Lecture 8. *Wednesday 6th November, 2019.* *Compiled: Thursday 15th September, 2022.*

Since $\sum_k \lambda_k^N = Z_N$ for $k = +, -, 1, \dots, n$, we have

$$\langle S_1 S_R \rangle_N = \frac{\sum_{ij} \langle t_j | \mathbb{S}_1 | t_i \rangle \lambda_i^{R-1} \langle t_i | \mathbb{S}_R | t_j \rangle \lambda_j^{N-R+1}}{\sum_{k=1}^n \lambda_k^N}$$

If we now multiply and divide by λ_+^N, we get

$$\langle S_1 S_R \rangle_N = \frac{\sum_{ij} \langle t_j | \mathbb{S}_1 | t_i \rangle (\lambda_i/\lambda_+)^{R-1} \langle t_i | \mathbb{S}_R | t_j \rangle (\lambda_j/\lambda_+)^{N-R+1}}{\sum_{k=1}^n (\lambda_k/\lambda_+)^N}$$

Remark. In the thermodynamic limit $N \to \infty$, only the terms with $j = +$ and $k = +$ will survive in the sum. Remind that R is fixed.

$$\langle S_1 S_R \rangle = \lim_{N\to\infty} \langle S_1 S_R \rangle_N = \sum_{i=\pm,1\dots n} \left(\frac{\lambda_i}{\lambda_+}\right)^{R-1} \langle t_+ | \mathbb{S}_1 | t_i \rangle \langle t_i | \mathbb{S}_R | t_+ \rangle$$

Rembember that $\lambda_+ > \lambda_- \geq \lambda_1 \geq \dots \geq \lambda_n$:

$$\langle S_1 S_R \rangle = \langle t_+ | \mathbb{S}_1 | t_+ \rangle \langle t_+ | \mathbb{S}_R | t_+ \rangle + \sum_{i\neq +}^n \left(\frac{\lambda_i}{\lambda_+}\right)^{R-1} \langle t_+ | \mathbb{S}_1 | t_i \rangle \langle t_i | \mathbb{S}_R | t_+ \rangle$$

Since one can prove

$$\lim_{N\to\infty} \langle S_R \rangle_1 = \langle t_+ | \mathbb{S}_1 | t_+ \rangle , \quad \lim_{N\to\infty} \langle S_R \rangle_N = \langle t_+ | \mathbb{S}_R | t_+ \rangle \tag{1}$$

we obtain

$$\langle S_1 S_R \rangle = \langle S_1 \rangle \langle S_R \rangle + \sum_{i\neq +} \left(\frac{\lambda_i}{\lambda_+}\right)^{R-1} \langle t_+ | \mathbb{S}_1 | t_i \rangle \langle t_i | \mathbb{S}_R | t_+ \rangle \tag{2}$$

Example 1: Show relation (1)

Let us prove (1) by a method analogous to that followed above.

$$\langle S_1 \rangle_N = \frac{1}{Z} \sum_{\{S\}} S_1 e^{-\beta \mathcal{H}_N} = \frac{1}{Z} \sum_{S_1} S_1 \langle S_1 | \mathbb{T}^N | S_1 \rangle = \frac{1}{Z} \sum_{S_1} S_1 \sum_i \langle S_1 | t_i \rangle \lambda_i^N \langle t_i | S_1 \rangle$$
$$= \frac{1}{Z} \sum_i \lambda_i^N \langle t_i | \mathbb{S}_1 | t_i \rangle = \frac{\sum_i (\lambda_i/\lambda_+)^N \langle t_i | \mathbb{S}_1 | t_i \rangle}{\sum_{k=1}^n (\lambda_k/\lambda_+)^N}$$

Taking the limit $N \to \infty$:

$$\langle S_1 \rangle = \lim_{N\to\infty} \langle S_1 \rangle_N = \langle t_+ | \mathbb{S}_1 | t_+ \rangle$$

The correlation function follows immediately from (2),

$$\Gamma_R = \langle S_1 S_R \rangle - \langle S_1 \rangle \langle S_R \rangle = \sum_{i\neq +}^n \left(\frac{\lambda_i}{\lambda_+}\right)^{R-1} \langle t_+ | \mathbb{S}_1 | t_i \rangle \langle t_i | \mathbb{S}_R | t_+ \rangle \tag{3}$$

Remark. Γ_R depends only on the eigenvalues and eigenvectors of the transfer matrix $\mathbb{T}$ and by the values of the spins S_1 and S_R.

