PHYS 8601 – Problem 5

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1 Introduction

In this work, we still study the two-dimensional square-lattice Ising model. Instead of doing importance sampling simulation many times, we use reweighting methods to generate new data from one sampling result. The reweighting method can save a large amount of computing time, but we cannot always get reliable results.

2 Histogram reweighting

The first step is to scan the importance sampling results measured at K_o. Different energy values are recorded and counted to generate a histogram $H(E)$. Then, from the histogram, we can estimate the probability distribution for arbitrary $K = K_o$ by

$$P_K(E) = \frac{H(E)e^{\Delta KE}}{\sum H(E)e^{\Delta KE}} \tag{1}$$

Finally, we estimate the specific heat per site by using the fluctuation relation

$$C_V(K) = \frac{k_B}{N} \times K^2 \left(\langle H(E)^2 \rangle - \langle H(E) \rangle^2 \right), \tag{2}$$

where the statistical quantities are calculated by using the weighted average

$$\langle f(E) \rangle_K = \sum f(E) \times P_K(E). \tag{3}$$

3 Results and Discussion

First we do a simple random sampling Monte Carlo simulation at infinite temperature and then we estimate the specific heat at other temperatures using the histogram of the energy values from the simulation. The result is marked in red in Fig. 1. We compare it with direct importance sampling simulation results (black curve in Fig. 1) and find the results by using reweighting method is totally wrong. The probability distribution is plotted (Fig. 2) and there are resonances exhibited. Because the specific heat at temperatures we are interested in are far away from the infinite temperature, we get very bad estimated results. The maximum is obtained at T=3.8.

We then perform another importance sampling simulation at T=3.8 and use reweighting method to generate specific heat at other temperatures (blue curve in Fig. 1). The result becomes much closer to the direct importance sampling results. Still, the probability distribution is plotted (Fig. 3). We can see that the probability curves are rapidly smooth. The maximum is obtained at T=2.4 which is very close to the real critical temperature.

Finally we do the importance sampling simulation at T=2.4 and apply reweighting method on the results. The specific heat (green curve in Fig. 1) calculated with reweighting method and direct sampling are in good agreement.

