Homework: Finite Size Scaling

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The Potts model is defines as

$$H(\{s_i\}) = -\frac{J}{2}\sum_{\langle ij\rangle}(2\delta_{s_is_j} - 1) - \sum_i h_{s_i} = H_J(\{s_i\}) + H_h(\{s_i\}) \tag{1}$$

where $s_i = 1, 2, ..., q$ takes q values and $J > 0$. The first part H_J is the two-body coupling term and H_h comes from external magnetic field. We focus on 2D case.

1 Generic questions

1) Can the free energy of a finite system be non-analytic ?

The free energy of a finite system is analytic. We know $F = -\frac{1}{\beta}\ln Z$, $Z = \sum_{\{s_i\}} e^{-\beta H(\{s_i\})}$ and the Hamiltonian is given in Eq.(1). In a finite system, the summation terms in the Hamiltonian is finite, thus the partition function Z is analytic and $\ln Z$ is analytic, making the free energy analytic. The problem of being non-analytic occurs when we take the thermodynamic limit by letting $N \to \infty$.

2) Do you expect the actual critical temperature of a finite dimensional system to be higher or lower than the one found with the mean-field approximation ?

The actual critical temperature of a finite dimensional system should be lower than that in the the mean-field approximation. Because in mean-field approximation of finite dimensional system, we neglect the fluctuations of the system, which tend to destroy the order, therefore making the mean-field critical temperature higher than the actual one. In the low-dimensional case, the effect of the fluctuations is significant, and the relative error caused by neglecting the fluctuations is large.

3) What's the degeneracy of the equilibrium state at $T < T_c$?

It's non-trivial to know the degeneracy of equilibrium state in general cases at $T < T_c$. Therefore, we first consider a simple case at $T = 0$. At $T = 0$, the system orders in one of the equivalent q equilibrium states and the degeneracy is given by $D = q$. At very low temperature, the system tend to have a majority of spins taking one of the q possible values, and a minority of spins taking the other $q-1$ possible values. Suppose there are $N-n$ spins taking one of the q values and n spins taking the other values ($n \ll N$), we give a very crude discussion of the degeneracy. First choose a value for the majority spins and there are q options, then choose the values for the rest spins and each has $(q-1)$ options, next randomly choose n sites in the lattice to accommodate the minority of spins and we have C_N^n options, therefore, the total degeneracy is given by $D = q(q-1)^n C_N^n$. For the cases where n is comparatively large (T is comparable with T_c), it's hard to know the degeneracy.

4) Which is the relation between the fluctuations of magnetisation and the linear magnetic susceptibility in an Ising model ? Derive it. How general is this ?

The relation between the fluctuations of magnetisation and linear magnetic susceptibility in the Ising model is given by

$$\chi = \frac{\partial \langle m \rangle}{\partial h} = \beta N(\left\langle m^2 \right\rangle - \langle m \rangle^2) \tag{2}$$

To derive it, we first write the definition of magnetisation

$$\langle m \rangle = \frac{1}{Z} \sum_{\{s_i\}} (\frac{1}{N} \sum_i s_i) e^{-\beta H(\{s_i\})} \tag{3}$$

with

$$H(\{s_i\}) = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i \tag{4}$$

Susceptibility is therefore given by

$$\begin{aligned}
\chi &= \left.\frac{\partial \langle m \rangle}{\partial h}\right|_{h\to 0} = \frac{\partial}{\partial h} \frac{1}{Z} \sum_{\{s_i\}} (\frac{1}{N} \sum_i s_i) e^{-\beta H(\{s_i\})} \\
&= \frac{\frac{\partial}{\partial h} \sum_{\{s_i\}} (\frac{1}{N} \sum_i s_i) e^{-\beta H(\{s_i\})}}{Z} - \frac{(\sum_{\{s_i\}} (\frac{1}{N} \sum_i s_i) e^{-\beta H(\{s_i\})}) \frac{\partial Z}{\partial h}}{Z^2} \\
&= \frac{\sum_{\{s_i\}} (\beta \sum_i s_i)(\frac{1}{N} \sum_i s_i) e^{-\beta H(\{s_i\})}}{Z} - \frac{(\sum_{\{s_i\}} (\frac{1}{N} \sum_i s_i) e^{-\beta H(\{s_i\})})(\beta \sum_{\{s_i\}} (\sum_i s_i) e^{-\beta H(\{s_i\})})}{Z^2} \\
&= \beta N(\left\langle m^2 \right\rangle - \langle m \rangle^2)
\end{aligned} \tag{5}$$

Note that the average value $\langle m \rangle$ and $\langle m^2 \rangle$ is calculated by setting $h \to 0$, which is independent of applied field.

This relation is also known as **fluctuation-dissipation theorem**, which is very general and model independent. It can be derived without knowing the specific form of the Hamiltonian H and only relies on the assumption of equilibrium.

5) Which is the relation between the fluctuations of the energy and the heat capacity ? Derive it.

The relation between the heat capacity and energy fluctuations is given by

$$C = \frac{\partial \langle E \rangle}{\partial T} = \frac{1}{k_B T^2}(\left\langle E^2 \right\rangle - \langle E \rangle^2) = \frac{1}{k_B T^2}\Delta^2 \langle E \rangle \tag{6}$$

For a system at thermal equilibrium with a reservoir at temperature T, the average energy of the system is

$$\langle E \rangle = \frac{1}{Z}\sum_{\mathcal{C}} E(\mathcal{C})e^{-\beta E(\mathcal{C})} \tag{7}$$

where the summation is taken over all the possible microscopic configurations $\mathcal{C}$.

Then following the definition of heat capacity (magnetic field is fixed), we obtain

$$\begin{aligned} C &= \frac{\partial \langle E \rangle}{\partial T} = \frac{\partial}{\partial T}\frac{\sum_{\mathcal{C}} E(\mathcal{C})e^{-\beta E(\mathcal{C})}}{Z} \\ &= \frac{\frac{\partial}{\partial T}\sum_{\mathcal{C}} E(\mathcal{C})e^{-\beta E(\mathcal{C})}}{Z} - \frac{\sum_{\mathcal{C}} E(\mathcal{C})e^{-\beta E(\mathcal{C})}\frac{\partial Z}{\partial T}}{Z} \\ &= \frac{1}{k_B T^2}[\frac{1}{Z}\sum_{\mathcal{C}} E(\mathcal{C})^2 e^{-\beta E(\mathcal{C})} - (\frac{1}{Z}\sum_{\mathcal{C}} E(\mathcal{C})e^{-\beta E(\mathcal{C})})^2] \\ &= \frac{1}{k_B T^2}(\left\langle E^2 \right\rangle - \langle E \rangle^2) = \frac{1}{k_B T^2}\Delta^2 \langle E \rangle \end{aligned} \tag{8}$$

which connects the heat capacity and energy fluctuations.

