

Tutorial 8, Statistical Mechanics: Concepts and applications 2019/20 ICFP Master (first year)

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Tutorial exercises

I. PHYSICS IN INFINITE DIMENSIONS

1. Ising model on the Bethe lattice

The model: Consider the Ising model on a Bethe lattice at inverse temperature β . The energy reads as

$$E(\{\sigma\}) = -J \left(\sum_{(i,j)} \sigma_i \sigma_j + h \sum_i \sigma_i \right), \quad (1)$$

and the first sum is over all the bonds of the Bethe lattice.

- (a) We define the dimensionality of a lattice as $d = \lim_{n \rightarrow \infty} \frac{\log c_n}{\log n}$, where $c_n = 1 + m_1 + \dots + m_n$ with m_1 the number of neighbors per site, m_2 the number of next-nearest neighbors, and so on. Show that, for some regular lattices you know, this definition is consistent with our intuition. Which is the dimensionality of the Bethe lattice?

: Let us consider simple hyper-cubic lattices. In 1D, $m_1 = m_2 = \dots = 2$, therefore $c_n = 1 + 2n$; the dimensionality is $\lim_{n \rightarrow \infty} \frac{\log(2n+1)}{\log n} = 1$. In 2D, it is simple to see that $m_n = 4n$, therefore $c_n = 1 + 4 \sum_{j=1}^n j = 1 + 2n(n+1)$; the dimensionality is $\lim_{n \rightarrow \infty} \frac{\log(1+2n^2+2n)}{\log n} = 2$. It is clear that we only have to determine the asymptotic behavior of c_n . In 3D, it is then sufficient to note that $m_n \sim n^2$ to get $d = 3$. If we apply the same definition to the Bethe lattice, for the central spin we obtain $m_n = q(q-1)^{n-1}$. Thus, $c_n = 1 + q \sum_{j=0}^{n-1} (q-1)^j = \frac{q^{n+1}-1}{q-1}$ and the dimensionality is $d = \infty$. (Note that for a spin different from the central one, m_n is slightly different, but still increases exponentially with n .)

- (b) Rewrite the probability of a configuration in the form

$$P(\{\sigma\}) = \frac{1}{Z} e^{\beta J h \sigma_0} \prod_{j=1}^q Q_n(\sigma_0 | \{\sigma\}^{(j)}), \quad (2)$$

where $\{\sigma\}^j$ are all the spins in the j -th subtree (we are labeling the spins as $\sigma_i^{(j,k,\dots)}$, where (j,k,\dots) identifies the specific branch and i is a redundant index equal to the number of the shell - Fig. ??).

: In the canonical description, the probability of a configuration is

$$P(\{\sigma\}) = \frac{1}{Z} e^{\beta J \sum_{(i,j)} \sigma_i \sigma_j + \beta J h \sum_i \sigma_i}, \quad (3)$$

where Z is the partition function. By isolating the contribution from the central spin of the Bethe lattice we find

$$P(\{\sigma\}) = \frac{1}{Z} \exp \left(\beta J h \sigma_0 + \beta J h \sum_i \sigma_i + \beta J \sigma_0 \sum_{k=1}^q \sigma_1^{(k)} + \beta J \sum_{k=1}^q \sum_{i=0}^{\infty} \sum_{\{k\}_i}^{q-1} \sigma_i^{(k,k_1,\dots,k_i)} \sigma_{i+1}^{(k,k_1,\dots,k_{i+1})} \right), \quad (4)$$

where, for $i = 0$, $\sigma_i^{(k, k_1, \dots, k_i)} \equiv \sigma_i^{(k)}$. Thus we have

$$Q_n(\sigma_0 | \{\sigma\}^{(j)}) = \exp\left(\beta J h \sum_{i=0}^{\infty} \sum_{\{k\}_i}^{q-1} \sigma_i^{(j, k_1, \dots, k_i)} + \beta J \sigma_0 \sigma_1^{(j)} + \beta J \sum_{i=0}^{\infty} \sum_{\{k\}_i}^{q-1} \sigma_i^{(j, k_1, \dots, k_i)} \sigma_{i+1}^{(j, k_1, \dots, k_{i+1})}\right). \quad (5)$$

(c) Show that $Q_n(\sigma_0 | \{\sigma\}^{(j)})$ satisfies the recurrence relation

$$Q_n(\sigma_0 | \{\sigma\}^{(j)}) = e^{\beta J \sigma_0 \sigma_1^{(j)} + \beta J h \sigma_1^{(j)}} \prod_{k=1}^{q-1} Q_{n-1}(\sigma_1^{(j)} | \{\sigma\}^{(j, k)}), \quad (6)$$

where $\{\sigma\}^{j, k}$ are all the spins in k -th brunch of the j -th subtree.

