Tutorial

3: Monte Carlo: The Ising model I

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Contents

1 Description **1**

2 A first visual inspection **1**

3 The histogram technique **2**

References **3**

1 Description

The code used during this tutorial is a Monte Carlo simulation of a 2D Ising model, adapted from the code of Wolfgang Wieser[1]. The moves are local ones, with an update according to the Metropolis method.

- As a first task you are required to understand the global arrangement of the code, and write the (missing) part of function `_FlipSpin()`, that implements the Metropolis update on one spin.

2 A first visual inspection

The code has many commands (`m`, `M`, `c`, ...), each one of those requires a different number of paramenters. The `m` command allows you to run the simulation for a given number of steps and,

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to dump snapshots of the configurations into `ppm` files. Remember: *always* redirect `stdout` to a textfile, since it will produce a gnuplot script, to be processed after the program terminates.

- Run the code to sample and dump 100 configurations.
- Look at the '`dump.*.ppm`' files with `display`, or animate the sequence using
  `animate -delay 10 dump.?.ppm dump.??.ppm`.
- Repeat the procedure for different temperatures (actually, at different values of the dimensionless parameter KT/J, where J is the coupling constant).
- What do you observe going from low temperatures ($\simeq 1.0$) to higher ones ($\simeq 3.5$) ?

The snapshots should be similar to what is shown in figure 1, displaying domains in the proximity of the phase transition, and random magnetization at higher temperatures.

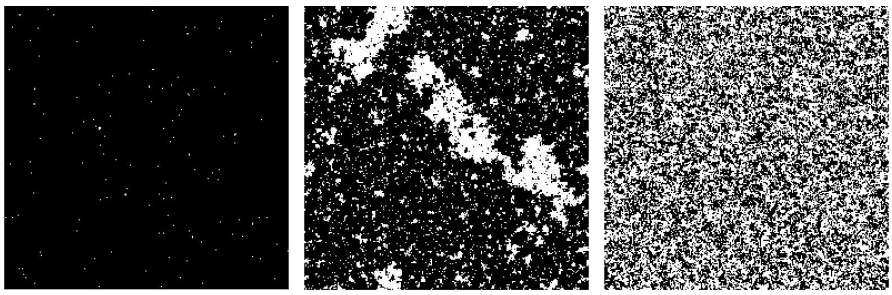

Figure 1: Configuration snapshots at three different values of KT/J: 1.3, 2.26 and 3.5

- Run the program (command `M` to obtain the magnetisation as a function of temperature for different lattice sizes.
- Compare the behavior of the Magnetization with the snapshos: are they consistent?
- Look at the phase transition: how does the lattice size influence it?

3 The histogram technique

The reweighting, or histogram technique[2] is a powerful tool to extract information on different temperature from a single simulation performed at a reference temperature $KT_0 = 1/\beta_0$: if the observable of interest can be written in terms of the energy only, the reweighting procedure is quite simple, requiring to sample only the probability $P_{\beta_0}(E)$ for the system of having energy E. Then, any observable $f(E)$ can be estimated at a different temperature using the formula

$$\langle f(E)\rangle(\beta) = \frac{\sum_i f(E_i) P_{\beta_0}(E_i) e^{-(\beta-\beta_0)E_i}}{\sum_i P_{\beta_0}(E_i) e^{-(\beta-\beta_0)E_i}} \tag{1}$$

- Launch a simulation to sample the probability histogram (command `m`) for a lattice size of 16: the output will be in the `P.<size>.<KT/J>.dat` file (hint: use about 1000 bins).
- Read and understand the script `reweight.sh`

The `reweight.sh` is a simple `awk` (see Ref.[3] for an introduction) script that performs exactly the integration described in Eq.(1), where the generic observable f is replaced by the energy $\langle E \rangle$ and its square $\left\langle E^2 \right\rangle$, to construct the specific heat

$$C(\beta) = \frac{\beta^2}{N_s^2} \left(\left\langle E^2 \right\rangle (\beta) - \langle E \rangle (\beta)^2 \right)$$

- Plot the resulting data: how much does the reweighted curve depend on the reference temperature?
- Compare the reweighted data with the explicit calculation, obtained using the `c` command of the program
- For which temperature intervals is the reweighted curve accurate?

The results should look like that presented in Fig.2

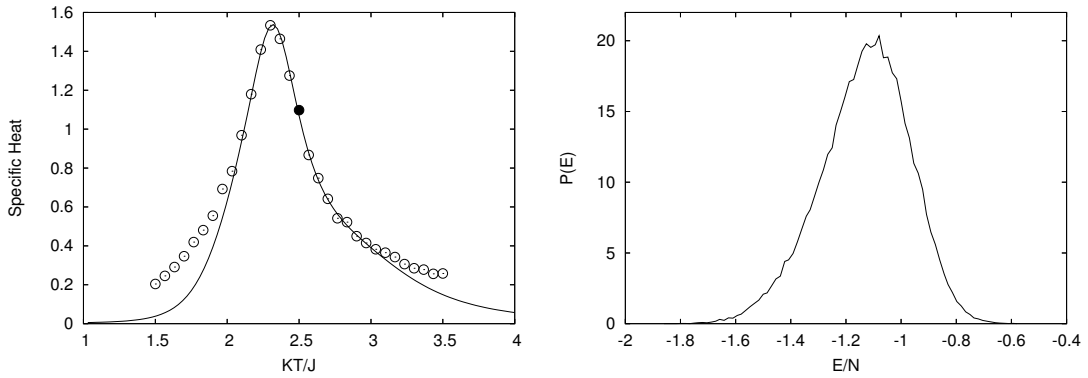

Figure 2: (a) Specific heat as a function of temperature: reweighted (solid line) from $KT/J = 2.5$ (full circle) and explicit computation (circles). (b) Histogram of $P(E)$

References

[1] `http://www.cip.physik.uni-muenchen.de/~wwieser/sim/isingmag/`

[2] Histograms and All That, in: Computer Simulations of Surfaces and Interfaces, NATO Science Series, II. Vol. 114 (Kluwer, Dordrecht, 2003), pp. 137 - 157 `http://www.physik.uni-leipzig.de/~janke/Paper/histograms.ps`

[3] `http://www.grymoire.com/Unix/Awk.html`