\downarrow + \uparrow\uparrow\downarrow\uparrow + \uparrow\downarrow\uparrow\uparrow + \uparrow\downarrow\uparrow\downarrow + \downarrow\downarrow\uparrow\uparrow + \downarrow\uparrow\uparrow\downarrow + \dots + \downarrow\downarrow\downarrow\downarrow$   
 $= 1 - 4 + 6 - 4 + 1 = 0$

v-  $\sum_{S_i=-1}^{+1} S_i^\ell = \begin{cases} 2 & \ell = \text{even} \\ 0 & \ell = \text{odd} \end{cases}, \quad \sum_{S_i} 1 = 2$

## Ising Model and Transfer Matrix

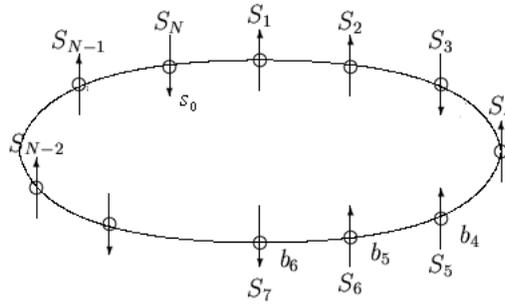
Exact solutions of the Ising model are possible in 1 and 2 dimensions and can be used to calculate the exact critical exponents for the two corresponding universality classes.

In one dimension, the Ising Hamiltonian becomes:

$$\begin{array}{ccccccc} \uparrow & \uparrow & \downarrow & \dots & \downarrow & \downarrow & \uparrow \\ s_0 & s_1 & s_2 & \dots & & & s_{N-1} \end{array}$$

$$H = -J \sum_{i=0}^N s_i s_{i+1} - h \sum_{i=0}^N s_i, \quad J, h > 0$$

which corresponds to  $N$  spins on a line. We will impose periodic boundary conditions on the spins so that  $s_N = s_0$ ,  $s_i = +1$  or  $-1$ . Thus, the topology of the spin space is that of a circle, see the figure.



With the definitions  $K = \beta J$  and  $H = \beta h$ , the partition function is then:

$$\begin{aligned} Z &= \sum_{\{s\}} e^{K(s_0 s_1 + s_1 s_2 + \dots + s_{N-1} s_0) + H(s_0 + s_1 + s_2 + \dots + s_{N-1})} \\ &= \sum_{\{s\}} e^{H(\frac{s_0}{2}) + K(s_0 s_1) + \beta h(\frac{s_1}{2})} e^{H(\frac{s_1}{2}) + K(s_1 s_2) + \beta h(\frac{s_2}{2})} \dots e^{H(\frac{s_{N-1}}{2}) + K(s_{N-1} s_0) + H(\frac{s_0}{2})} \\ &\equiv \sum_{\{s\}} P_{0,1} P_{1,2} \dots P_{N-1,0} \end{aligned}$$

Where

$$P_{i,i+1} = e^{H(\frac{s_i}{2}) + K(s_i s_{i+1}) + H(\frac{s_{i+1}}{2})}$$

In order to carry out the spin sum, let us define a matrix  $P$  with matrix elements:

$$\begin{aligned} \langle s | P | s' \rangle &= e^{H(\frac{s}{2}) + K(s s') + H(\frac{s'}{2})}, \\ \langle 1 | P | 1 \rangle &= e^{K+H}, \quad \langle -1 | P | -1 \rangle = e^{K-H}, \\ \langle -1 | P | 1 \rangle &= \langle 1 | P | -1 \rangle = e^{-K} \end{aligned}$$

The matrix  $\mathbf{P}$  is called the *transfer matrix*. Thus, the matrix  $P$  is a 2 x2 matrix given by

$$P = \begin{matrix} & s_{i+1} = 1 & s_{i+1} = -1 \\ \begin{matrix} s_i = 1 \\ s_i = -1 \end{matrix} & \begin{pmatrix} e^{K+H} & e^{-K} \\ e^{-K} & e^{K-H} \end{pmatrix} \end{matrix}$$

From the matrix rules, the larger  $\lambda_+$  and smaller  $\lambda_-$  eigenvalues are calculated as:

$$\begin{aligned} \lambda_+ + \lambda_- &= \text{Tr}(P) = e^{K+H} + e^{K-H} = 2e^K \cosh(H) \\ \lambda_+ \lambda_- &= \det(P) = e^{K+H} e^{K-H} - e^{-K} e^K = e^{2K} - e^{-2K} = 2 \sinh(K) \end{aligned}$$

Solving for  $\lambda_{\pm}$ , one finds:

$$\lambda_{\pm} = e^K \left[ \cosh(H) \pm \sqrt{\sinh^2(H) + e^{-4K}} \right]$$

The trace of  $P^N$  is given by:

$$Z_N = \text{Tr}(P^N) = \lambda_+^N + \lambda_-^N = \lambda_+^N \left[ 1 + (\lambda_- / \lambda_+)^N \right] \underset{N \rightarrow \infty}{\sim} \lambda_+^N$$

### Free energy:

In the thermodynamic limit, the free energy per spin is given by:

$$f = -k_B T \lim_{N \rightarrow \infty} \frac{1}{N} \ln Z_N = -k_B T \ln \lambda_+$$

As  $\beta \rightarrow \infty$

$$f = -k_B T \lim_{\beta \rightarrow \infty} \ln \lambda_+ = -k_B T \ln \left\{ e^K [\cosh(H) + \sinh(H)] \right\} = -J - h$$

which is the energy per spin as expected.