The relation above can also be written in terms of energy density $\langle e \rangle = \langle E \rangle / N$

$$c = \frac{\partial \langle e \rangle}{\partial T} = k_B \beta^2 N(\left\langle e^2 \right\rangle - \langle e \rangle^2) \tag{9}$$

The derivation is similar and thus not shown here.

2 The $q = 2$ (Ising case)

Now we focus on the $q = 2$ case. Potts model, whose Hamiltonian is given by Eq.(1), should be equivalent to Ising model. Note that we put a coefficient **2** in front of $\delta_{s_i s_j}$ so that it matches the Hamiltonian in the Ising model. When s_i and s_j is equivalent, $2\delta_{s_i s_j} - 1$ gives 1; otherwise, $2\delta_{s_i s_j} - 1$ gives -1.

2.1 Data analysis

1) Use the information about the energy density given in the datafile to deduce whether the contributions $s_i s_j$, with i and j nearest neighbours on the lattice, are summed once or twice.

From the Hamiltonian in Eq.(1), we know that the system favors ferromagnetism at low temperature with a majority of sites taking the same spin. Therefore, at very low temperature and zero magnetic field, the energy of the system is approximately given by

$E_0 = -\frac{J}{2}\sum_{\langle i,j\rangle} 1 = -\frac{J}{2}\sum_i \sum_{j\in\partial i} 1 = -\frac{J}{4}Nz = -\frac{Jz}{4}L^2$. Set $J = 1$, the energy density $e = \frac{E}{L^2}$ and we obtain $-e_0 = \frac{z}{4}$, where z is the coordination number of each lattice site.

From data files $OUT2dL\#Th0$, we can read the energy density $(-e)$ and magnetization (m) at $T = 0.56729633$ for systems with different sizes. The magnetisations of the four systems are all approximately 1, which implies that the systems at such temperature are indeed well ferromagnetic. The energy density $-e$ is given by 1.99, which indicates that the coordination number z is equal to 8 instead of 4 as we usually have in the 2D Ising model. This indicates that we count the nearest neighbour interactions twice for each site, therefore, **the nearest neighbour interactions are summed twice.**

2) Plot the magnetisation density m as a function of temperature in the absence of magnetic field, for different values of the linear size L. Discuss the curves. If you guessed the critcal temperature T_c from them, would it be close to the exact value ?

We plot the magnetisation as a function of temperature for different sizes, as shown in Fig.(1). From the curves we know that magnetisation m decreases with increasing temperature. The decrease is becoming sharper and sharper with increasing size of the system. The non-analytic behavior of magnetisation in the vicinity of critical temperature is becoming more obvious with increasing system size because the finite-size effect is reduced.

Ideally at critical temperature, the derivative of m w.r.t T should diverge, therefore, we assume the temperature at which the curves is steepest is the critial temperature. It is determined and marked in the figure, with $T_c^{read} \approx 1.17$ (see the vertical green dashed line). The exact value of critical temperature is given by

$$k_B T_c = \frac{J}{\ln\left(1+\sqrt{q}\right)} \tag{10}$$

And we calculate $T_c^{exact} = 1.134$. The result we guess from the figure is not far from the exact value, with an error of 3%.

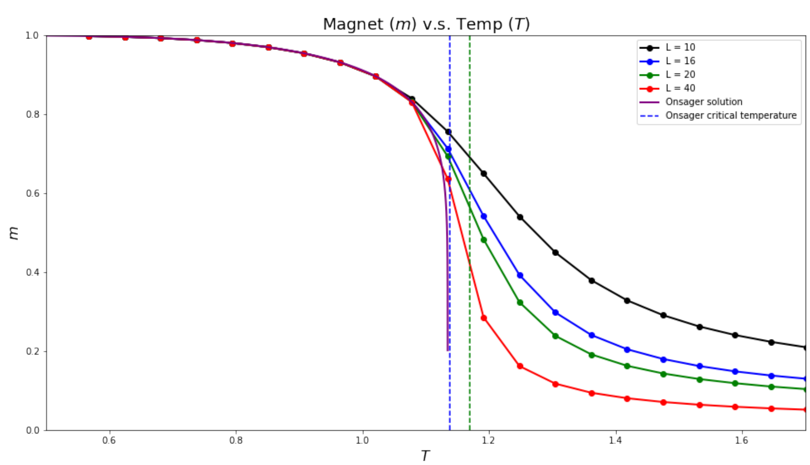
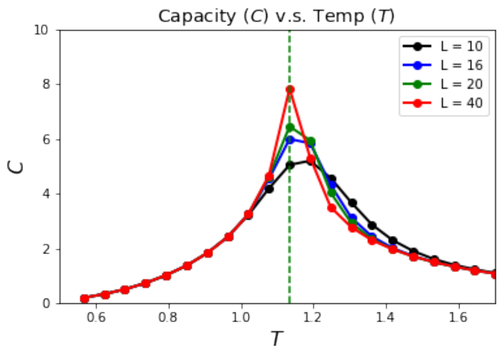
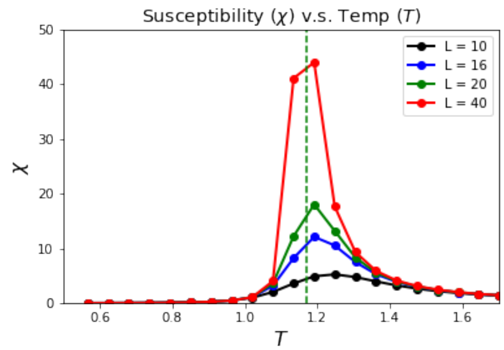


Figure 1: Magnetisation as a function of temperature for different sizes

More precisely, we can plot the susceptibility and capacity as a function of temperature for different sizes using the data in the data files. The expressions for susceptibility and capacity are given by Eq.(2) and Eq.(9) and the relevant curves are shown in Fig.(2). The peak positions in both figures gives the critical temperature. From capacity v.s. temperature figure we know the critical temperature is located at $T_c \approx 1.135$ and from susceptibility v.s. temperature figure we know the critical temperature is located at $T_c \approx 1.165$.



(a)



(b)

Figure 2: (a) Heat capacity v.s. temperature for different sizes; (b) Susceptibility v.s. temperature for different sizes

3) Write down the equation that determines the mean-field magnetisation density. What do you conclude about the mean-field critical temperature ?

