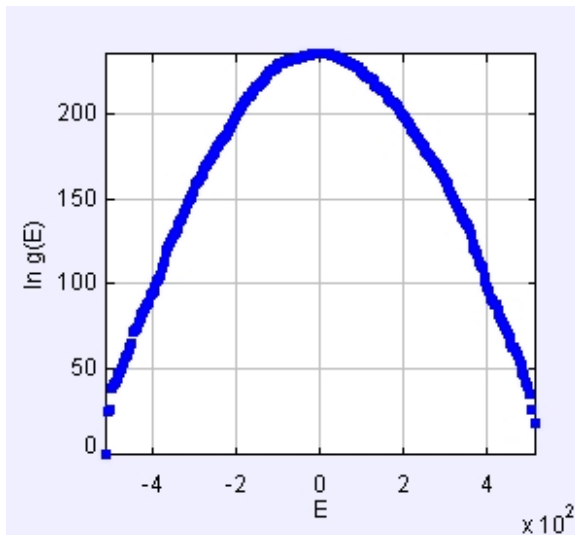## Density of States of the Two-Dimensional Ising Model:

STP IsingDensityOfStates

FIG. 1: Plot of the density of states generated by `stp_IsingDensityOfStates`.

I. INTRODUCTION

The STP `IsingDensityOfStates` program computes the density of states of the two-dimensional Ising model using the Wang-Landau algorithm. The default is a lattice of linear dimension $L = 16$ (for a total of $N = L^2$ spins).

   STP `IsingDensityOfStates` is part of a suite of Open Source Physics programs that model aspects of Statistical and Thermal Physics (STP). The program is distributed as a ready-to-run (compiled) Java archive. Double clicking the `stp_IsingDensityOfStates.jar` file will run the program if Java is installed on your computer. Additional programs can be found by searching ComPADRE for Open Source Physics, STP, or Statistical and Thermal Physics.

II. DESCRIPTION

The probability that a system in equilibrium with a heat bath at temperature T has energy E is given by

$$P(E, \beta) = \frac{g(E)e^{-\beta E}}{Z}, \tag{1}$$

where Z is the partition function and $g(E)$ is the number of states with energy E. If $g(E)$ is known, we can calculate the mean values of various thermal properties. For example, the

mean energy can be expressed as

$$<E> = \frac{1}{Z} \sum Eg(E)e^{\beta E}. \tag{2}$$

Hence, the quantity $g(E)$ is of much interest.

In the following we discuss a Monte Carlo algorithm for directly computing $g(E)$. To be concrete we apply the algorithm to the two-dimensional Ising model. In this case the energy is a discrete variable and hence the quantity we wish to compute is the number of spin configurations with the same energy. If we were to apply the algorithm to a system for which the energy is continuous, we would compute the number of states with energy between E and $E + \Delta E$, that is $g(E)\Delta E$. In this case, $g(E)$ would be the density of states. It is common to refer to $g(E)$ as the density of states even when we really mean the number of states.

Suppose that we were to try to compute $g(E)$ by doing a random walk in energy space by flipping the spins at random and accepting all configurations that we obtain in this way. The histogram of the energy, $H(E)$, the number of visits to each possible energy E of the system, would converge to $g(E)$ if the walk visited all possible configurations. In practice, it would be impossible to realize such a long random walk given the extremely large number of configurations. For example, the Ising model on a $L = 10$ square lattice has $2^{100} \approx 1.3 \times 10^{30}$ spin configurations.

Another limitation of a simple random walk to determine $g(E)$ is that the walk would spend most of its time visiting the same energy values over and over again and would not reach the values of E that are less probable. The idea of the Wang-Landau algorithm is to do a random walk in energy space by flipping single spins at random and accepting the changes with a probability that is proportional to the reciprocal of the density of states. In this way energy values that would be visited often using a simple random walk would be visited less often because they have a larger density of states. There is only one problem – we don't know the density of states. We will see that the Wang-Landau algorithm estimates the density of states at the same time that it does a random walk in phase space.

Double click on the `jar` file to run the program. When you click on the `Initialize` button followed by the `Start` button, several windows will open and you will see a plot of the energy histogram, the probability distribution $P(E)$ at temperature T as given by Eq. (1), the current estimate of the density of states $\tilde{g}(E)$, and the specific heat as a function of temperature. The simulation also returns the number of Monte Carlo steps (mcs) the iterations and the modification factor f.

Once you `Stop` the simulation, you may click on `New` and can change the temperature T and size of the lattice L by typing in a number. (After you type in a value, the box remains yellow, which signifies that the program has not incorporated the new value until you press Enter). A list of the parameters is given in Section V.

III. ALGORITHM

The Wang-Landau algorithm for estimating the density of states of the Ising model can be summarized as follows:

1. Start with an initial arbitrary configuration of spins and a guess for the density of states. The simplest guess is to set $\tilde{g}(E) = 1$ for all possible energies E.

2. Choose a spin at random and make a trial flip. Compute the energy before, E_1, and after the flip, E_2, and accept the change with probability

$$p(E_1 \rightarrow E_2) = \min(\tilde{g}(E_1)/\tilde{g}(E_2), 1) \tag{3}$$

Equation (3) implies that if $\tilde{g}(E_2) \leq \tilde{g}(E_1)$, the state with energy E_2 is always accepted; otherwise, it is accepted with probability $\tilde{g}(E_1)/\tilde{g}(E_2)$. That is, the state with energy E_2 is accepted if a random number $r \leq \tilde{g}(E_1)/\tilde{g}(E_2)$.

