Advanced Statistical Physics

Homework: Finite Size Scaling

October 2022

This homework is intended to familiarize you with the use of the finite size scaling technique to characterize continuous and discontinuous phase transitions. It illustrates its application to data of the two dimensional Potts model.

The **Potts model** is defined as follows [1],

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

with the $= 1, \dots, N$ spins, s_i, taking q values, graphically represented as colors, $s_i = 1, \dots, q$. The coupling constant J is positive $J > 0$. The symbol $\delta_{s_i s_j}$ is a Kronecker delta. The constant subtracted from it ensures that the energy is the one of the Ising model for $q = 2$. The sum $\sum_{\langle ij\rangle}$ runs over nearest neighbours on a lattice with linear size L. For definiteness, we will focus on the two dimensional case. The magnetic field contributions h_{s_i} can be seen as acting (favouring) one of the q possible spin configurations.

We defined the two contributions to the Hamiltonian, $H_J(\{s_i\})$ from the two-body coupling, and $H_h(\{s_i\})$ from the magnetic field contribution, for later convenience.

Take this system in equilibrium with a thermal bath at inverse temperature $\beta = 1/(k_B T)$ and no applied field. On the square lattice, and in the infinite size limit there is a critical temperature at

$$k_B T_c = \frac{J}{\ln(1+\sqrt{q})} \tag{2}$$

which separates a high temperature paramagnetic phase, from a low temperature ordered phase. In the latter, the system orders in one of the equivalent q equilibrium states. Typical equilibrium low temperature configurations have a majority of spins taking one of the q possible values, and a minority taking the other $q-1$ values, and being due to thermal fluctuations. Equilibrium configurations above, at, and below the critical temperature of a $q = 3$ model are shown in Fig. 1.

The thermal phase transition - under no applied field - is continuous for $q = 2, 3, 4$ and discontinuous for $q > 4$. The case $q = 2$ boils down to the bidimensional Ising model.

We will apply the finite size scaling technique to analyse numerical Monte Carlo data for this model.

Many experimental realizations of this model are described in [1].

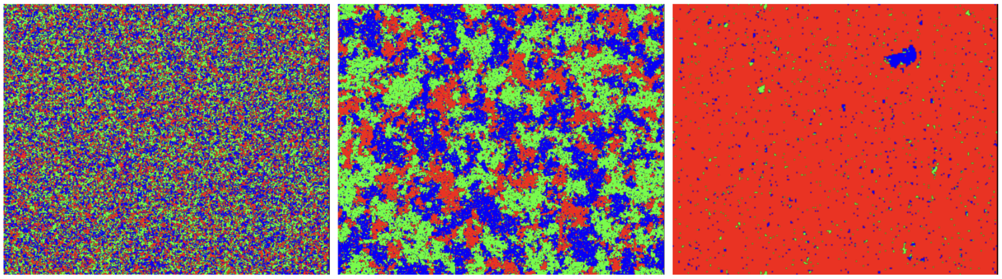

FIG. 1 – *Three typical equilibrium configurations of the $q = 3$ bidimensional Potts model above T_c (left), at T_c (center) and below T_c (right).*

1 Generic questions

We start with a series of general questions. Justify your answers.

1. Can the free-energy of a finite size system be non-analytic?
   no, it's the logarithm of a sum of a finite number of terms, each of them analytic with respect to β times the parameters in the Hamiltonian (J, h). More precisely, if there are no non-analyticities in the Hamiltonian, the Boltzmann factor $e^{-\beta H}$ is also analytic, and the $\ln Z$ is analytic too. .
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?
   MF usually over-estimates order, so $T_c^{\rm MF} > T_c$, with T_c the actual critical temperature of the finite dimensional model. An example is given by the $q = 2$ Ising case on the square lattice. From Eq. (2), $T_c = J/(1 + \sqrt{2})$ while $T_c^{\rm MF} = zJ = 4J$, which is higher than the previous one.
3. What is the degeneracy of the equilibrium state at $T < T_c$?
   q. Below T_c there is ferromagnetic order and there are q such choices.
4. Which is the relation between the fluctuations of the magnetisation and the linear magnetic susceptibility in an Ising model? Derive it. How general is this?
   FDT. Look at the lecture notes for a proof.
5. Which is the relation between the fluctuations of the energy and the heat capacity? Derive it.
   It is the equilibrium FDT again. Using $C_v = \partial \langle H \rangle / \partial T$ and $\langle H \rangle = -Z^{-1} \partial Z / \partial \beta$,
   $$C_v = \beta^2 \langle (H - \langle H \rangle)^2 \rangle = k_B \beta^2 \left(\langle H^2 \rangle - \langle H \rangle^2 \right)$$