Define the mean-field magnetisation density $m = \frac{1}{N}\langle|\sum_i s_i|\rangle$, which is slightly different from the defintion in the lectures, and follow the same procedure of mean-field approximation (we have a coupling $\frac{J}{2}$ instead of J), we arrive at

$$m = \tanh\left[\beta(Jzm/2 + h)\right] \tag{11}$$

Note that here $m \geq 0$. For $T > T_c^{MF}$ there is only one solution $m = 0$ and for $T < T_c^{MF}$ there are two solutions $m = 0$ and $m = m_1 > 0$ at zero magnetic field. We will only reserve the upper half plane in $m - T$ phase diagram.

For 2D Ising model, we know the critical temperature is given by $T_c^{MF} = 2$. As we discussed in Question 2, the mean-field critical temperature $T_c^{MF} = 2$ is much larger than the exact value $T_c = 1.134$. This is because we neglect the fluctuations of the system in mean-field approximation, which tend to destroy the order so that the order will be preserved at higher temperature in MFA. When $d = 2$, the effect of the fluctuations is significant, and the relative error caused by neglecting the fluctuations is large.

4) Find in the literature Onsager's expression for m and trace it in the same plot. Compare to the numerical data.

Onsager's expression for m is given by [1]

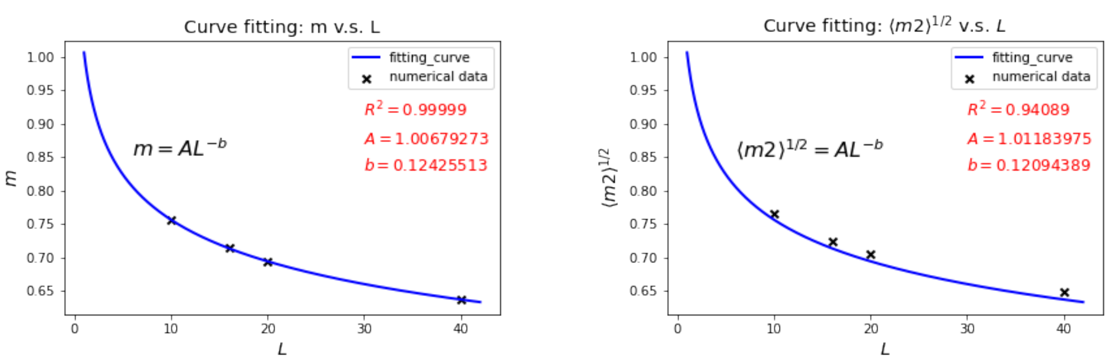
$$m(h=0,T)=\begin{cases}0, & T>T_c\\ \{1-(\sinh(2\beta J))^{-4}\}^{\frac{1}{8}}, & T<T_c\end{cases} \tag{12}$$

Note that in our model, we have to replace J by $J/2$. We plot it in the same figure as magnetisation v.s. temperature figure, i.e. Fig.(1), the purple line.

Comparing Onsager expression and the numerical data, we know that the exact critical temperature obtained from Onsager expression is slightly smaller than that we obtained before. Some long range fluctuations are not considered due to finite size, which pushes up the critical temperature. Furthermore, Onsager found that magnetisation is strictly 0 above critical temperature, which is consistent with the mean field solution and our common sense. But here numerical data curves exhibit a large tail due to finite size effects. The numerical data at low temperature is well consistent with Onsager expression, because the system is well ordered at low temperature and contains very few fluctuations, therefore finite size effects don't play an important role.

5) One can determine the ratio exponent β/ν from the relation $\langle m2\rangle^{1/2}(T_c)\sim L^{-\beta/\nu}$. We can also use the expression for m in the fourth column in the files since they have the absolute value. Plot $\langle m2\rangle^{1/2}$ or this m as a function of L and determine the exponent. Determine from Onsager's exact expression for m the exponent β in $d=2$. Compare to what you found with data analysis, setting $\nu=1$.

We plot m as a function of size L in Fig.(3a) and do the curve fitting. Following the same procedure, we plot $\langle m2\rangle^{1/2}$ as a function of size L in Fig.(3b) and do the curve fitting. The results are presented in the graph. The exponent β/ν is given by 0.124 in the left graph and 0.121 in the right one. 0.124 is more convincing because the curve fitting is better ($R^2=0.99999$).



(a) (b)

Figure 3: (a) Curve fitting for m v.s. L; (b) Curve fitting for $\langle m2\rangle^{1/2}$ v.s. L

Using Onsager's exact expression for m (see Eq.(12), we can deduce the critical exponent β using $m\sim(\frac{T_c-T}{T_c})^{\beta}$. Let $-t=\frac{T_c-T}{T_c})^{\beta}$, we do the variable transformation from T to t and

[1] Kerson Huang, Statistical mechanics, John Wiley & Sons, p391

the expression is given by

$$m(h=0,T) = [1-(\sinh\frac{1}{T})^{-4}]^{1/8} = [1-\sinh(\frac{1}{T_c}\frac{1}{1-(-t)})^{-4}]^{1/8} \tag{13}$$

Note that

$$\begin{aligned}\sinh(\frac{1}{T_c}\frac{1}{1-(-t)}) &= \frac{1}{2}(e^{\frac{1}{T_c}\frac{1}{1-(-t)}} - e^{-\frac{1}{T_c}\frac{1}{1-(-t)}})\\ &= \frac{1}{2}[(1+\sqrt{2})^{1+(-t)+(-t)^2+...} - (\sqrt{2}-1)^{1+(-t)+(-t)^2+...}]\\ &= \frac{1}{2}[(1+\sqrt{2})(1+\ln(1+\sqrt{2})((-t)+(-t)^2+...)+O(((-t)+(-t)^2+...)^2))\\ &\quad -(\sqrt{2}-1)(1+\ln(\sqrt{2}-1)((-t)+(-t)^2+...)+O(((-t)+(-t)^2+...)^2))]\\ &= 1+\alpha(-t)+O(t^2)\end{aligned} \tag{14}$$

where $\alpha = \frac{(1+\sqrt{2})\ln(1+\sqrt{2})-(\sqrt{2}-1)\ln(\sqrt{2}-1)}{2} \approx 1.2464$.

Then we have

$$\begin{aligned}m(h=0,-t) &= [1-\sinh(\frac{1}{T_c}\frac{1}{1-(-t)})^{-4}]^{1/8}\\ &= [1-(1+\alpha(-t)+O(t^2)^{-4}]^{1/8}\\ &= [1-1+4\alpha(-t)+O(t^2)]^{1/8}\\ &\sim (-t)^{1/8}\end{aligned} \tag{15}$$

Therefore, the critical exponent is given by $\beta = 0.125$. Setting $\nu = 1$, we obtain $\beta/\nu = 0.125$. The exact result obtained here is quite close to the result obtained using data analysis.