**The magnetization:** becomes

$$m = \left( \frac{\partial f}{\partial h} \right) = - \left( \frac{\partial \ln \lambda_+}{\partial (H)} \right) = \frac{\sinh(H) + \frac{\sinh(H) \cosh(H)}{\sqrt{\sinh^2(H) + e^{-4K}}}}{\cosh(H) + \sqrt{\sinh^2(H) + e^{-4K}}}$$

Which is regular as  $H \rightarrow 0$ , since  $\cosh(H) \rightarrow 1$  and  $\sinh(H) \rightarrow 0$ , itself vanishes. Thus, there is no magnetization at any finite temperature in one dimension, hence no nontrivial critical point.

**Example:** It was that the exact eigenvalues of the periodic Ising model is given by:

$$\lambda_{\pm} = e^K \left[ \cosh(H) \pm \sqrt{\sinh^2(H) + e^{-4K}} \right], \quad \beta = 1/kT, \quad K = \beta J \text{ and } H = \beta h$$

For  $H = 0$ , simplify the expression:

$$\begin{aligned} \lambda_{\pm} &= e^K \left[ \cosh(H) \pm \sqrt{\sinh^2(H) + e^{-4K}} \right] = e^K \left[ 1 \pm \sqrt{e^{-4K}} \right] = e^K \pm e^{-K}, \quad \beta = 1/kT, \\ &\Rightarrow \lambda_+ = 2 \cosh(K), \quad \lambda_- = 2 \sinh(K), \end{aligned}$$

Consequently

$$\lambda = \lambda_+^N + \lambda_-^N = [2 \cosh(K)]^N + [2 \sinh(K)]^N = \lambda_+^N \left[ 1 + (\lambda_- / \lambda_+)^N \right];$$

$$= \{2 \cosh(K)\}^N (1 + y^N) \approx \{2 \cosh(K)\}^N$$

Where  $y = \tanh(K)$

Then find the following:

i-  $F = -\frac{1}{\beta} \ln(\lambda)$  in the extreme limits, i.e.  $T \rightarrow 0$  and  $T \rightarrow \infty$ .

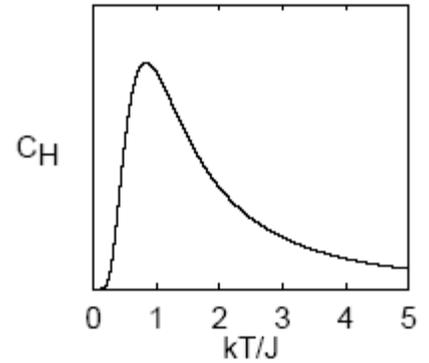
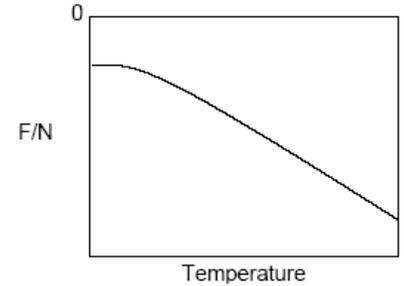
Ans:  $F = -\frac{1}{\beta} \ln(\lambda) = -NkT \ln\{2 \cosh(K)\}$

ii-  $E = -\frac{\partial}{\partial \beta} \ln(\lambda)$

Ans:  $E = -\frac{\partial}{\partial \beta} \ln(\lambda) = -NJ \tanh(K)$

ii-  $C = -\frac{\partial E}{\partial T}$  in the extreme limits, i.e.  $T \rightarrow 0$  and  $T \rightarrow \infty$ , and find  $T$  at maximum  $C$ .

Ans:  $C = -\frac{\partial E}{\partial T} = NK \left[ \frac{K}{\cosh(K)} \right]^2$



**Note:**

$$Z_N = \{2 \cosh(K)\}^N;$$

$$F = -\frac{1}{N} \ln Z_N = -\ln\{2 \cosh(K)\} = -\ln\{e^{J/T} + e^{-J/T}\}$$

$$= -\ln(e^{J/T}) - \ln\{1 + e^{-2J/T}\}$$

As  $T \rightarrow 0$

$$F \approx -\frac{J}{T} - e^{-2J/T}$$

The first term, even though it looks like it blows up at  $T \rightarrow 0$ , is actually regular. It simply says that the ground state energy is  $-J$  per spin. It could be removed by a constant shift of energy, for example. The second term is singular. So the singular part of the free energy behaves as:

$$F_{\text{singular}} \approx -e^{-2J/T}$$

The correlation length is

$$\xi = \frac{1}{\ln\left(\frac{\lambda_+}{\lambda_-}\right)} = \frac{1}{\ln\left(\frac{1}{\tanh K}\right)} \approx \frac{1}{2} e^{2J/T}$$