: This is a direct consequence of (5). In addition, this holds true also replacing n by $m \leq n$.

(d) Define $g_n(\sigma_0) = \sum_{\{\sigma\}^{(j)}} Q_n(\sigma_0 | \{\sigma\}^{(j)})$ and write a recurrence relation for $x_n = \frac{g_n(-)}{g_n(+)}$. Show that, by consistency, $g_0(\sigma_0)$ must be set equal to 1.

: By summing (6) over the spins $\{\sigma\}^{(j)}$ in the j -th subtree we obtain

$$\begin{aligned} \sum_{\{\sigma\}^{(j)}} Q_n(\sigma_0 | \{\sigma\}^{(j)}) &= \sum_{\{\sigma\}^{(j)}} e^{\beta J \sigma_0 \sigma_1^{(j)} + \beta J h \sigma_1^{(j)}} \prod_{k=1}^{q-1} Q_{n-1}(\sigma_1^{(j)} | \{\sigma\}^{(j, k)}) = \\ &= \sum_{\sigma_1^{(j)}} e^{\beta J \sigma_0 \sigma_1^{(j)} + \beta J h \sigma_1^{(j)}} \prod_{k=1}^{q-1} \sum_{\{\sigma\}^{(j, k)}} Q_{n-1}(\sigma_1^{(j)} | \{\sigma\}^{(j, k)}), \end{aligned} \quad (7)$$

which means

$$g_n(\sigma_0) = \sum_{\sigma_1^{(j)}} e^{\beta J \sigma_0 \sigma_1^{(j)} + \beta J h \sigma_1^{(j)}} [g_{n-1}(\sigma_1^{(j)})]^{q-1} \equiv \sum_{\sigma = \pm 1} e^{\beta J \sigma_0 \sigma + \beta J h \sigma} [g_{n-1}(\sigma)]^{q-1}. \quad (8)$$

Consequently, we have

$$x_n = \frac{e^{\beta J - \beta J h} x_{n-1}^{q-1} + e^{-\beta J + \beta J h}}{e^{-\beta J - \beta J h} x_{n-1}^{q-1} + e^{\beta J + \beta J h}}. \quad (9)$$

Let us consider the case $n = 1$. We have (j is a given integer between 1 and q)

$$g_1(\sigma_0) = \sum_{\sigma_1^{(j)}} e^{\beta J \sigma_0 \sigma_1^{(j)} + \beta J h \sigma_1^{(j)}}, \quad (10)$$

which is equivalent to (8) if we define $g_0(\pm) = 1$.

(e) Express the local magnetization $\langle \sigma_0 \rangle$ as a function of x_n .

: The local magnetization is given by

$$\langle \sigma_0 \rangle = \sum_{\{\sigma\}} \sigma_0 P(\{\sigma\}), \quad (11)$$

which, using (2), reads as

$$\langle \sigma_0 \rangle = \frac{\sum_{\{\sigma\}} \sigma_0 e^{\beta J h \sigma_0} \prod_{j=1}^q Q_n(\sigma_0 | \{\sigma\}^{(j)})}{\sum_{\{\sigma\}} e^{\beta J h \sigma_0} \prod_{j=1}^q Q_n(\sigma_0 | \{\sigma\}^{(j)})}. \quad (12)$$

This can be rewritten in a compact form using the definition of g_n and x_n as follows:

$$\langle \sigma_0 \rangle = \frac{\sum_{\sigma_0} \sigma_0 e^{\beta J h \sigma_0} [g_n(\sigma_0)]^q}{\sum_{\sigma_0} e^{\beta J h \sigma_0} [g_n(\sigma_0)]^q} = \frac{-e^{-\beta J h} [g_n(-)]^q + e^{\beta J h} [g_n(+)]^q}{e^{-\beta J h} [g_n(-)]^q + e^{\beta J h} [g_n(+)]^q} = \frac{-e^{-\beta J h} x_n^q + e^{\beta J h}}{e^{-\beta J h} x_n^q + e^{\beta J h}}. \quad (13)$$

In conclusion, the magnetization is unequivocally determined by the value of x_n .

(f) What happens in the thermodynamic limit $n \rightarrow \infty$? Does the model exhibit ferromagnetism?