6) Make the scaling plots for the magnetisation densities close to the critical point, with $t = (T - T_c)/T_c$.

In this question, we first do some derivations about the finite size corrections of magnetisation density near the critical point. First we know that $m \sim t^\beta$ and correlation length $\xi \sim t^{-\nu}$, which indicate that $m \sim \xi^{-\beta/\nu}$. However, near the critical point the correlation length ξ tends to infinity and the size of the system $L \ll \xi$, which leads to finite size effects. Therefore, near critical point $m \sim L^{-\beta/\nu}$ and $t \sim L^{-1/\nu}$. We can define a scaling variable $m' = mL^{\beta/\nu}$ and $t' = tL^{1/\nu}$, and assumably we have scaling invariance near the critical point, i.e. $m' = t'^\beta$. To verify this, one should plot $m' = mL^{\beta/\nu}$ as a function of $t' = tL^{1/\nu}$ and check if the critical exponent remains unchanged with the new scaling variable.

We plot $mL^{\beta/\nu}$ as a function of $tL^{1/\nu}$ in Fig.(4). Here we use the fitting parameters from the last question by setting $\beta = 0.124$ and $\nu = 1$. The four curves coincide very well around critical temperature, which means that the finite size effect is eliminated by doing the scaling.

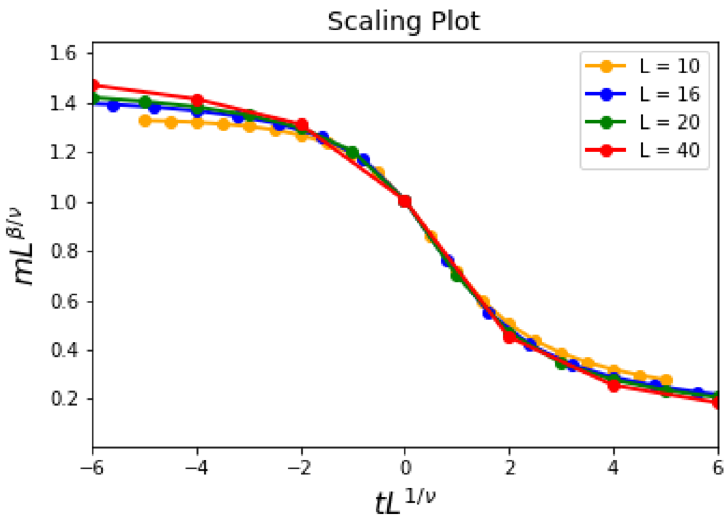


Figure 4: Scaling plot for magnetisation density

7) Consider now the applied field dependence of the magnetisation in the Ising model in $d = 2$. Confront the numerical data for $m(h)$ to the mean field predictions and to Onsager's result. Which one represents better the data? Think about using a double logarithmic representation to make the algebraic dependence easy to visualize.

We plot $\ln m$ as a function of $\ln h$ for different sizes L in Fig.(5). For $L = 16, 20, 40$, one can observe very good linear relations. Linear fitting results are given in the graphs. We know that fitting parameter δ obtained from systems with different sizes are given by 14.88, 14.79, 15.43, which is close to 15, as indicated by Onsager's result.

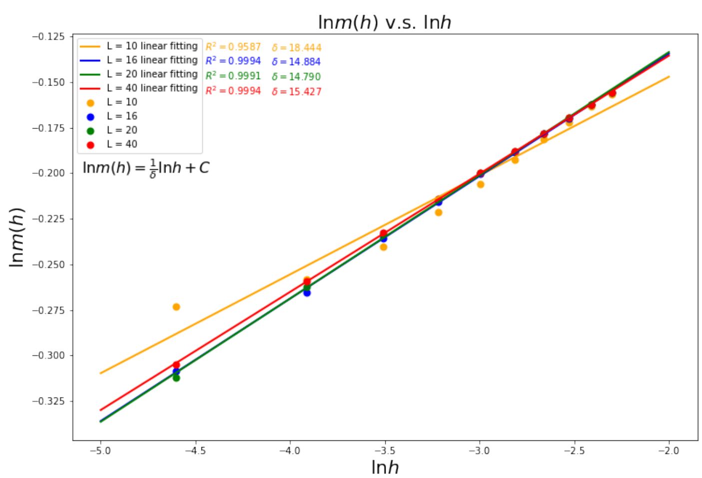


Figure 5: $\ln m(h)$ as a function of $\ln h$ for different sizes and linear fitting

8) Use now the more detailed data in the critical region that you can find in the files. Make

plots of the linear magnetic susceptibility in the $2d$ model using the data. Do you see the expected qualitative behaviour?

Imagine that the maximum value in this plot scales as

$$\chi_{max}(L) \propto (T_c(L) - T_c(L \to \infty))^{-\gamma} \propto L^{\gamma/\nu} \tag{16}$$

where $T_c(L \to \infty)$ is here a fitting parameter to be compared later to Onsager's exact value. Proceed as follows:

(a) Apply some smoothing of the data;

(b) Estimate the pair $(T_c(L), \chi_{max}(L))$ for each L, where $T_c(L)$ is the position of the maximum and $\chi_{max}(L)$ the height at the maximum;

(c) Make a power law fit of the maximum location $T_c(L) = T_c(L \to \infty) - cL^{-1/\nu}$ and find estimates for the infinite size T_c and the exponent ν;

(d) Get γ from $\chi_{max} \sim L^{\gamma/\nu}$;

(e) Compare all values with Onsager's exact ones.

The linear susceptibility χ is plotted as a function of T using more detailed data, as shown in Fig.(6). Note that we have already plotted χ v.s. T in Fig.(2b), but this one has more data, thus being more precise. We use spline interpolation to obtain a smooth curve for these four systems and obtain relevant peak positions and peak heights, which are indicated in the figure. Note that for $L = 10$ system the peak is not very evident, but it can be seen clearly if one zooms in.

