PHYS 8601 – Problem 5

Yier Wan

April 13, 2018

1 Introduction

In this work, we still study the two-dimensional square-lattice Ising model. Instead of sampling the probability distribution at a fixed temperature, a random walk is performed in energy space to extract an estimate for the density of states. The procedure of generating energy density is completely independent on temperature. The time-consuming job of data generation only needs to be done once. Thermodynamic properties can then be determined by weighting the density of states by the appropriate Boltzmann factor.

2 Algorithm

We want to perform a random walk in the energy space, but an unbiased random walk is difficult to realize. The 16×16 square lattice Ising model has $2^{16\times16}$ spin configurations.

1. We begin to initialize the density of states to be uniform: $g(E) = 1$ with E to be all the possible values of the system energy.

2. The we flip the spins according to the probability

$$p(E_1 \to E_2) = \min\left(\frac{g(E_1)}{g(E_2)}, 1\right), \tag{1}$$

   where E_1 is the energy before flipping and E_2 is the energy that would result if the spin were flipped.

3. No matter the spin flipping is accepted or not, we update the density of states for each spin-flip trial,

$$g(E) \to g(E) \times f_i, \tag{2}$$

   where E is the energy of the resultant state and f_i is modification factor. A suitable choice for initial modification factor is $f = f_0 = e^1 \approx 2.71828$.

4. During the random walk, we also accumulate the histogram $H(E)$ in energy space. When the histogram is observed to be "flat", the process is interrupted by setting all histogram entries to zero and reducing the next modification factor, $f_{i+1} = \sqrt{f_i}$.

   Note that the spin configuration and the density of states are not reset. We keep using the existing $g(E)$ as the starting point for further improvement. We typically use whether $\min(H(E))$ is greater than 70% of the mean value to decide when to reduce the modification factor.

The thermodynamic quantities can be computed by

$$\langle X \rangle = \frac{\sum_E X(E) g(E) \exp(-E/k_B T)}{\sum_E g(E) \exp(-E/k_B T)}. \tag{3}$$

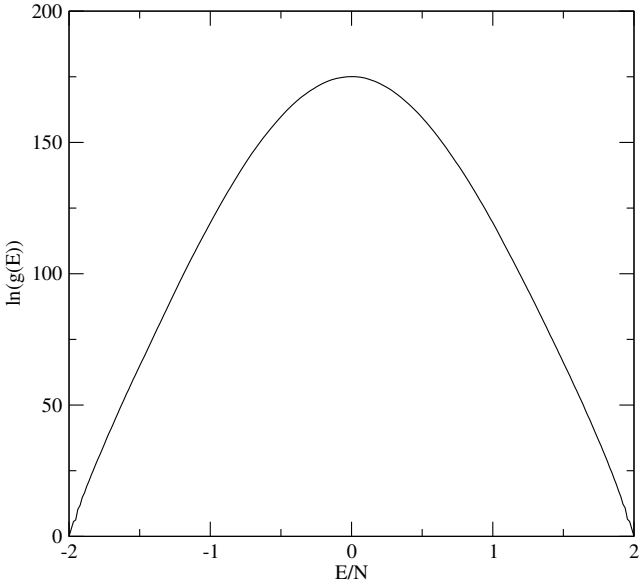

Fig. 1. Logarithm of the density of states, $\ln[g(E)]$, of the 2D Ising model for $L = 16$.

Because $g(E)$ can become very big, the logarithm of the density of states, $\ln(g(E))$, is actually used int the simulation. So Eq. 3 can be rewritten as

$$\langle X \rangle = \frac{\sum_E X(E) \exp(\ln(g(E)) - E/k_B T - m)}{\sum_E \exp(\ln(g(E)) - E/k_B T - m)}, \tag{4}$$

where m is a constant to avoid big values because of the exponent. Here we choose $m = mean(\ln g(E))$.

3 Results

In the Wang-Landau sampling, we run 500000 MCS in total. The histogram is checked every 1000 MCS. If 70% of the histogram entries are greater than the mean values of the histogram, we consider the histogram to be "flat" and reset the histogram as well as the modification factor. $\ln[g(E)]$ has very big values, so we rescale it by subtracting $\min(\ln[g(E)])$. The final modification factor for the random walk is $\ln(f_{final}) = 0.000122$. This result can be further improved by being more strict to the flatness of the histogram and including more MCS to finally end up with $\ln(f_{final})$ closer to zero.

Fig. 1 shows the density of states. The curve looks smoothly with a little resonance at tails. However, in Fig. 2, the weighted probability doesn't look good, especially for $T = 2.3J/k$. It might result from the limited numbers of simulations, which makes the thermal quantities questionable.

Table 1 shows thermal quantities calculated from the sampled results. It also contains results obtained from Metropolis sampling. We run 100000 MCS for each temperature in Metropolis sampling. Data from the first 5000 MCS are thrown away. Internal energy and specific heat obtained from Metropolis and Wang-Landau simulations are close. The time spent on the two different methods is close, but thermal quantities at all the temperatures can be generated from this finish Wang-Landau simulations, while to get thermal quantities at different temperatures by using Metropolis sampling we need to a lot more simulations at each temperature.

In general, Wang-Landau sampling can save us more time. And if we run enough MCS at the beginning, we can get reliable results with small uncertainty.

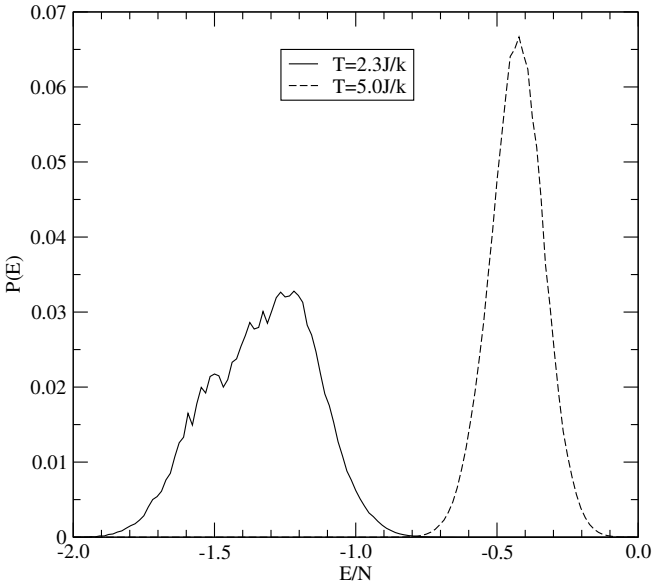

Fig. 2. Weighted probability $P(E) = \frac{g(E)\exp(-E/k_BT)}{\sum_E g(E)\exp(-E/k_BT)}$ fot the $L = 16$ Ising model.

Table 1: Metropolis VS Wang-Landau Sampling

	U/N $(T = 2.3J/k)$	C_V/N $(T = 2.3J/k)$	U/N $(T = 5.0J/k)$	C_V/N $(T = 5.0J/k)$
Metropolis	-1.405204	1.533375	-0.427954	0.097273
Wang-Landau	-1.330995	1.684409	-0.430056	0.095696