2 The $q = 2$ (Ising case)

The data in `www.lpthe.jussieu.fr/~leticia/TEACHING/ICFP/Homework-2022` have been produced by M. Picco (LPTHE) using the Swendsen-Wang (two dimensional) cluster algorithms which allow one to speed up the Monte Carlo simulations close to the critical point, and equilibrate samples of much larger sizes than the single spin flip Monte Carlo codes. In the following we measure $k_B T$ in units of J or, equivalently, we set $J = 1$, and, furthermore, also $k_B = 1$.

The first two files have data for the Ising model ($q = 2$)

The $2d$IM at different T and $h = 0$	OUT2dL#Th0
The $2d$IM at different h and $T = T_c$	OUT2dL#Tch

The label # close to L means that the values of the system sizes, L, are placed there in the names of the files. For example, OUT2dL4Tch contains data for the model with linear size $L = 4$, at the (zero field) critical temperature, and under different applied fields.

The columns of OUT2dL#Th0 are organised as

$$L \qquad 1/\beta \qquad h \qquad m \qquad -e \qquad L^2\sigma_m^2 \qquad L^2\sigma_H^2 \qquad \#\,\text{samp}$$

and the ones of OUT2dL#Tch as

$$L \qquad 1/\beta \qquad h \qquad m \qquad -e_J \qquad -e \qquad \sigma_m^2 \qquad L^2\sigma_{H_J}^2 \qquad L^2\sigma_H^2 \qquad \#\,\text{samp}$$

with the definitions

$$\begin{aligned}
m &= \frac{1}{L^d}\left\langle \left| \sum_i s_i \right| \right\rangle , & m2 &= \left\langle \left(\frac{1}{L^d} \sum_i s_i \right)^2 \right\rangle , & \sigma_m^2 &= m2 - m^2 , \\
e_J &= \frac{1}{L^d} \langle \beta H_J(\{s_i\}) \rangle & e &= \frac{1}{L^d} \langle \beta H(\{s_i\}) \rangle & \sigma_{H_J}^2 &= e2_J - e_J^2 \\
e2_J &= \frac{1}{L^{2d}} \left\langle (\beta H_J(\{s_i\}))^2 \right\rangle & e2 &= \frac{1}{L^{2d}} \left\langle (\beta H(\{s_i\}))^2 \right\rangle & \sigma_H^2 &= e2 - e^2
\end{aligned} \tag{3}$$

samp gives the number of samples used to calculate the averages. Note that H has been multiplied by β in the definitions of e, e_J, $e2$ and $e2_J$.

The file OUTL#h0close zooms close to the thermal phase transition at zero field.

2.1 Data analysis

1. Use the information about the energy density given in the data-file OUT2dL#Th0 to deduce whether the contributions $s_i s_j$, with i and j nearest neighbours on the lattice, are summed once or twice.

   At zero temperature the value $-e = 2$ is approached. This means that $\frac{1}{2}\sum_{\langle ij \rangle} = \frac{1}{2}\sum_i \sum_{\partial i} 1$ with $\partial i = 1, \dots, z$ the coordination of the lattice. One recovers in this way $e = -\frac{1}{2} 4 = -2$. The energy density is measured in units of the coupling

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 these curves. If you guessed the critical temperature T_c from them, would it be close to the exact value in Eq. (1)?

   The plots are in Fig. 3 where we display the magnetisation density as a function temperature over the coupling strength, for several system sizes.