A much simpler formula is obtained for the correlation length (??). Taking the limit $R \to \infty$ the ratio (λ_-/λ_+) dominates the sum and hence

$$
\begin{aligned}
\xi^{-1} &= \lim_{R\to\infty} \left\{ -\frac{1}{R-1} \log |\langle S_1 S_R\rangle - \langle S_1\rangle \langle S_R\rangle| \right\} \\
&= \lim_{R\to\infty} \left\{ -\frac{1}{R-1} \log \left[\left(\frac{\lambda_-}{\lambda_+}\right)^{R-1} \langle t_+| \, \mathbb{S}_1 \, |t_-\rangle\langle t_-| \, \mathbb{S}_R \, |t_+\rangle \right] \right\} \\
&= -\log \left[\left(\frac{\lambda_-}{\lambda_+}\right) \right] - \lim_{R\to\infty} \frac{1}{R-1} \log \langle t_+| \, \mathbb{S}_1 \, |t_-\rangle\langle t_-| \, \mathbb{S}_R \, |t_+\rangle \\
&= -\log \left(\frac{\lambda_-}{\lambda_+}\right)
\end{aligned}
$$

The important result is

$$
\xi^{-1} = -\log \left(\frac{\lambda_-}{\lambda_+}\right) \tag{4}
$$

It means that the *correlation length does depend only on the ratio between the two largest eigenvalues of the transfer matrix* $\mathbb{T}$.

0.0.1 Results for the *1-dim* Ising model

Let us now return to the example of the nearest neighbour Ising model in a magnetic field, to obtain explicit results for the bulk free energy f_b, the correlation function Γ and the correlation length ξ.

Recall that the transfer matrix of such a system is given by

$$
\mathbb{T} = \begin{pmatrix} \exp(K+h) & \exp(-K) \\ \exp(-K) & \exp(K-h) \end{pmatrix}
$$

Now, let us calculate the eigenvalues:

$$
|\mathbb{T} - \lambda \mathbb{1}| = (e^{K+h} - \lambda)(e^{K-h} - \lambda) - e^{-2K} = 0
$$

The two solutions are

$$
\lambda_\pm = e^K \cosh(h) \pm \sqrt{e^{2K}\sinh^2(h) + e^{-2K}} \tag{5}
$$

The free energy

The free energy is

$$
\begin{aligned}
f_b &\equiv \lim_{N\to\infty} \frac{-k_B T}{N} \log Z_N(K,h) \\
&= -k_B T \lim_{N\to\infty} \frac{1}{N} \log \left[\lambda_+^N \left(1 + \left(\frac{\lambda_-}{\lambda_+}\right)^N \right) \right] \\
&= -k_B T \log \lambda_+
\end{aligned}
$$

and inserting the explicit expression of λ_+ for the Ising model, we get

$$
\begin{aligned}
f_b &= -k_B T \log \left(e^K \cosh h + \sqrt{e^{2K}\sinh^2(h) + e^{-2K}} \right) \\
&= -K k_B T - k_B T \log \left(\cosh(h) + \sqrt{\sinh^2(h) + e^{-4K}} \right)
\end{aligned} \tag{6}
$$

Remark. Remember that $K \equiv \beta J, h \equiv \beta H$.

Exercise 1

Check that if $h = 0$ we get back the expression found previously with the iterative method. What is the importance of boundary conditions?