3. After step 2 the energy of the system is E. (E is E_2 if the change is accepted or remains at E_1 if the change is not accepted.)

4. The other part of the Wang-Landau algorithm is to multiply the current estimate $\tilde{g}(E)$ by the modification factor $f > 1$

$$\tilde{g}(E) = f\tilde{g}(E). \tag{4}$$

We also update the energy histogram $H(E)$ as

$$H(E) = H(E) + 1. \tag{5}$$

Because $\tilde{g}(E)$ becomes very large, in practice we work with the logarithm of the density of states, so that $\ln(\tilde{g}(E))$ will fit into double precision numbers. Therefore, each update of the density of states is implemented as

$$\ln(\tilde{g}(E)) \rightarrow \ln(\tilde{g}(E)) + \ln(f). \tag{6}$$

and the ratio of the density of states is computed as $\exp[\ln(\tilde{g}(E_1)) - \ln(\tilde{g}(E_2))]$.

5. A reasonable choice of the initial modification factor is $f = f_0 = e \approx 2.71828\ldots$. If f_0 is too small, the random walk will need a very long time to reach all possible energies. Too large a choice of f_0 will lead to large statistical errors.

6. Proceed with the random walk in energy space until a "flat" histogram $H(E)$ is obtained, that is, until all the possible energy values are visited an approximately equal number of times. Of course, it is impossible to obtain a perfectly flat histogram, and we will say that $H(E)$ is "flat" when $H(E)$ for all possible E is not less than Δ of the average histogram $<H(E)>$; Δ is chosen according to the size and the complexity of the system and the desired accuracy of the density of states. For the two-dimensional Ising model on small lattices, Δ can be chosen to be as high as 0.95, but for large systems the criterion for flatness will never be satisfied if Δ is too close to unity.

7. Once the flatness criterion has been satisfied, reduce the modification factor f using a function such as $f_1 = \sqrt{f_0}$, reset the histogram to $H(E) = 0$ for all values of E, and begin the next iteration of the random walk during which the density of states is modified by f_1 at each trial flip. The density of states is not reset during the simulation. We continue performing the random walk until the histogram $H(E)$ is again flat.

8. Reduce the modification factor, $f_{i+1} = (f_i)^{1/2}$, reset the histogram to $H(E) = 0$ for all values of E, and continue the random walk. Stop the simulation when f is smaller than a predefined value (such as $f_{\text{final}} = \exp(10^{-8}) \approx 1.00000001$). The modification factor acts as a control parameter for the accuracy of the density of states during the simulation and also determines how many Monte Carlo sweeps are necessary for the entire simulation.

At the end of the simulation, the algorithm provides only a relative density of states. To determine the normalized density of states we can either use the fact that the total number of states for the Ising model is

$$\sum_E g(E) = 2^N, \tag{7}$$

or that the number of ground states (for which $E = -2N$) is 2. The latter normalization guarantees the accuracy of the density of states at low energies which is important in the calculation of thermodynamic quantities at low temperatures. If we apply the former condition, we cannot guarantee the accuracy of $g(E)$ for energies at or near the ground state, because the rescaling factor is dominated by the maximum density of states. We can use

one of these two normalization conditions to obtain the absolute density of states, and use the other normalization condition to check the accuracy of our result.

IV. QUESTIONS

1. First choose $L = 2$. How many states are there for each value of E? Run the simulation and verify that the computed density of states is close to your exact answer.

2. Choose larger values of L, for example, $L = 16$. Describe the qualitative energy dependence of $g(E)$.

3. Compute the specific heat as a function of temperature and describe its qualitative temperature dependence. Is there any evidence of a phase transition?

4. *Determine the value of the specific heat C at $T = T_c = 2/\ln(1 + \sqrt{2}) = 2.269$ as a function of L and make a log-log plot of C versus L. If your data for C is sufficiently accurate, you will find that the log-log plot of C versus L is not a straight line but shows curvature. The reason is that the critical exponent α equals zero for the two-dimensional Ising model, and hence

$$C \approx C_0 \ln L. \tag{8}$$

Is your data for C consistent with this form? The constant C_0 is approximately 0.4995.

V. INPUT AND OUTPUT PARAMETERS

Parameter	Description
L	Linear dimension of lattice.
T for $P(E)$	Temperature.

TABLE I: Control parameters.

Parameter	Description
mcs	Number of Monte Carlo steps per spin.
iteration	Number of iterations of the modification factor f.
f	Modification factor.

TABLE II: Output parameters.

VI. REFERENCES

- D. P. Landau, Shan-Ho Tsai, and M. Exler, "A new approach to Monte Carlo simulations in statistical physics: Wang-Landau sampling," Am. J. Phys. **72**, 1294–1302 (2004).

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- J. Kim, J. E. Straub, and T. Keyes, "Statistical-temperature Monte Carlo and molecular dynamics algorithms," Phys. Rev. Lett. **97**, 050601-1–4 (2006). The authors discuss a novel Monte Carlo algorithm that samples the temperature as a function of the energy.

VII. RELATED CURRICULAR PACKAGES

This model is described Chapter 5 of *Statistical and Thermal Physics* by H. Gould and J. Tobochnik available on ComPADRE. For the two-dimensional Ising model, see `stp_Ising2D.jar`. Other resources are available for Statistical and Thermal Physics from `osp_stp.jar` or searching ComPADRE for STP, OSP, or Statistical and Thermal Physics.

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