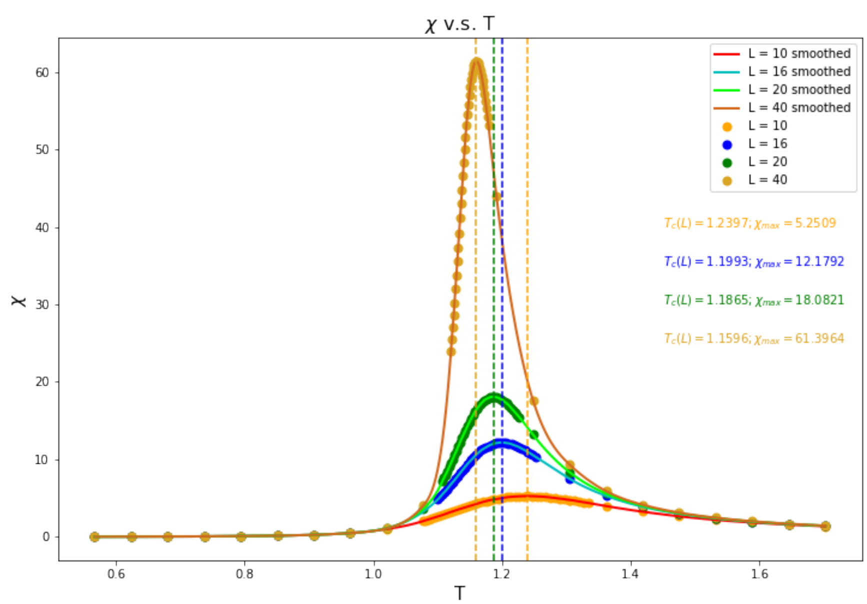


Figure 6: Linear susceptibility χ as a function of T for different sizes (Numerical data are plotted in circles and the curve is smoothed using spline interpolation).

The qualitative behavior is quite understandable. First we observe a shift in the position of the maximum, which corresponds to the finite size critical temperature, namely $T_c(L)$ –

$T_c(L \to \infty)$ decreases with L. Second, the width of the peak (L) decreases with L. Third, the peak height $\chi_{max}(L)$ increases with L.

In finite size system, the behavior of physical quantities is analytic, even at the critical point. Therefore, we will not see the divergence behavior but only a peak. Near critical point, we know in principle $\chi \sim \xi^{\gamma/\nu}$, with correlation length $\xi \to \infty$. In finite size system, $\chi \sim L^{\gamma/\nu}$, which explains that χ_{max} increases with L. Critical temperature decreases with increasing L, because more fluctuations will be included and order is more easily to be destroyed. Besides, the larger the system, the more exact the critical behavior will be. Therefore, we will have smaller and smaller peak width, which finally leads to divergence behavior.

Peak positions and peak heights are given in the figure above. Thus, we can make a power law fit of the maximum location $T_c(L) = T_c(L \to \infty) - cL^{-1/\nu}$. The fitting result is that

$$\nu = 0.9926, \quad T_c(L \to \infty) = 1.133, \quad c = -1.0812 \tag{17}$$

with $R^2 = 0.99995$.

Then we fit $\chi_{max} = AL^{\gamma/\nu}$ with $\nu = 0.9926$, the fitting result is $\gamma = 1.7529$ with $R^2 = 0.99999$.

All the fitting result is given in Tab.(1). One can find that these two match very well.

Parameters	Onsager's exact values	fitting results
T_c	1.134	1.133
ν	1	0.9926
γ	1.75	1.7529

Table 1: Fitting results and Onsager's exact results

9) How would you exploit the data in the files to find the exponent α?

First, it's tricky to use the relation between critical exponents to calculate the value of α. Since that we already know $\nu = 0.9926$ from Tab.(1). Using Josephson's identity $2-\alpha = \nu d$, we obtain $\alpha = 0.0148$, which is of course close to Onsager's exact value $\alpha = 0$.

Besides, we could follow the same procedure as Question (8) to determine α. First plot heat capacity C as a function of T for systems with different sizes and carry out smoothing using spline interpolation, as shown in Fig.(7a). The peak positions and height are indicated in the figure.

One could observe similar characteristic as question (8). First, the critical temperature decreases with size L; second, the peak height increases with size L; third, the width of the peak decreases with size L. The explanation is similar as above.

We know that $C \sim |T-T_c|^{-\alpha}$ and $\xi \sim |T-T_c|^{-\nu}$ near critical point, therefore, $C \sim \xi^{\alpha/\nu}$. Due to the finite size, we have $C \sim L^{\alpha/\nu}$.

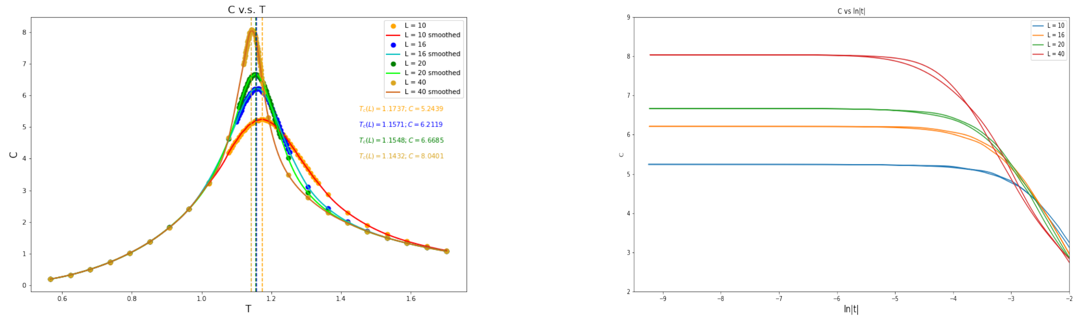
First, we make a power law fit of the maximum location $T_c(L) = T_c(L \to \infty) - cL^{-1/\nu}$. The fitting result is that

$$\nu = 0.9771, \quad T_c(L \to \infty) = 1.134 \tag{18}$$

with $R^2 = 0.9561$.

Then we fit $C_{max} = AL^{\alpha/\nu}$ with $\nu = 0.9771$. The fitting result is $\alpha = 0.299$ with $R^2 = 0.993$.

But we know that Onsager's exact solution gives $\alpha = 0$. There must be something hidden in the data set that we haven't found yet.



(a) (b)

Figure 7: (a) Heat capacity C as a function of T for different sizes, curves smoothed using spline interpolation (peak positions and peak heights are given in the figure); (b) Heat capacity C as a function of $\ln|t|$ for different sizes.

We searched some literatures and found that [2] the behavior near the critical point of the heat capacity given by Onsager is

$$C \approx -Nk_B \frac{1}{\pi}(\frac{2J}{k_B T_c})^2 \ln|1 - \frac{T}{T_c}| \tag{19}$$

Denote $\frac{T-T_c}{T_c} = t$, we obtain $C \sim -\ln|t|$ near the critical point. To capture this feature, we plot heat capacity C as a function of $\ln|t|$ using the smooth data by setting $t = \frac{T-T_c(L)}{T_c}$ for different sizes, as shown in Fig.(7b). It can be observed that near the critical temperature ($|t| \to -\infty$) capacity C do not vary with $\ln|t|$, which suggests that $C \sim -\ln|t|$.

To determine critical exponent α, we write $C \sim |t|^{-\alpha} \sim -\ln|t|$. Therefore, $\alpha = \lim_{t\to 0} -\frac{\ln(-\ln|t|)}{\ln|t|} = 0$. Finally, we obtain critical exponent $\alpha = 0$, which is consistent with the exact value.