Solution. If $h = 0$, we obtain

$$\begin{aligned} f_b &= -Kk_BT - k_BT\log\left(1 + \frac{1}{e^{2K}}\right) = -k_BT\big(\log e^K + \log\big(1 + e^{-2K}\big)\big) \\ &= -k_BT\log\big(e^K + e^{-K}\big) = -k_BT\log\left(2\frac{e^K + e^{-K}}{2}\right) \\ &= -k_BT\log(2\cosh K) = -k_BT\log\left(2\cosh\left(\frac{J}{k_BT}\right)\right) \end{aligned}$$

The choice of boundary conditions becomes irrelevant in the thermodynamic limit, $N \to \infty$.

Let us now consider the limits $T \to 0$ and $T \to \infty$ by keeping H fixed and J fixed.

- Case: $T \to 0 \Rightarrow K \to \infty, h \to \infty$.

$$e^{-4K} \overset{K\to\infty}{\longrightarrow} 0$$
$$\sqrt{\sinh^2 h} \overset{h\to\infty}{\sim} \sinh(h)$$

We have

$$\cosh h + \sinh h \sim \frac{2e^h}{2} \simeq e^h$$

and

$$f \overset{\substack{h\to\infty \\ K\to\infty}}{\sim} -Kk_BT - k_BT\log e^h \sim -J - H \quad const \tag{8}$$

Therefore, as $T \to 0^+$, f goes to a constant that depends on J and H.

- Case: $T \to \infty \Rightarrow K \to 0, h \to 0$. In this case we suppose also that H and J (fixed) are also finite.

$$e^{-4K} \simeq 1$$
$$\sqrt{\sinh^2 h + e^{-4K}} \sim \sqrt{1}$$

Since $\cosh h \overset{h\to 0}{\sim} 1$:

$$f_B \sim -Kk_BT - k_BT\log\left(1 + 1\right) \sim -J - k_BT\ln 2 \tag{10}$$

Therefore, as $T \to \infty$, the free energy goes linearly to zero, as in Figure 1.

The magnetization

This can be obtained by differentiating the negative of the free energy with respect to the magnetic field H (or by using equation (1)):

$$m = -\frac{\partial f_b}{\partial H} = -\frac{1}{k_BT}\frac{\partial f_b}{\partial h} = \frac{\partial}{\partial h}\left[\log\left(\cosh(h) + \sqrt{\sinh^2(h) + e^{-4K}}\right)\right]$$

The result is

$$m = \frac{\sinh h + \frac{\sinh h\cosh h}{\sqrt{\sinh^2 h + e^{-4K}}}}{\cosh h + \sqrt{\sinh^2 h + e^{-4K}}} = \frac{\sinh h}{\sqrt{\sinh^2 h + e^{-4K}}} \tag{11}$$

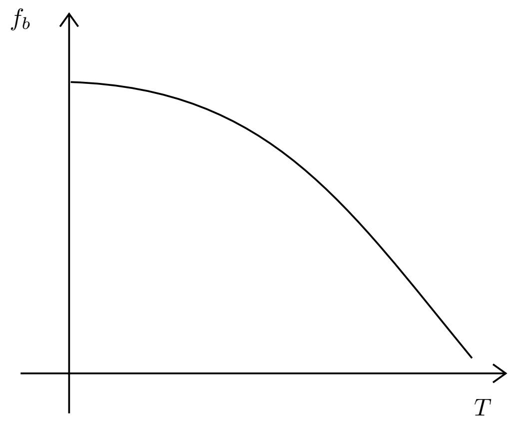

Figure 1: Plot of the free energy f_b in function of the temperature T. For $T \to 0$, the free energy becomes constant, while for $T \to \infty$ it goes linearly to zero.

