A MONTE CARLO COMPUTATION OF THE ENTROPY, THE FREE ENERGY AND THE EFFECTIVE POTENTIAL. USE OF DISTRIBUTION FUNCTIONS

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A method to compute the entropy and the free energy of lattice systems is proposed. The method using the distribution functions is applied to the two-dimensional Ising model and results which agree with the exact ones are obtained. The effective potential is computed as well.

1. Introduction. In recent studies on lattice gauge theories, almost all quantities computed in Monte Carlo (MC) simulations are "expectation value" type ones, i.e. averages over the MC time, such as the internal energy, the Wilson loop and chiral order parameter. On the other hand, the possibility to measure quantities of the "probability sum (partition function)" type, such as the entropy and the free energy, is almost ignored and forgotten. In this note we propose a method to compute such quantities: the entropy and the free energy.

A revived interest in computing the entropy on the MC simulations was stirred by Ma [1] several years ago. His method is, however, limited to small-size systems due to the algorithm and the run time. On the other hand, our method presented here, which is an extension of the "multistage sampling" method by Valleau and Card [2] to the lattice model, can be applied to fairly large systems (typically 40 × 40 square lattice in this article).

The point of our method is to keep a record of the energy distribution $P(E, T)$ through the MC time. From the distribution functions $P(E, T)$ at successive temperatures, we can compute the entropy, the free energy and even the effective potential. These problems are discussed in the two-dimensional Ising model [3], because some exact results are known for this model and it is suitable to examine our method.

2. Computations of the entropy and the free energy. Let us consider the two-dimensional Ising model to illustrate our method. The energy of the Ising model is given by

$$H = -\sum \sigma\sigma', \tag{1}$$

where the σ's take values ± 1, and the summation is taken for nearest neighbor pairs. The partition function at temperature T is given by

$$Z(T) = \mathrm{Tr}\exp(-H/T) = \sum_E W(E)\exp(-E/T), \tag{2}$$

where $W(E)$ is the density of states.

Then the function $P(E, T)$, defined by

$$P(E, T) = W(E)\exp(-E/T)/Z(T), \tag{3}$$

is the probability that the system has an energy E at temperature T, that is, the energy distribution function. Although such a distribution function is not a thermodynamical quantity, it is very useful and informative as will be seen below. From eq. (3) we get an identity:

$$Z(T_1)/Z(T_2) = [P(E, T_2)/P(E, T_1)] \times \exp(E/T_2 - E/T_1), \tag{4}$$

which may look a little bit strange: the right-hand side is independent of E. This "identity" is, however, very useful in extracting physics from MC simulations, because simulations give us the quantity $P(E, T)$ di-

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rectly; strictly speaking one gets a quantity $P_{MC}(E, T) \approx N_{MC}P(E, T)$, where N_{MC} is the number of MC sweeps. Moreover the check of E-independence in eq. (4) is a good test whether the MC procedure simulates the equilibrium of the system well. This check will be shown in the actual computations later (see table 1).

Because the partition function $Z(T)$ gives the free energy $F(T)$ through the relation $Z(T) = \exp(-F/T)$, we can rewrite eq. (4) as follows,

$$\Delta(F/T) \equiv F(T_2)/T_2 - F(T_1)/T_1$$

$$= \ln[P(E, T_2)/P(E, T_1)] + (E/T_2 - E/T_1). \quad (5)$$

The entropy difference is also expressed by

$$\Delta S \equiv S(T_2) - S(T_1)$$

$$= [U(T_2)/T_2 - U(T_1)/T_1] - \Delta(F/T), \quad (6)$$

where the internal energy $U(T)$ is given by

$$U(T) = \sum_E EP(E, T), \quad (7)$$

which is an "expectation value" type quantity and can be measured easily in MC simulations. Using eqs. (5), (6) and the boundary condition at $T = \infty$, $F/T \to -S(T = \infty) = -N \ln 2$, where N is the system size, the number of spins, we can compute the free energy and the entropy at arbitrary temperature by connecting the differences at several temperatures, as far as the overlap exists in the $P(E, T)$'s at each step.

Now let us describe the results of actual MC simulations. We did simulations by the heat bath algorithm of the Ising model on a 10×10 square lattice (periodic boundary condition) over 400 000 MC sweeps. The energy distribution functions at various temperatures are shown in fig. 1. At the critical temperature $T_c = 2.269$ the distribution becomes flat, which implies that the energy fluctuation is large, although it is not truly critical because of the finiteness of the system. For smaller values of T and E, the data points appear to fall on two separate curves. This is due to the relative difference in probabilities of finding neighboring pairs (say, down pairs) and of finding separate pairs in the sea of up spin ground state. In table 1 the E-independence of eq. (4) is shown for typical cases. We see from the table that the MC method simulates the equilibrium very well although it takes only a small fraction of samples from all possible states ($N_{MC}/2^N \approx 10^{-25}$).

