Advanced Statistical Physics

Homework: Finite Size Scaling

October 2023

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.

To be returned in **pdf format** by email to `leticia@lpthe.jussieu.fr` before the 12ve of November at 24:00.

Write clearly your **names** and **Master**.

We define the **Potts model** as follows [1],

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

with the $= 1, \ldots, N$ spins, s_i, taking q values, graphically represented as colors, $s_i = 1, \ldots, q$. The coupling constant J is positive $J > 0$. The symbol $\delta_{s_is_j}$ 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 $\beta = 1/(k_BT)$ and no applied field. Renaming $Jq \mapsto J$, on the square lattice, and in the infinite size limit there is a critical temperature at

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

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

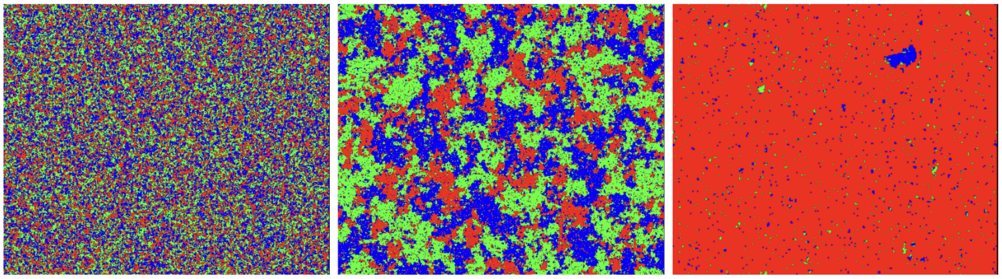

FIG. 1 – *Three typical equilibrium configurations of the $q = 3$ bidimensional Potts model above T_c (left), at T_c (center) and below T_c (right).*

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].

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?
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?
3. What is the degeneracy of the equilibrium state of the q Potts model at $T < T_c$?
4. Prove that the first term in the energy function (1) boils down to the Ising model one for $q = 2$. (Transform the s_i variables into Ising ones and re-write H_J conveniently to prove this statement.)
5. 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?
6. Which is the relation between the fluctuations of the energy and the heat capacity? Derive it.

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_BT 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 2dIM at different T and $h = 0$	OUT2dL#Th0
The 2dIM at different h and $T = T_c$	OUT2dL#Tc

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, OUT2dL4Tc 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#Tc 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 files OUTL#h0close zoom 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_is_j, with i and j nearest neighbours on the lattice, are summed once or 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 these curves. If you guessed the critical temperature T_c from them, would it be close to the exact value in Eq. (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?
4. Find in the literature Onsager's expression for m and trace it in the same plot. Compare to the numerical data.

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 the data analysis, setting $\nu = 1$.
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
   $$\chi_{\max}(L) \propto (\beta_c(L) - \beta_c(L \to \infty))^{-\gamma} \propto L^{\gamma/\nu} \tag{4}$$
   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.
9. How would you exploit the data in the files to find the exponent α?

2.2 The Binder cumulant

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

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

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 $T < T_c$.

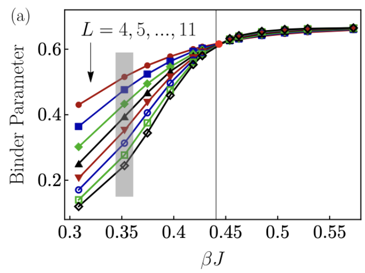

FIG. 2 – *The Binder parameter for the 2d Ising model.*

2. Find the condition on $\overline{P}$ so that P at $T \sim T_c$ is normalized.
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).
   (b) Evaluate U_L at low T using (6).
   (c) Find the scaling form of U_L close to T_c using (7).
   (d) Consider the case $T = T_c$ and take $\xi/L \to \infty$. Is there any L dependence of U_L left?
   (e) In Fig. 2 we show the Binder parameter defined above for the $2d$ Ising Model. Explain what you see.

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.

1. Explain the results shown in Fig. 3.

(a)

(b)

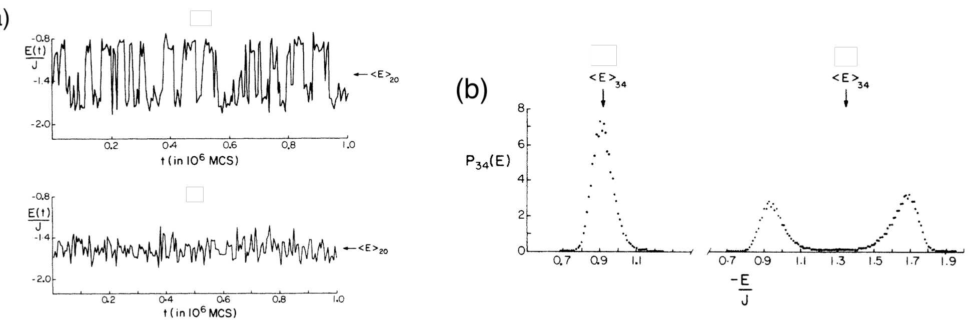

FIG. 3 – *(a) The energy density of a 2d Potts model, on a square lattice with linear size $L = 20$, with $q = 10$ (above) compared to the one of a $q = 2$ case along two Monte Carlo runs (data every 5×10^3 MC steps are shown). (b) The histograms of the energy densities measured in a Monte Carlo simulation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