- Case: $T > 0$ fixed, $H \to 0 \Rightarrow h \to 0$.

$$\sinh h \sim h \sim 0,$$
$$\cosh h \sim 1$$

In zero field $h \to 0$, we have $m \to 0$ for all $T > 0$. It means that there is no spontaneous magnetization!

The magnetic susceptibility

$$\chi_T \equiv \frac{\partial m}{\partial H} = \frac{1}{k_B T} \frac{\partial m}{\partial h} \tag{13}$$

If we consider the case $h \ll 1$, it is convenient first expand the (11) for $h \to 0$ and take the derivative to get χ_T.

Since $\sinh(h) \sim h + h^3$ and $\cosh(h) \sim 1 + h^2$, we have

$$m \overset{h \ll 1}{\sim} \frac{h(1 + e^{2K})}{1 + e^{-2K}}$$

If we now derive with respect to h

$$\chi_T = \frac{1}{k_B T} \frac{\partial m}{\partial h} \overset{h \ll 1}{\approx} \frac{1}{k_B T} \frac{(1 + e^{2K})}{(1 + e^{-2K})}$$

- Case: $T \to \infty \Rightarrow K \to 0$.

$$e^{2K} \simeq e^{-2K} \simeq 1$$

The *Curie's Law* for paramagnetic systems is:

$$\boxed{\chi_T \sim \frac{1}{k_B T}} \tag{14}$$

- Case: $T \to 0 \Rightarrow K \to \infty$.

$$e^{-2K} \simeq 0$$

The *Curie's Law* for paramagnetic systems is:

$$\boxed{\chi_T \sim \frac{1}{k_B T} e^{2K} \sim \frac{1}{k_B T} e^{2J/k_B T}} \tag{15}$$

The correlation length

$$\xi^{-1} = -\log\left(\frac{\lambda_-}{\lambda_+}\right) = -\log\left[\frac{\cosh h - \sqrt{\sinh^2 h + e^{-4K}}}{\cosh h + \sqrt{\sinh^2 h + e^{-4K}}}\right] \tag{16}$$

For $h = 0$, we have $\cosh h \to 1, \sinh h \to 0$:

$$\xi^{-1} = -\log\left[\frac{1 - e^{-2K}}{1 + e^{-2K}}\right] = -\log\left[\frac{1}{\coth K}\right]$$

Therefore:

$$\xi = \frac{1}{\log(\coth K)}, \quad \text{for } h = 0 \tag{17}$$

- Case: $T \to 0 \Rightarrow K \to \infty$.

$$\coth K = \frac{e^K + e^{-K}}{e^K - e^{-K}} \overset{K\to\infty}{\simeq} 1 + 2e^{-2K} + \dots \quad \overset{K\to\infty}{\longrightarrow} 1$$

  It implies

$$\xi \overset{K\gg 1}{\sim} \frac{1}{\ln(1 + 2e^{-2K})} \sim \frac{e^{2K}}{2}$$

  Hence,

$$\xi \overset{T\to 0}{\sim} \frac{1}{2} e^{J/k_B T} \tag{18}$$

  It diverges exponentially $\xi \to \infty$ as $T \to 0$.

- Case: $T \to \infty \Rightarrow K \to 0$.

$$\coth K = \frac{e^K + e^{-K}}{e^K - e^{-K}} \overset{K\to 0}{\simeq} \frac{1 + K + \frac{K^2}{2} + 1 - K + \frac{K^2}{2}}{1 + K + \frac{K^2}{2} - 1 + K - \frac{K^2}{2}} \sim \frac{2 + 2\frac{K^2}{2}}{2K} \sim \frac{1 + K^2}{K}$$

$$\xi^{-1} = \log(\coth K) \overset{K\to 0}{\sim} \ln\frac{1}{K} + \ln(1 + K^2) \sim +\infty$$

  Therefore

$$\xi \overset{K\to 0}{\longrightarrow} 0$$

  More precisely,

$$\xi \overset{K\to 0}{\sim} \frac{1}{\ln(1/K) + \ln(1 + K^2)} \overset{K\to 0}{\sim} -\frac{1}{\ln K} \tag{19}$$

0.1 Classical Heisenberg model for *d=1*

Now, let us suppose to study something different from the Ising model. Indeed, from a physicist's point of view the Ising model is highly simplified, the obvious objection being that the magnetic moment of a molecule is a vector pointing in any direction, not just up or down. One can build this property, obtaining the classical Heisenber model. We do not anymore assume spin that can assume values as -1 or +1, but spin that can assume a continuous value. Unfortunately, this model has not been solved in even two dimensions [**?**].