Finally we can compute the entropy and the free energy from the obtained distributions by the procedure described above. The results are shown in fig. 2 (the internal energy and the free energy) and fig. 3 (the entropy). The exact results of Onsager's solution

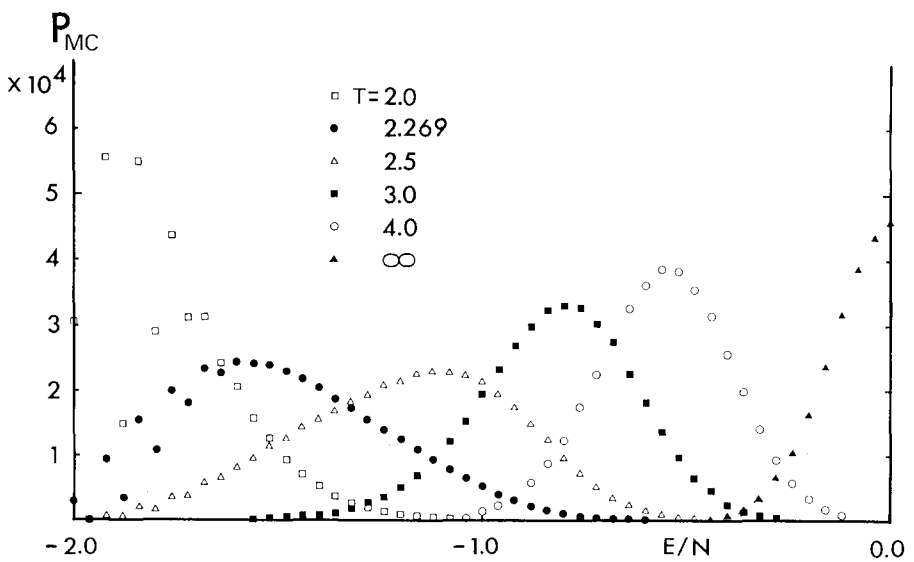

Fig. 1. The energy distribution functions at various temperatures of the Ising model.

Table 1
A check of Monte Carlo simulations (E-independence of eq. (4)). The numbers in parentheses are derived from the tail part and may contain large statistical errors.

E	$F/T\|_{2.5} - F/T\|_{2.0}$	$F/T\|_{3.0} - F/T\|_{2.5}$
−176	15.091	(6.327)
−168	15.116	(6.624)
−160	15.083	(6.616)
−152	15.082	(6.449)
−144	15.110	(6.518)
−136	15.102	6.577
−128	15.094	6.599
−120	15.111	6.602
−112	(15.142)	6.577
−104	(15.155)	6.573
−96	(15.014)	6.581
−88	(15.461)	6.573
−80	(14.453)	6.584

[4] are also given in figs. 2 and 3. The agreement with the exact curve is very good. Differences in the curves of the internal energy and the entropy are due to the finite size effect. The deviations from the exact curves (i.e. thermodynamic limit values) are of the order of $1/N$, that is, a few percent. Such flaw might be improved by the finite size scaling analysis.

Before closing this section, one comment is in order. According to the statistical mechanics, the entropy is expressed by

$$S(T) = \sum_E P(E, T) \ln[W(E)/P(E, T)], \tag{8}$$

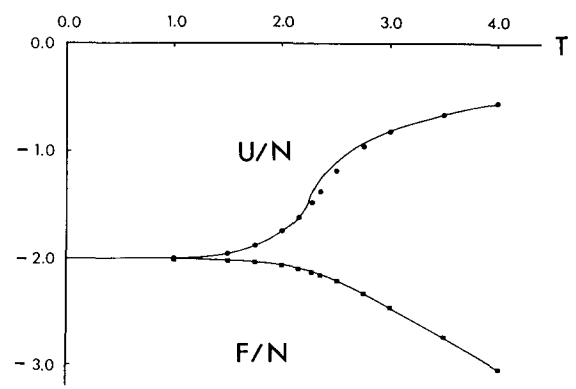

Fig. 2. The Ising model internal energy and the free energy versus temperature. The solid lines are the exact results.