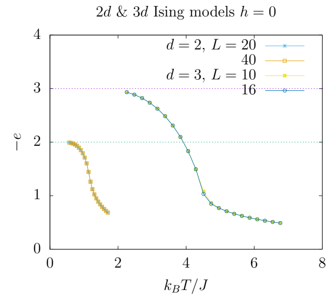

FIG. 2 – *Minus the energy density as a function of temperature over the coupling constant J.*

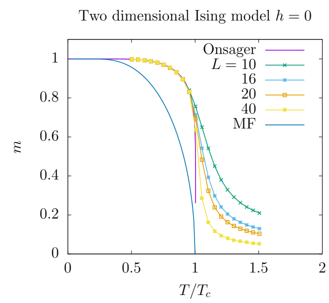

FIG. 3 – *The magnetisation density as a function temperature over critical temperature, for several system sizes, in the 2d. The Onsager exact solution is really close to the numerical data. The mean-field expression is quite far from it (it is better in three dimensions).*

The curves smoothly go from 1 at $T \sim 0$ to 0 at $T \gg J$. The change from the low-T to the high-T behaviour gets sharper for increasing L.

The guess for T_c would be very close $T_c = J/\ln(1+\sqrt{2}) \sim 1.13$, the exact value ($k_B = 1$).

3. Write down the equation that determines the mean-field magnetisation density (for the sum convention identified in the previous item). What do you conclude about the mean-field critical temperature?

   The mean-field equation predicts the critical temperature $k_B T_c/J = z = 4$, well above the values found in the simulation, which are very close to $T_c = 1/(1+\sqrt{2}) \sim 1.13$, the exact value. T_c is non-universal and depends on many details so the MF approximation cannot give it exactly in any finite d.

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

   Onsager's solution yields $m = [1 - \sinh^{-4}(\beta J)]^{1/8}$. The critical temperature is given by $[\sinh(\beta_c J)]^2 = 1$, and yields $T_c \sim 1.13$. The exponent $\beta = 1/8$ can be read from this expression after expanding close to the critical point.

In Fig. 3 we plot m against T/T_c. The numerical data are very close to the Onsager curve but quite far from the mean-field one, which is also shown in blue. We note that the larger L, the closer the data points are to the Onsager expression, something natural since the latter holds for $L \to \infty$.

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.

   Figure 4 investigates $m \sim L^{-\beta/\nu}$. The double logarithmic plot on the right demonstrates that $\beta/\nu = 1/8$, predicted by Onsager's solution represents the data very accurately. The mean-field $\beta/\nu = 1/2$ would have been completely off the data points.

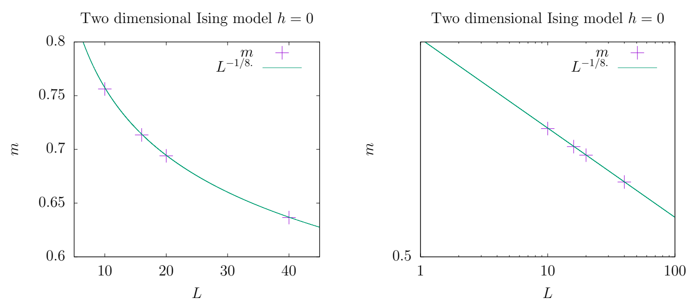

FIG. 4 – *The (absolute value of the) magnetization density at the critical temperature and zero field for four system sizes. The dependence $m \sim L^{-\beta/\nu}$ in linear scale and in double log scale.*

   Determine from Onsager's exact expression for m the exponent β in $d = 2$. Compare to what you found with the data analysis, setting $\nu = 1$.

   Just expanding $\beta = 1/8$.

6. Make the scaling plots for the magnetisation densities close to the critical point, with $t \equiv (T - T_c)/T_c$
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 visualise.
8. Use now the more detailed data in the critical region that you can find in the files called OUTL#h0close. Make plots of the linear magnetic susceptibility in the $2d$ model using the data in OUT2dL#Th0. Do you see the expected qualitative behaviour?
   Imagine that the maximum value in this plot scales as

$$\chi_{\max}(L) \propto (\beta_c(L) - \beta_c(L \to \infty))^{-\gamma} \propto L^{\gamma/\nu} \tag{4}$$