Let us take a $d = 1$ dimensional lattice. In the classical Heisenberg model, the spins are unit length vectors $\vec{\mathbf{S}}_i$, i.e. $\vec{\mathbf{S}}_i \in \mathbb{R}^3$, $\left|\vec{\mathbf{S}}_i\right|^2 = 1$ (continuous values on the unit sphere). We have

$$\vec{\mathbf{S}}_i = (S_i^x, S_i^y, S_i^z)$$

with periodic boundary condition

$$\vec{\mathbf{S}}_{N+1} = \vec{\mathbf{S}}_1$$

Assuming $H = 0$, the model is defined through the following Hamiltonian:

$$-\beta\mathcal{H}(\{\vec{\mathbf{S}}\}) = K\sum_{i=1}^{N}\vec{\mathbf{S}}_i \cdot \vec{\mathbf{S}}_{i+1} \quad (+\sum_i \vec{\mathbf{h}} \cdot \vec{\mathbf{S}}_i) \tag{20}$$

This model satisfies $O(3)$ symmetry. In the transfer matrix formalism:

$$Z_N(K) = \sum_{\{\vec{\mathbf{S}}\}} e^{-\beta\mathcal{H}} = \sum_{\{\vec{\mathbf{S}}\}} e^{K\sum_{i=1}^{N}\vec{\mathbf{S}}_i\cdot\vec{\mathbf{S}}_{i+1}} = \mathrm{Tr}\big(\mathbb{T}^N\big) \tag{21}$$

where

$$\left\langle \vec{\mathbf{S}}_i \middle| \mathbb{T} \middle| \vec{\mathbf{S}}_{i+1} \right\rangle = e^{K\vec{\mathbf{S}}_i\cdot\vec{\mathbf{S}}_{i+1}}$$

Similarly to the Ising case,

$$\mathbb{T} = \sum_i |t_i\rangle\, \lambda_i\, \langle t_i|$$

and

$$\mathbb{T}_D = \mathbb{P}^{-1}\mathbb{T}\mathbb{P}$$

The problem is computing the eigenvalues λ_i of $\mathbb{T}$.

Formally, we should find

$$\exp\Big[K\vec{\mathbf{S}}_1 \cdot \vec{\mathbf{S}}_2\Big] = \left\langle \vec{\mathbf{S}}_1 \middle| \mathbb{T} \middle| \vec{\mathbf{S}}_2 \right\rangle = \sum_{i\in\text{eigenvalues}} \lambda_i \left\langle \vec{\mathbf{S}}_1 \middle| t_i \right\rangle \left\langle t_i \middle| \vec{\mathbf{S}}_2 \right\rangle = \sum_i \lambda_i f_i(\vec{\mathbf{S}}_1) f^*(\vec{\mathbf{S}}_2)$$

Remark. We start by noticing that the term $e^{K\vec{\mathbf{S}}_1\cdot\vec{\mathbf{S}}_2}$ is similar to the plane wave $e^{i\vec{\mathbf{q}}\cdot\vec{\mathbf{r}}}$, that in scattering problems is usually expanded in spherical coordinates. Plane wave can be expanded as a sum of spherical harmonics as

$$e^{i\vec{\mathbf{q}}\cdot\vec{\mathbf{r}}} = 4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{l}(i)^l j_l(qr) Y^*_{lm}(\hat{\mathbf{q}}) Y_{lm}(\hat{\mathbf{r}})$$

where

$$j_l(qr) = -\frac{(i)^l}{2}\int_0^\pi \sin(\theta) e^{iqr\cos(\theta)} P_l(\cos(\theta))\,\mathrm{d}\theta$$

are the *spherical Bessel functions*, while the $P_l(\cos(\theta))$ are the *Legendre polynomial* of order l.