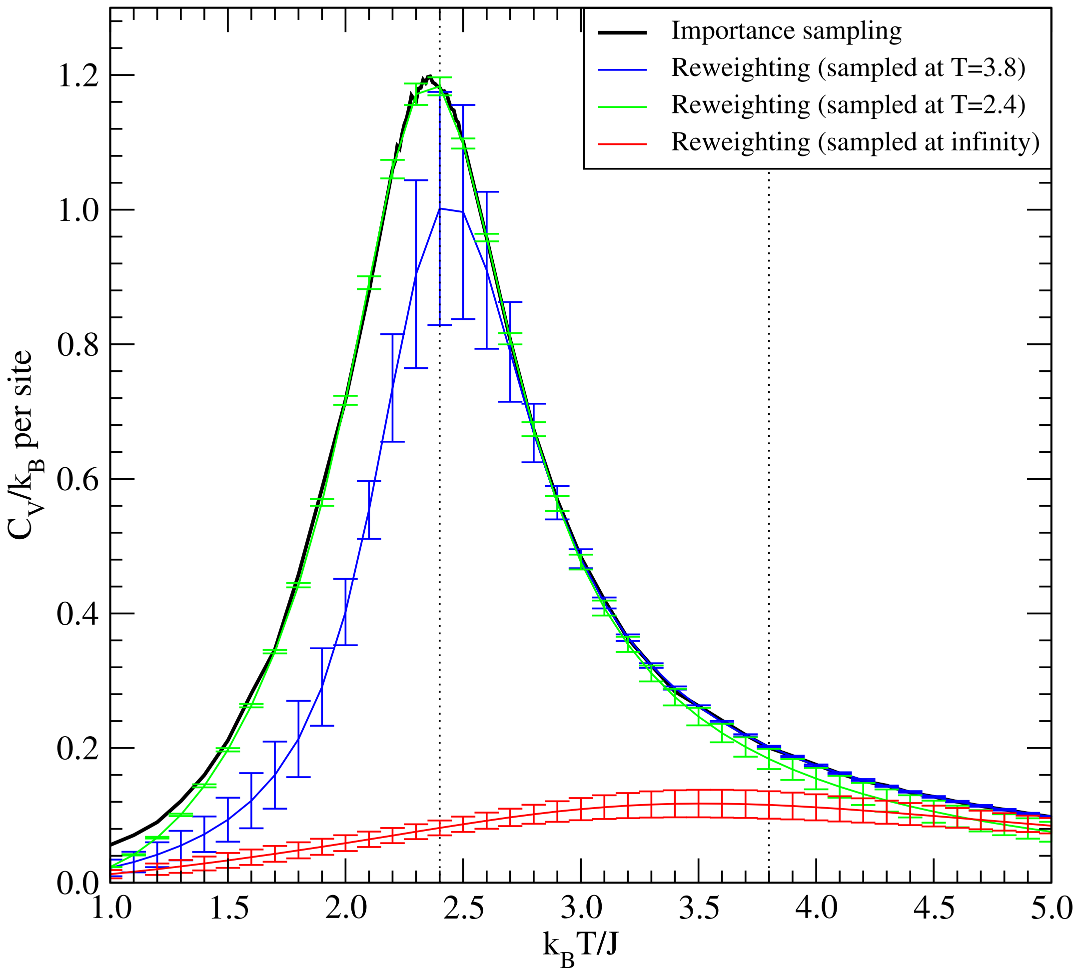

Figure 1: Specific heat as a function of temperature.

So, if we want to get excellent results near phase transition, it's better to do the direct importance sampling near the critical temperature. It doesn't need to be so accurate. We can start from any reasonable temperature and then resampling at the "effective transition temperature" obtained from the reweighting method. And then keep doing this a couple of times until we get converged results.

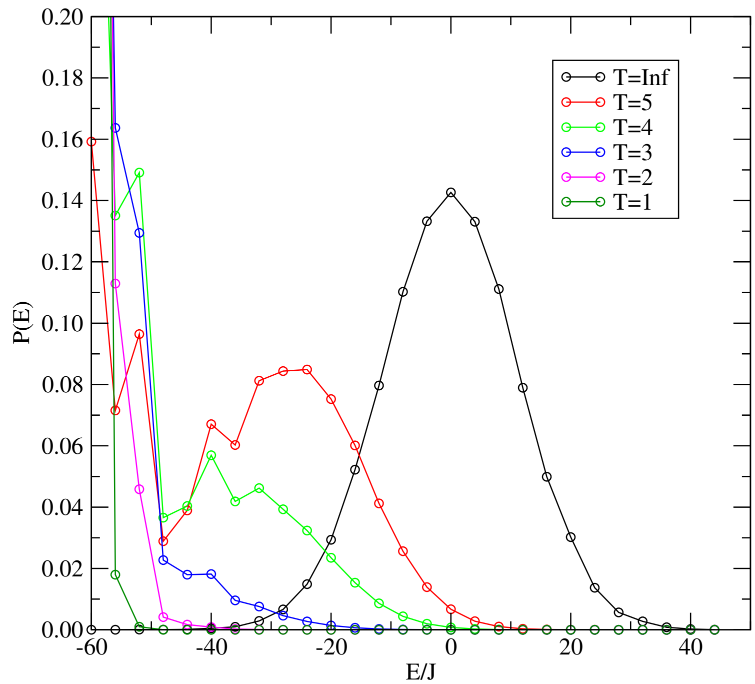

Figure 2: Probability distribution.

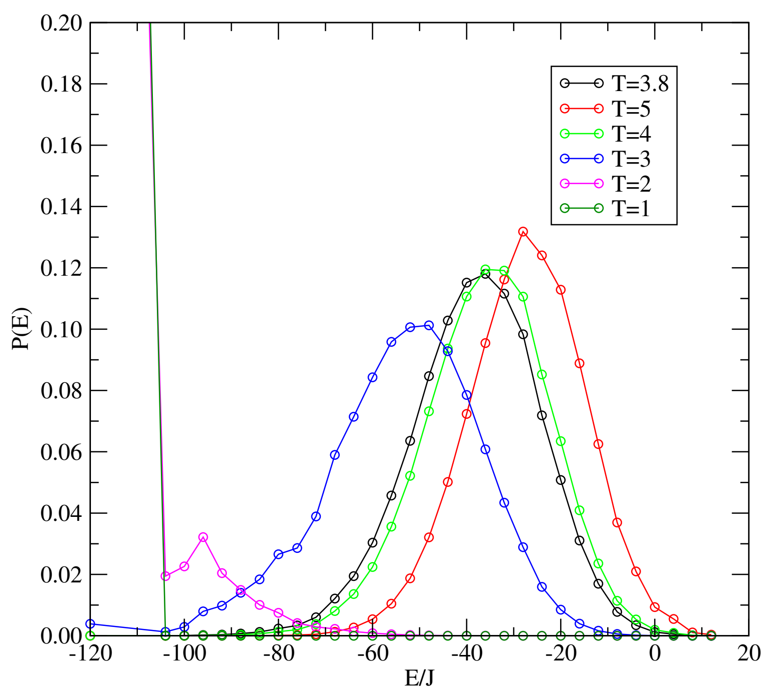

Figure 3: Probability distribution.