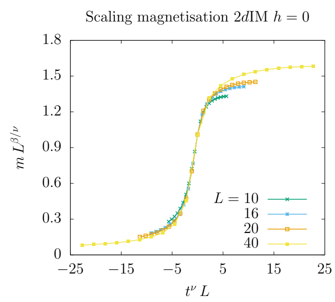

FIG. 5 – *Scaling plots of m. The critical temperature is $k_B T_c/J = 1.13$ and the exponents are $\beta = 1/8$ and $\nu = 1$.*

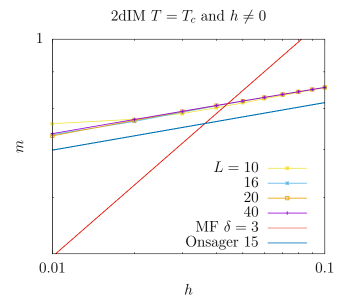

FIG. 6 – *Log-log plot of the magnetisation as a function of the applied magnetic field with the temperature held fixed at T_c. Comparison to mean-field and the Onsager result.*

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

(a) Apply some smoothing of this data (e.g. with gnuplot, the "smooth bezier" option to the "plot" command).

(b) Estimate the pair $(\beta_c(L), \chi_{\max}(L))$ for each L, where $\beta_c(L)$ 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 $\beta_c(L) = \beta_c(L \to \infty) - cL^{-1/\nu}$. This is a three parameter fit, $\beta_c(L \to \infty)$, c, ν, and serves to find estimates for the infinite size β_c and the exponent ν.

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

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

We read from the smooth $\chi(\beta,L)$ curves:

L	β_c	$\chi_{\max}$
10	0.77	5.10
16	0.81	9.12
20	0.82	11.81
40	0.85	23.36

Estimates $\beta_c(L \to \infty)$ to 0.88, which is in agreement with what we have from Onsager's solution, and $1/\nu$ to 0.87, which is not very precise, since $\nu = 1$ in Onsager's solution. Also from the $\chi_{\max}(L)$ plot $\gamma/\nu \sim 1.04$, while $\gamma = 1.23$ in Onsager's.

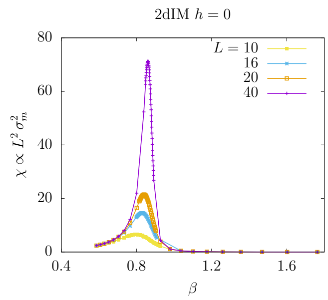

FIG. 7 – *The magnetisation fluctuations as a function of temperature with more details close to the transition in the 2d case.*

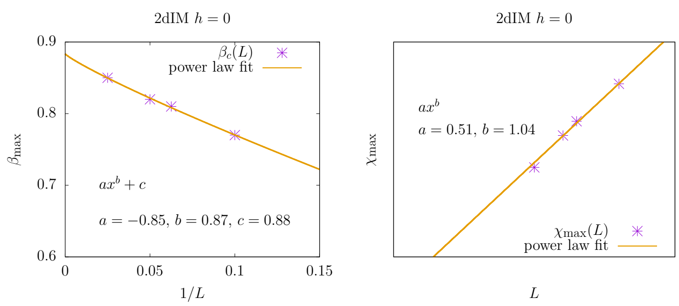

FIG. 8 – *The (β,χ) of the maximum as a function of L and their fits.*

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

   Using the FDT or else using the relation $\alpha + 2\beta + \gamma = 2$ between critical exponents. We have already estimated β and γ from the data, this equation then yields α.

2.2 The Binder cumulant

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

$$P_L(m) = \begin{cases} \dfrac{L^{d/2}}{(2\pi k_B T \chi_L)^{1/2}}\, e^{\frac{-m^2 L^d}{(2k_B T \chi_L)}} & T > T_c \quad (5) \\ \dfrac{L^{d/2}}{(2\pi k_B T \chi_L)^{1/2}} \left[\dfrac{1}{2}\, e^{\frac{-(m-\overline{m}_L)^2 L^d}{(2k_B T \chi_L)}} + \dfrac{1}{2} e^{\frac{-(m+\overline{m}_L)^2 L^d}{(2k_B T \chi_L)}} \right] & T < T_c \quad (6) \\ L^{\beta/\nu}\, \overline{P}(m L^{\beta/\nu}, L/\xi) & T \sim T_c \quad (7) \end{cases}$$

with $\overline{m}_L = |\langle m \rangle|$. These forms are a Gaussian centered at zero, two Gaussian centered at the (symmetric) mean values, and a form satisfying finite size scaling.