From a formal comparison we have

$$\vec{\mathbf{S}}_1 \leftrightarrow \hat{\mathbf{S}}_1, \qquad \begin{cases} i\vec{\mathbf{q}}\cdot\vec{\mathbf{r}} = iqr \\ K\vec{\mathbf{S}}_1\cdot\vec{\mathbf{S}}_2 = K\left|\vec{\mathbf{S}}_1\right|\left|\vec{\mathbf{S}}_2\right| = K \end{cases} \tag{22}$$

multiplying by $(-i)$ we can write

$$qr = -iK\left|\vec{\mathbf{S}}_1\right|\left|\vec{\mathbf{S}}_2\right| = -iK \tag{23}$$

In our case, we have $\hat{\mathbf{q}} = \vec{\mathbf{S}}_1, \hat{\mathbf{r}} = \vec{\mathbf{S}}_2$. Hence,

$$e^{K\vec{\mathbf{S}}_1\cdot\vec{\mathbf{S}}_2} = 4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{l}(i)^l j_l(-iK) Y^*_{lm}(\vec{\mathbf{S}}_1) Y_{lm}(\vec{\mathbf{S}}_2) = \sum_i \lambda_i f_i(\vec{\mathbf{S}}_1) f^*(\vec{\mathbf{S}}_2) \tag{24}$$

where

$$\lambda_i = \lambda_{lm}(K) = 4\pi(i)^l j_l(-iK) \tag{25}$$

Remark. Note that λ_i does not depend on m!

If $l = 0$, the largest eigenvalue is:

$$\lambda_+ = \lambda_0(K) = 4\pi j_0(-iK) = 4\pi \frac{\sinh K}{K}$$

and

$$\lambda_- = \lambda_1(K) = 4\pi i j_1(-iK) = 4\pi \left[\frac{\cosh K}{K} - \frac{\sinh K}{K^2} \right]$$

Exercise 2

Given the largest eigenvalue λ_+,

$$\lambda_+ = 4\pi \frac{\sinh K}{K}$$

find the bulk free energy density of the model and discuss its behaviour in the limits of low ($T \to 0$) and high ($T \to \infty$) temperatures.

Solution. The bulk free energy is

$$f_b = -k_B T \log \lambda_+ = -k_B T \log \left(4\pi \frac{\sinh K}{K} \right)$$

Remind that $K \equiv \beta J$ and consider the limits

- Case: $T \to 0 \Rightarrow K \to \infty$.

$$f_b = -\frac{J}{K} \log \left(4\pi \frac{\sinh K}{K} \right) \overset{K \to \infty}{\sim} \frac{J}{K} \log \left(\frac{K}{\sinh K} \right)$$

  Hence,

$$f_b \overset{K \to \infty}{\sim} 0$$

- Case: $T \to \infty \Rightarrow K \to 0$.

$$\sinh K \overset{K \to 0}{\sim} K$$

$$\Rightarrow f_b = -k_B T \log \left(4\pi \frac{\cancel{K}}{\cancel{K}} \right) = -k_B T \log(4\pi)$$

  In this case the free energy f_b goes linearly with respect to the temperature.

How can we violate the hypothesis of the Perron-Frobenius theorem hoping to find a phase transition also in a $d = 1$ model? One of the hypothesis of the Perron-Frobenius theorem is the one in which $A_{ij} > 0$ for all i, j. Hence, one possibility is to build a model in which its transfer matrix has same A_{ij} that are equal to zero also for $T \neq 0$.