2.2 The Binder cumulant

Assume that for **finite but large** L the distribution of fluctuating order parameter is

$$P_L(m) = \begin{cases} \frac{L^{d/2}}{(2\pi k_B T \chi_L)^{1/2}} e^{\frac{-m^2 L^d}{2k_B T \chi_L}}, & T > T_c \\ \frac{L^{d/2}}{(2\pi k_B T \chi_L)^{1/2}} \frac{1}{2}[e^{\frac{-(m-\bar{m}_L)^2 L^d}{2k_B T \chi_L}} + e^{\frac{-(m+\bar{m}_L)^2 L^d}{2k_B T \chi_L}}], & T < T_c \\ L^{\beta/\nu} \bar{P}(mL^{\beta/\nu}, L/\xi), & T \sim T_c \end{cases} \tag{20}$$

[2] Onsager L. Crystal statistics. I. A two-dimensional model with an order-disorder transition. Physical Review, 1944, 65, 117.

with $\bar{m}_L = |\langle m \rangle|$. Note that here $|\langle m \rangle|$ corresponds to spontaneous magnetisation below critical temperature for infinite size systems, $|\langle m \rangle| \neq 0$.
1) Relate χ_L to the moments of m in the cases $T > T_c$ and $T < T_c$.

$T > T_c$, according to the probability distribution, which is a Gaussian located at $m = 0$ with variance $\sigma^2 = \frac{k_B T \chi_L}{L^d}$. We have

$$\begin{cases} \langle m \rangle_L = 0 \\ \langle m^2 \rangle_L = \sigma^2 = \frac{k_B T \chi_L}{L^d} \\ \langle m^3 \rangle_L = 0 \\ \langle m^4 \rangle_L = 3\sigma^4 = 3\frac{k_B^2 T^2 \chi_L^2}{L^{2d}} \end{cases} \tag{21}$$

χ_L is related to the second order moment $\langle m^2 \rangle_L$ by

$$\chi_L = \frac{\langle m^2 \rangle_L L^d}{k_B T} \tag{22}$$

$T < T_c$, the distribution is a combination of two Gaussian peaks positioned at $\bar{m}_L$ and $-\bar{m}_L$ with equal weight. It's not easy to find

$$\begin{cases} \langle m \rangle_L = 0 \\ \langle m^2 \rangle_L = \sigma^2 + \bar{m}_L^2 = \frac{k_B T \chi_L}{L^d} + \bar{m}_L^2 \\ \langle m^3 \rangle_L = \bar{m}_L^3 + 3\bar{m}_L \sigma^2 = \bar{m}_L^3 + 3\bar{m}_L \frac{k_B T \chi_L}{L^d} \\ \langle m^4 \rangle_L = 3\sigma^4 + 6\sigma^2 \bar{m}_L^2 + \bar{m}_L^4 = 3\frac{k_B^2 T^2 \chi_L^2}{L^{2d}} + 6\bar{m}_L^2 \frac{k_B T \chi_L}{L^d} + \bar{m}_L^4 \end{cases} \tag{23}$$

χ_L is related to the second order moment $\langle m^2 \rangle_L$ by

$$\chi_L = \frac{(\langle m^2 \rangle_L - \bar{m}_L^2) L^d}{k_B T} \tag{24}$$

2) Find the condition on $\bar{P}$ so that P at $T \sim T_c$ is normalized.

The general expression for $\bar{P}$ is not known, however, we can determine some conditions that such functions should satisfy. First write down the normalization condition

$$\int_{-\infty}^{\infty} dm L^{\beta/\nu} \bar{P}(m L^{\beta/\nu}, L/\xi) = 1 \tag{25}$$

Moreover we know under such probability distribution $\langle m \rangle_L = 0$ at $T \sim T_c$, therefore, we also have

$$\int_{-\infty}^{\infty} dm m L^{\beta/\nu} \bar{P}(m L^{\beta/\nu}, L/\xi) = 1 \tag{26}$$

Introduce a scaling parameter $m' = m L^{\beta/\nu}$, and note that when $T \sim T_c$, $L \ll \xi$ for large but finite L. Eq.(25) and Eq.(26) become

$$\begin{cases} \int_{-\infty}^{\infty} dm' \bar{P}(m', 0) = 1 \\ \int_{-\infty}^{\infty} dm' m' \bar{P}(m', 0) = 0 \end{cases} \tag{27}$$

Eq.(27) are the conditions that $\bar{P}$ should satisfy.

3) The functional form of the distribution close to T_c is generally not known. The possible deviations from the Gaussian are studied with kurtosis or Binder parameter which is defined as

$$U_L = 1 - \frac{\langle m^4 \rangle_L}{3 \langle m^2 \rangle_L^2} \tag{28}$$

a) Evaluate U_L at high T using (5).

$T > T_c$, for large but finite L we can calculate the binder parameter using Eq.(21)

$$U_L = 1 - \frac{\sigma^4}{3(\sigma^2)^2} = 0 \tag{29}$$

which means that for large but finite size system, the binder parameter will be 0 when $T > T_c$.

For the systems with finite but not large L, the probability distribution is not given by a Gaussian distribution, therefore, U_L is not always 0. But as long as T is large enough, i.e. $T \to \infty$, $U_L \to 0$. The reason is as follows. For large T spins are correlated on a finite length ξ, and we can divide the system into small blocks of size ξ and assume no correlations between these blocks. The correlation length ξ decreases with increasing temperature so that the number of such spin blocks will increase. Then the system can be seen as the sum of a large number of independent identical variables, which by Central Limit Theorem (CLT) will give again a Gaussian distribution, therfore we still have $\lim_{T\to\infty} U_L \to 0$.

To sum up here, we know that $\lim_{T\to\infty} U_L = 0$ and $\lim_{L\to\infty} U_L = 0$.

b) Evaluate U_L at low T using (6).