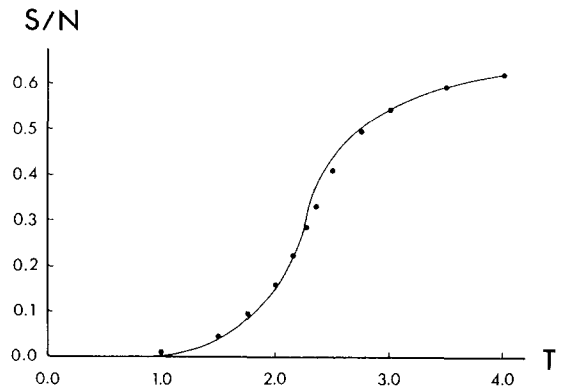

Fig. 3. The Ising model entropy versus temperature. The solid line is the exact result.

where the density of states $W(E)$ is nothing but the $P(E, T = \infty)$ times 2^N. Here we have another method of computing the entropy from the MC simulations. This procedure, which is similar to Ma's one, works well for the small-size case (as for 4×4). It fails, however, for larger sizes or for lower temperatures because $W(E)$ does not overlap $P(E, T)$ due to the limited MC sweeps.

3. Computation of the effective potential. The effective potential, or the Helmholtz potential as a function of the temperature and the order parameter, is a very important quantity to discuss the phase transition. The effective potential for the Ising model can be computed in MC simulations as follows. We introduce a symmetry breaking field (magnetic field) into the hamiltonian,

$$H = -\sum \sigma\sigma' - h \sum \sigma. \tag{9}$$

Now from the Gibbs free energy defined by $F(T, h) = -T \ln(\mathrm{Tr}\, \mathrm{e}^{-H/T})$, we get the effective potential $V(T, m)$:

$$V(T, m) = F(T, h) + hN\langle\sigma\rangle, \tag{10}$$

where the magnetization $m = \langle\sigma\rangle$ is the order parameter, and the field h is regarded as a function of m implicitly (i.e. the Legendre transformation).

The method discussed in the previous section can be used in computing the effective potential $V(T, m)$, through $F(T, h)$ according to eq. (10). Because the procedure is almost the same, we give only the results.

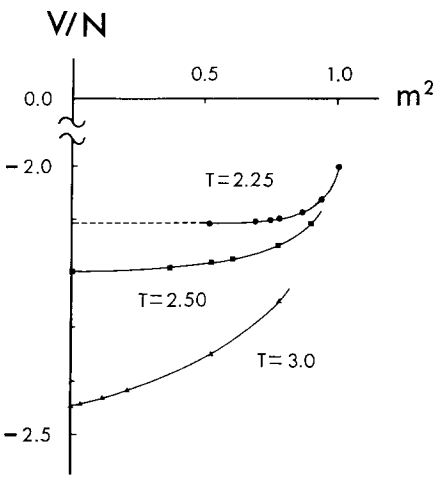

Fig. 4. The effective potential (the Helmholtz free energy) of the Ising model.

Each of the 20 000 MC sweeps were done on the 40×40 lattice. Not only the internal energy and the energy distribution, but also the correlation functions $\langle \sigma_0 \sigma_L \rangle$ were measured. Fig. 4 shows the effective potential at several temperatures below and above T_c, where the value of m^2 was determined by the extrapolation of $\langle \sigma_0 \sigma_L \rangle$ to large L. Unlike the usual curve of the effective potential in some texts, the absolute value of $V(T, m)$ is obtained here. Although such an energy shift of $V(T, m)$ at different temperatures is ignored in usual perturbative calculations (e.g. in the ϕ^4 theory) as the energy renormalization, it becomes crucial for some coupled systems. Our method will provide effective information for such cases.

For temperatures above T_c the value m^2 goes to zero without the external field, which is realized as a minimum in the effective potential. At temperatures below T_c, however, the correlation $\langle \sigma_0 \sigma_L \rangle$ tends to a finite m^2: spontaneous magnetization. The region in which m is smaller than that value becomes unstable: the dotted line in fig. 4 shows this part. To compute the effective potential in this region, another new technique is required and will be left for future work.

4. Conclusions. The energy distribution function is used effectively to compute the entropy and the free energy in the MC simulations. Applying the method to the two-dimensional Ising model, we obtained the entropy and the free energy which agree with the exact values quite well. In the same way, the effective potential was also computed.

The applications of our method to the four-dimensional lattice gauge models are in progress. The MC computation of the effective potential in a lattice gauge theory can relate it to the perturbative calculation in the continuum theory. And the lattice computation will give, in principle, the full quantum corrections. It can provide also the details of the symmetry breaking in the cosmological phase transition. We expect that the present method will provide decisive information about the properties of such phase transitions.

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