: In order to compute the magnetization in the thermodynamic limit, we must determine $x_\infty = \lim_{n \rightarrow \infty} x_n$. This corresponds to a fixed point of the equation (cf. (9))

$$x = f(x) = \frac{e^{\beta J - \beta J h} x^{q-1} + e^{-\beta J + \beta J h}}{e^{-\beta J - \beta J h} x^{q-1} + e^{\beta J + \beta J h}}. \quad (14)$$

Specifically, it is the point reached applying iteratively the equation starting from $x = x_0 = 1$. First, we note that $x = 1$ is a fixed point for $h = 0$. Let us then consider the behavior in the limit of weak field. If (14) has only one solution, from the schematic plot of the function, we realize that the fixed point is stable ($f'(1) < 1$). On the other hand, the fixed point is not stable if $f'(1) > 1$ (in that case there must be more solutions, in particular, three). If the fixed point is not stable, x_∞ will depend on the sign of h , even in the limit $h \rightarrow \infty$. This is the signature of ferromagnetism. To see it clearly, we can reinterpret (14) as a condition that gives h for given x :

$$2\beta J h(x) = \log\left(\frac{e^{2\beta J} - x}{e^{2\beta J} x - 1} x^{q-1}\right). \quad (15)$$

Since the exponential on the left hand side is positive, x must be in the interval $(e^{-2\beta J}, e^{2\beta J})$. Let us now differentiate the equation with respect to $\log x$. We find

$$2\beta J x h'(x) = q - 1 - \frac{2 \sinh(2\beta J)}{2 \cosh(2\beta J) - x - 1/x}. \quad (16)$$

If β is large enough, $2\beta J x h'(x)$ is positive for $x \approx 1$ and approaches $-\infty$ for $x \rightarrow e^{\pm 2\beta J}$. In addition, from (15) it follows that $h(1) = 0$. Thus, there must be another value of $x \neq 1$ where $h(x) = 0$.

(g) Show that there is a phase transition ($q > 2$) and compute the critical temperature.

: This could be solved by identifying the temperature at which $2\beta J x h'(x)$ changes sign. Alternatively, one can compute $f'(1)$. This is given by

$$f'(1) = (q-1) \frac{\sinh(2J\beta)}{1 + \cosh(2(1+h)J\beta)}. \quad (17)$$

The critical temperature corresponds to the solution to the equation $f'(1) = 1$ for $h = 0$

$$(q-1) \sinh(2J\beta_c) = 1 + \cosh(2J\beta_c) \Rightarrow e^{2J\beta_c} = \frac{q}{q-2}, \quad (18)$$

where we have taken the unique positive solution to the equation for $e^{2J\beta_c}$. If $q > 2$, the critical temperature is finite, so there is a finite-temperature phase transition.

- (h) Expand around the critical temperature and show that, in the limit of small h and temperature close to the critical one, the magnetization $\langle \sigma_0 \rangle$ satisfies

$$\beta J h = \langle \sigma_0 \rangle^3 b\left(\frac{T - T_c}{T_c \langle \sigma_0 \rangle^2}\right), \quad (19)$$

where

$$b(x) = \frac{1}{2}(q-2)x \log \frac{q}{q-2} + \frac{(q-1)(q-2)}{3q^2}. \quad (20)$$

Which are the values of the critical exponents β and δ ?

- : We consider the model at inverse temperature $\beta < \beta_c$ close to the inverse critical temperature. For small h , x is close to 1, and it is convenient to parametrize it as $x = e^{-2s}$, with s close to 0. By series expanding (15) around $s = 0$ we find

$$\beta J h(e^{2s}) = [\coth(\beta J) - q + 1]s + \frac{1}{3} \frac{\cosh(\beta J)}{\sinh^3(\beta J)} s^3 + O(s^5). \quad (21)$$

At temperature close to the critical temperature, $t = \beta^{-1}\beta_c - 1 \approx 0$, therefore we can expand the expressions in the limit of small t . We easily find

$$\beta_c J h(e^{2s}) = q(q-2) \left[\beta_c J t s + \frac{1}{3}(q-1)s^2 + O(t^2 s, t s^3, s^5) \right]. \quad (22)$$

From (13) the magnetization is given by

$$\langle \sigma_0 \rangle = \tanh(\beta J h + q s). \quad (23)$$

From (22) we see that h is much smaller than s (the leading term is multiplied by t), thus we have

$$s = q^{-1} \langle \sigma_0 \rangle + O(h, \langle \sigma_0 \rangle^3). \quad (24)$$

Plugging this into (22) gives

$$\beta J h(e^{2s}) = \langle \sigma_0 \rangle^3 b(t / \langle \sigma_0 \rangle^2) + O(t^2 \langle \sigma_0 \rangle, t \langle \sigma_0 \rangle^3, \langle \sigma_0 \rangle^5), \quad (25)$$

where $b(x)$ is given by (20).

The critical exponent β and δ can be extracted directly from this expression, indeed in general we have

$$\beta J h \sim \langle \sigma_0 \rangle | \langle \sigma_0 \rangle |^{\delta-1} \tilde{b}(t | \langle \sigma_0 \rangle |^{-\frac{1}{\beta}}), \quad (26)$$

for some scaling function $\tilde{b}(x)$. In conclusion, we find $\beta = \frac{1}{2}$ and $\delta = 3$.