$T < T_c$, for large but finite L we can calculate the binder parameter using Eq.(23)

$$U_L = 1 - \frac{3\sigma^4 + 6\sigma^2 \bar{m}_L^2 + \bar{m}_L^4}{3(\sigma^2 + \bar{m}_L)^2} = \frac{2\bar{m}_L^4}{3(\sigma^2 + \bar{m}_L^2)^2} \tag{30}$$

When $T \to 0$ or $L \to \infty$, $\sigma^2 = \frac{k_B T \chi_L}{L^d} \to 0$ and we have

$$\lim_{T\to 0} U_L = \frac{2}{3} \tag{31}$$

$$\lim_{L\to\infty} U_L = \frac{2}{3} \tag{32}$$

For small T (but not necessarily 0), we have

$$\begin{aligned} U_L &\approx 1 - \frac{\bar{m}^4 + 6\sigma^2 \bar{m}_L^2}{3(\sigma^2 + \bar{m}_L^2)^2} = 1 - \frac{1}{3}[1 + 6(\sigma/\bar{m}_L)^2][\frac{1}{(1 + (\sigma/\bar{m}_L)^2)^2}] \\ &\approx 1 - \frac{1}{3}[1 + 6(\sigma/\bar{m}_L)^2][1 - 2(\sigma/\bar{m}_L)^2] \approx \frac{2}{3} - \frac{4}{3}(\frac{\sigma}{\bar{m}_L})^2 = \frac{2}{3} - \frac{4}{3}\frac{\chi_L k_B T}{L^d \bar{m}_L^2} \end{aligned} \tag{33}$$

c) Find the scaling form of U_L close to T_c using (7).

Close to T_c we have

$$\left\langle m^2 \right\rangle_L = \int_{-\infty}^{\infty} dm m^2 L^{\beta/\nu} \bar{P}(mL^{\beta/\nu}, L/\xi) \tag{34}$$

$$\left\langle m^4 \right\rangle_L = \int_{-\infty}^{\infty} dm m^4 L^{\beta/\nu} \bar{P}(mL^{\beta/\nu}, L/\xi) \tag{35}$$

After some rescaling,

$$\left\langle m^2 \right\rangle_L = (L^{\beta/\nu})^{-2} \int_{-\infty}^{\infty} dm' m'^2 \bar{P}(m', L/\xi) \tag{36}$$

$$\left\langle m^4 \right\rangle_L = (L^{\beta/\nu})^{-4} \int_{-\infty}^{\infty} dm' m'^4 \bar{P}(m', L/\xi) \tag{37}$$

Therefore, we have

$$\begin{aligned} U_L &= 1 - \frac{\langle m^4 \rangle_L}{3 \langle m^2 \rangle_L} = 1 - \frac{\int_{-\infty}^{\infty} dm' m'^4 \bar{P}(m', L/\xi)}{3[\int_{-\infty}^{\infty} dm' m'^4 \bar{P}(m', L/\xi)]^2} \\ &= g_U(L/\xi) \end{aligned} \tag{38}$$

The scaling form of U_L close to T_c is given by $U_L = g_U(L/\xi)$, which is a function of L/ξ.

Note that $\xi \sim t^{-\nu}$ close to T_c, therefore, $U_L = g_U(L/\xi) = g_U(t^\nu L) = \tilde{g_U}(tL^{1/\nu})$.

d) Consider the case $T = T_c$ and take $\xi/L \to \infty$. Is there any L dependence of U_L left ?

When $T = T_c$ and the system has finite size L, it's easy to see $L/\xi \to 0$. Therefore, $U_L = g_U(L/\xi) \to g_U(0)$, which is independent of L. This indicates that the binder parameter U_L should be the same for any finite L at $T = T_c$. Therefore, we can determine the critical temperature by plotting binder parameter for different size's critical temperature is given by the intersection point.

e) In Fig.(8) we show the Binder parameter defined above for the $2d$ Ising model. Explain what you see.

In Fig.(8), we observe that:

- The binder parameter v.s. β curves for different sizes intersect at one point, which gives $\beta_c J \approx 0.44$, i.e. $T_c \approx 1.136$.
- U_L tends to approximately $2/3$ at low temperature (is equal to $2/3$ if $T = 0$) while tends to 0 at high temperature (is equal to 0 if we take the limit of $T \to \infty$) for a system with size L ($\forall$ L).
- When $T > T_c$, with symmetry unbroken, the Binder parameter decreases with increasing system size; while for $T < T_c$, in a symmetry breaking magnetic phase, U_L increases with L.

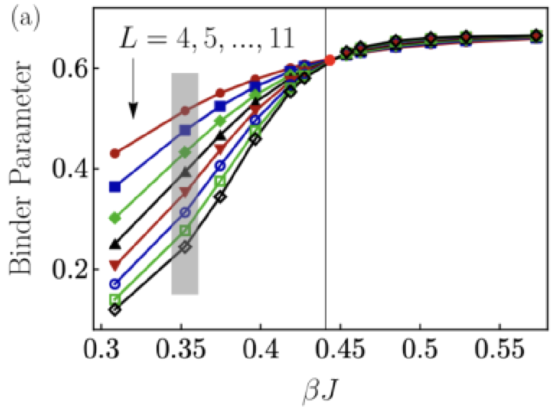


Figure 8: The Binder parameter for the $2d$ Ising model

The illustrations regarding the three observations are as follows:

1. As we argue in part (d), at critical temperature $T = T_c$, the Binder parameter $U_L = g_U(L/\xi) \to g_U(0)$ is size independent, therefore, all curves w.r.t. different sizes should have the same value, which suggests the intersection of these curves. Furthermore, the critical temperature read from the graph is given by 1.136, quite consistent with the exact value.

2. The second observation can be understood using the calculation result in part (a) and (b). For a system with size L, in part (a) we explain that $\lim_{T\to\infty} U_L = 0$ and for T large but not ∞, $U_L \neq 0$ because the distribution deviates from the Gaussian distribution. And in part (b) we explain that $\lim_{T\to 0} U_L = 2/3$.

3. First we consider a fixed small temperature $T < T_c$. According to Eq.(33) we have $U_L \approx \frac{2}{3} - \frac{4}{3}\frac{\chi_L k_B T}{L^d \bar{m}_L^2}$. Therefore, we know that U_L increases with L. Then we consider a fixed large temperature $T > T_c$, the correlation length ξ is finite and fixed. Use the same "coarse grain" argument, we divide the system (of size L) into block spins of size ξ (which is the correlation length of spins) and assume no correlation between different blocks. The large system can be seen as a sum of $(L/\xi)^d$ independent identical variables, which behaves more and more like the Gaussian distribution with increasing L. Thus U_L becomes closer and closer to 0 accordingly with increasing L.

3 The large q Potts model

We now turn to the study of the Potts model with large value of q, and we focus on its energy (in the absence of any applied field) and its statistical properties.