1. Relate χ_L to the moments of m in the cases $T > T_c$ and $T < T_c$.

   At $T > T_c$ the distribution is Gaussian with zero mean $\langle m \rangle = 0$. The variance is $\sigma^2 = \langle m^2 \rangle = k_B T \chi_L / L^d$
   At $T < T_c$ the distribution is a superposition of two Gaussian weights with the same variances but non-zero averages, with the same magnitude but different sign. The full distribution is symmetric with respect to $m \mapsto -m$. Thus the average of m vanishes. Of course, if one restricts the sum over m to only positive (or negative) values, then the result is not zero. In the $L \to \infty$ limit it approaches the typical value of m, the one at which the peak attains its maximum.
   The variance is $\sigma^2 = \langle m^2 \rangle = k_B T \chi_L / L^d + (\overline{m}_L)^2$

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

   $\int du\ \overline{P}(u,L/\xi) = 1$.

3. The functional form of the distribution close to T_c is in general not know, The possible deviations from the Gaussian are studied with the kurtosis or Binder parameter which is defined as

$$U_L \equiv 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2} \ . \tag{8}$$

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

   $U_L \sim L^{-d}$

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

   $U_L = 2/3$ (having already taken the limit $L \to \infty$)

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

   $U_L \sim 1 - \tilde{\chi}_4(L/\xi)/(\tilde{\chi}_2(L/\xi))^2$

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

   No. $U_L \sim 1 - \tilde{\chi}_4(0)/(\tilde{\chi}_2(0))^2$. Crossing of curves at T_c

   (e) In Fig. 9 we show the Binder parameter defined above for the $2d$ Ising Model. Explain what you see.

   The high T and low T limits found above are recovered. The curves cross at T_c where the L dependence disappears. This is a very useful method to determine T_c.

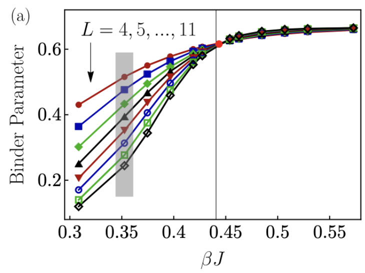

FIG. 9 – *The Binder parameter for the* 2*d Ising model.*

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.

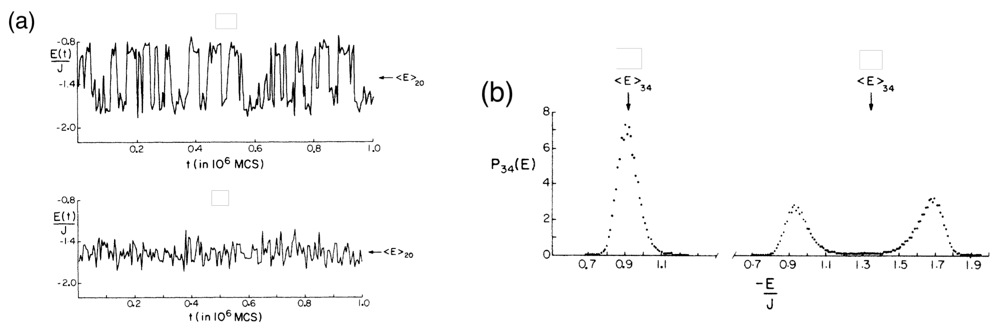

FIG. 10 – *(a) The energy density of a* 2*d Potts model, on a square lattice with linear size* $L = 20$, *with* $q = 10$ *(above) compared to the one of a* $q = 2$ *case along two Monte Carlo runs (data every* 5×10^3 *MC steps are shown). (b) The histograms of the energy densities measured in a Monte 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. Comment on Fig. 10.

   In (a) for $q = 10$ we see jumps between two values of the energy while for $q = 2$ there are only relatively small fluctuations around a single value. The histograms are shown in (b), where we see a single peak at high T representing the energy of the paramagnetic state and its fluctuations (approximately Gaussian). At the phase transition there are two peaks, one corresponds to the paramagnetic state while the other to an ordered state. The transition for q large is of first order and there is coexistence.