The last approximate equality works at  $T \rightarrow 0$ . Their product, in the limit  $T \rightarrow 0$  is thus

$$\xi F_{\text{singular}} = -\frac{1}{2}$$

Which is a universal number (does not depend on parameters)

**H.W.** With the eigenvector of the Ising matrix in 2-dimensions, calculate the magnetization per spin, the correlation function, and the correlation length, and check if they behave in a sensible way. (Go to the discussion in sections 3.3 and 3.4 of Goldenfeld)

**H.W.** Write down the transfer matrix for the one-dimensional spin-1 Ising model in zero field which is described by the Hamiltonian

$$H = -J \sum_{i=0}^N s_i s_{i+1}, \quad J > 0, \quad s_i = \pm 1, 0$$

Hence calculate the free energy per spin of this model and show that it has the expected behavior in the limits  $T \rightarrow 0$  and  $T \rightarrow \infty$ .

[Answer:  $f = -kT \ln\{(1+2 \cosh \beta J + [(2 \cosh \beta J - 1)^2 + 8]^{1/2})/2\}$  .]

While the one-dimensional Ising model is a relatively simple problem to solve, the two-dimensional Ising model is *highly* nontrivial. It was only the pure mathematical genius of Lars Onsager that was able to find an analytical solution to the two-dimensional Ising model. This, then, gives an exact set of critical exponents for the  $d = 2$  and  $n = 1$  universality class. To date, the three-dimensional Ising model remains unsolved.

Here, the Onsager results will be stated as:

In the thermodynamic limit, the final result at zero field is:

$$f(T) = -kT \ln [2 \cosh(2\beta J)] - \frac{kT}{2\pi} \int_0^\pi d\phi \ln \frac{1}{2} \left( 1 + \sqrt{1 - K^2 \sin^2 \phi} \right)$$

where

$$K = \frac{2}{\cosh(2\beta J) \coth(2\beta J)}$$

The energy per spin is

$$e(T) = -2J \tanh(2\beta J) + \frac{K}{2\pi} \frac{dK}{d\beta} \int_0^\pi d\phi \frac{\sin^2 \phi}{\Delta(1 + \Delta)}$$

where

$$\Delta = \sqrt{1 - K^2 \sin^2 \phi}$$

The magnetization, then, becomes

$$m = \left\{ 1 - [\sinh(2\beta J)]^{-4} \right\}^{1/8}$$

for  $T < T_c$  and 0 for  $T > T_c$ , indicating the presence of an order-disorder phase transition at zero field. The condition for determining the critical temperature at which this phase transition occurs turns out to be

$$2 \tanh^2(\beta J) = 1$$

$$kT_c \approx 2.269185J$$

Near  $T = T_c$ , the heat capacity per spin is given by

$$\frac{C(T)}{k} = \frac{2}{\pi} \left( \frac{2J}{kT_c} \right)^2 \left[ -\ln \left( 1 - \frac{T}{T_c} \right) + \ln \left( \frac{kT_c}{2J} \right) - \left( 1 + \frac{\pi}{4} \right) \right]$$

Thus, the heat capacity can be seen to diverge logarithmically as  $T \rightarrow T_c$ .

The critical exponents computed from the Onsager solution are

$$\alpha = 0 \quad (\text{log divergence})$$

$$\beta = \frac{1}{8}$$

$$\gamma = \frac{7}{4}$$

$$\delta = 15$$

which are a set of exact exponents for the  $d = 2$  and  $n = 1$  universality class.

$$\ln Z = n \ln(\lambda), \quad \lambda = e^{\beta J} \cosh(\beta \mu B) + \sqrt{e^{2\beta J} \sinh^2(\beta \mu B) + e^{-2\beta J}}$$

EXAMPLE:

In terms of  $J, \mu B$  and  $T$ , find the average magnetization (per spin) for the 1-d Ising model.

Since the magnetic field enters the Hamiltonian as  $-\mu \vec{B} \cdot \vec{\sigma}$ , the average spin is

$$\langle \sigma \rangle = \frac{1}{n} \frac{d \ln Z}{d(\beta \mu B)}$$

This gives,

$$\langle \sigma \rangle = \frac{\sinh(\beta \mu B) + \frac{\cosh(\beta \mu B) \sinh(\beta \mu B)}{\sqrt{\sinh^2(\beta \mu B) + e^{-4\beta J}}}}{\cosh(\beta \mu B) + \sqrt{\sinh^2(\beta \mu B) + e^{-4\beta J}}}$$

$$= \frac{\sinh(\beta \mu B)}{\sqrt{\sinh^2(\beta \mu B) + e^{-4\beta J}}}$$