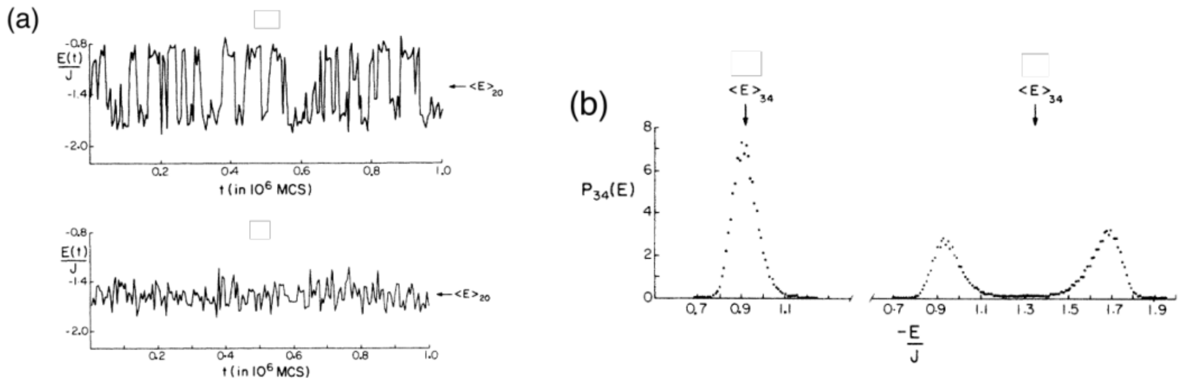


Figure 9: (a) The energy density of a $2d$ Potts model, on a square lattice with linear size $L = 20$, with $q = 10$ (above) compared to the one of a $q = 2$ case along two Monte Carlo runs (data every 5×10^3 MC steps are shown). (b) The histograms of the energy densities measured in a Monte Carlo simulation of the $q = 10$ Potts model with $L = 34$ away from its transition (left) and at the transition T_c. The averaged values are indicated.

1) Explain the results shown in the figure.

- From Fig.(9a) we observe that $q = 10$ Potts model has a larger mean value of internal energy and a larger variance of internal energy than those in the case $q = 2$ (keeping T and L the same). The minimum value of both models are approximately the same.
- From Fig.(9b) we observe that away from the transition T_c there is only one peak in the internal energy distribution, which evolve into two smaller peaks with a small gap when T approaches T_c.

Regarding the first observation, there will be more equilibrium configurations for systems with larger q at fixed temperature, which indicates that the entropy of the system is larger. Thus the energy fluctuations is larger for $q = 10$ Potts model. Besides, $q = 10$ Potts model has larger mean value of internal energy, possibly because the energy fluctuations in this model is larger than $q = 2$ model, and the probability to have larger energy is greater, leading to a larger mean value.

Regarding the second observation, the emergence of two peaks at critical temperature is due to the fact that large q ($q > 4$) Potts model experience a first order phase transition. Away from T_c (for $T > T_c$ or $T < T_c$) the energy of the system is mainly located around its mean value, while two phases, whose correlation lengths are both finite at T_c, will coexist at transition temperature, resulting in the two peaks in the distribution of energy density. The gap between these two peaks reflects the latent heat in the first order phase transition.

Remark: the following content is an additional part, which is not included in the first version .pdf file we submitted, but it indeed helps explain the first observation in a half-quantitative way.

We want to demonstrate that the mean value of the energy in the Potts model increases with larger q at a fixed temperature T. Treat the system in a mean field way and then the total energy is the sum of energy per site, with each site contributing the same energy. Now we just need to focus on the energy contribution of one site, which comes from the coupling between its 4 nearest neighbors and itself. The local mean field Hamiltonian is written as

$$H_{loc}^{eff} = H_i^{eff} = -J/2 \sum_{s_j, j \in \partial i} \delta_{s_i, s_j} + \text{const.} \tag{39}$$

where the summation is over all the nearest neighbors. Set $J = 1$ for simplicity.

The groundstate configurations of this effective local Hamiltonian are those in which the 4 nearest neighbors take the same spin as the local site. We denote this state as $|0\rangle$ with $E(|0\rangle) = -1/2 \times 4 = -2$ and degeneracy $D(|0\rangle) = q$. The probability to have such configurations is given by Boltzmann factor $P(|0\rangle) = e^{-\beta E(|0\rangle)} = e^{2\beta}$. The first excited state configurations are those in which one of the nearest neighbors takes a different spin from the local site and the other three take the same. We denote this state as $|1\rangle$ with $E(|1\rangle) = -1/2 \times 3 = -1.5$ and $D(|1\rangle) = q(q-1)C_4^1 \sim 4q^2$ (Note that C_4^1 appears because we need to choose one of the four neighbors to have a different spin). The probability to have such configurations is given by Boltzmann factor $P(|1\rangle) = e^{-\beta E(|1\rangle)} = e^{1.5\beta}$. Following the same procedure, the relevant quantities are calculated for the second, third, fourth excited states and the results are given in Tab.(2) below. Note that T is fixed, therefore, inverse temperature β is a constant and we set it to be 1 for simplicity.

States	E	D	P
$\|0\rangle$	-2	q	$e^{2\beta} \sim e^2$
$\|1\rangle$	-1.5	$4q^2$	$e^{1.5\beta} \sim e^{1.5}$
$\|2\rangle$	-1	$6q^3$	$e^{1\beta} \sim e^1$
$\|3\rangle$	-0.5	$4q^4$	$e^{0.5\beta} \sim e^{0.5}$
$\|4\rangle$	0	q^5	1

Table 2: Energy, degeneracy and probability of groundstate, first, second, third , fourth excited state configurations of the local effective Hamiltonian

Now we can calculate the mean value of energy

$$\langle e \rangle = \frac{\sum_i E(|i\rangle) P(|i\rangle) D(|i\rangle)}{\sum_i P(|i\rangle) D(|i\rangle)} \tag{40}$$

which gives

$$\langle e \rangle = \frac{-2qe^2 - 6q^2 e^{1.5} - 6q^3 e^1 - 2q^4 e^{0.5}}{qe^2 + 4q^2 e^{1.5} + 6q^3 e^1 + 4q^4 e^{0.5} + q^5} \tag{41}$$

Plot $\langle e \rangle$ as a function of q, as shown in Fig.(10), we notice that the mean value of energy density increases with q. Thus we provide a half-quantitative way to demonstrate that the mean value of the energy in the Potts model increases with larger q at a fixed temperature T using the mean-field treatment.

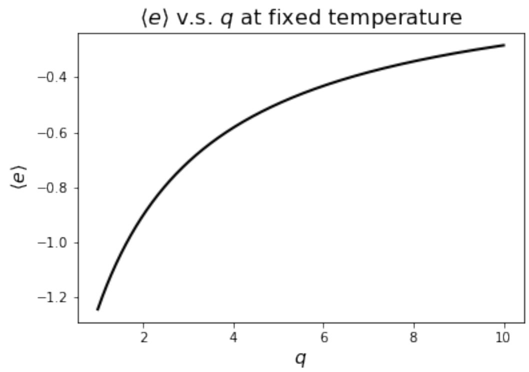


Figure 10: Mean energy density as a function of q at fixed temperature within mean-field approximation.