A MONTE CARLO COMPUTATION OF "ENTROPY" AND "FREE ENERGY" FOR THE Z(3) LATTICE GAUGE MODEL

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A method to compute the entropy and the free energy of lattice systems, which uses distribution functions generated by a Monte Carlo simulation, is applied to the standard Z(3) gauge model. Clear evidence for the first-order phase transition is found near the self-dual point $\beta_{sd} \cong 0.67$. The effective potential for the Wilson line is computed as well.

1. Introduction

In the usual Monte Carlo (MC) studies on lattice gauge theories, the possibility to measure quantities of "probability sum (partition function)" type, such as the entropy, the free energy and also the effective potential, has been almost forgotten. In order to realize the above possibility, the present authors developed the "multistage sampling" method by Valleau and Card [1] and applied it to the Ising model on a fairly large (40 × 40) square lattice [2]. Computed values of the free energy and the entropy agree nicely with the exact ones. The effective potential as a function of the magnetization was also computed by applying an external field to the system and Legendre-transforming the resulting free energy.

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 at successive temperatures T, we can compute the free energy, the entropy and even the effective potential. This method can be applied directly to lattice gauge systems at zero temperature, since they are regarded as statistical systems with a temperature which is equal to the inverse gauge coupling β^{-1}: the distribution functions $P(A, \beta)$ with respect to β and A = action/β are used instead of the $P(E, T)$. In the following we will use for brevity the statistical mechanics terminology such as entropy, free energy and internal energy regarding this correspondence. In other words, here we consider a phase transition of the zero temperature Z(3) gauge system with respect to the gauge coupling constant.

2. Computational method

For definiteness, let us consider the four-dimensional Z(3) gauge model on an $N^3 \times N_t$ lattice. The extension of the method to other gauge models will be trivial. N (N_t) is the size in the Euclidean space (time) direction. The action is given by

$$\beta A = \beta \,\mathrm{Re}\left(\sum_{\mathrm{P_t}} [1 - U(\mathrm{P_t})] + \sum_{\mathrm{P_s}} [1 - U(\mathrm{P_s})]\right), \quad (1)$$

where $U(\mathrm{P_t})$ ($U(\mathrm{P_s})$) is the product of the link variables U_ϱ ($U_\varrho = \exp(\mathrm{i}2\pi n_\varrho/3)$, $n_\varrho = 0, 1, 2$) around the boundary of a time-like plaquette $\mathrm{P_t}$ (space-like plaquette $\mathrm{P_s}$). The partition function is given by

$$Z(\beta) = \prod_{\text{links}} \sum_{n_\varrho=0}^{2} \exp(-\beta A). \quad (2)$$

This can also be expressed as a sum with respect to A, i.e., the action divided by β,

$$Z(\beta) = \sum_{A} W(A) \exp(-\beta A), \quad (3)$$

where $W(A)$ stands for the density of states with respect to A.

The point of the method is to use the distribution function $P(A, \beta)$ which represents the probability for the system to have a value A for a given coupling constant β, and is defined by

$$P(A, \beta) = W(A) \exp(-\beta A)/Z(\beta). \quad (4)$$

From eq. (4) we get an identity:

$$Z(\beta_1)/Z(\beta_2) = [P(A,\beta_2)/P(A,\beta_1)] \times \exp(\beta_2 A - \beta_1 A). \quad (5)$$

From eq. (5) we see that the combination of the right-hand side must be independent of A. The distribution functions are obtained through the MC procedure, and the confirmation of the approximate A-independence in eq. (5) proves to be a nice check to see if the MC procedure actually simulates the thermal equilibrium of the system.

Since the "free energy" is related to the partition function as $-\beta F(\beta) = \ln Z(\beta)$, we can rewrite eq. (5) as

$$\beta_2 F(\beta_2) - \beta_1 F(\beta_1) = \ln[P(A,\beta_2)/P(A,\beta_1)] + (\beta_2 A - \beta_1 A). \quad (6)$$

Thanks to this formula, starting from the boundary values $-(\beta F)\,(\beta = 0.0) = \ln \Sigma_A W(A) = 4N^3 N_t \ln 3$ and $-(\beta F)\,(\beta = \infty) = \ln$ (gauge volume) $= N^3 N_t \ln 3$, we can compute the free energy successively up to an arbitrary β, as far as the overlap exists in the $P(A,\beta)$ at each step. The "entropy" can be obtained easily by the relation

$$S(\beta) = \beta[U(\beta) - F(\beta)], \quad (7)$$

where the "internal energy" $U(\beta)$ is computed as the expectation value of A = action/β,

$$U(\beta) = \sum_A A\,P(A,\beta) = N^3 N_t\, 3\,\mathrm{Re}[\langle 1 - U(\mathrm{P_t})\rangle + \langle 1 - U(\mathrm{P_s})\rangle], \quad (8)$$

which is measured in the MC simulation.

In order to get the effective potential for the Wilson line $L(x)$, which is the order parameter of the deconfinement transition at zero temperature, we introduce a global-Z(3)-symmetry breaking field H. Actually we adopt the following action:

$$\beta A_{\mathrm{H}} = \beta\left(A - HN_t \sum_x \mathrm{Re}\,L(x)\right), \quad (9)$$

where $\mathrm{Re}\,L(x)$ is expressed, using the time-like link variable $n_0(x,t)$ on a site (x,t), as

$$\mathrm{Re}\,L(x) = \cos\left(\sum_t 2\pi n_0(x,t)/3\right). \quad (10)$$

The "free energy" $F(\beta,H)$ can be obtained by the same procedure as explained above, and the effective potential can be computed as the Legendre transform of $F(\beta,H)$,

$$V(\beta, \langle \mathrm{Re}\,L\rangle) = F(\beta,H) + H\langle \mathrm{Re}\,L\rangle N^3 N_t. \quad (11)$$

3. Entropy, free energy and effective potential

We did MC simulations of the Z(3) gauge model by the heat bath algorithm on a $6^3 \times 3$ lattice. Discarding the first 1000–3000 sweeps depending on the β values (or relaxation times), we measured the "internal energies", $\langle \mathrm{Re}\,L\rangle$'s and the distribution functions through 14 000 sweeps for $H = 0.0$, and through 12 000 sweeps for other H values.

Results from strong coupling and duality. Before showing the MC results, we summarize here the results for $H = 0.0$ from the lower order expansions with respect to β and their reflections in the large-β region deduced from self-duality [3]. From the naive expansion for the partition function of eq. (2), we obtain the "free energy" per site up to third order as [4]

$$f(\beta) = F(\beta)N^{-3}N_t^{-1} \cong -4\ln 3/\beta + 6 - 3\beta/2 - \beta^2/4. \quad (12)$$

The "internal energy" per site can be computed by differentiating $\beta f(\beta)$ with respect to β as

$$u(\beta) = U(\beta)N^{-3}N_t^{-1} = \partial(\beta f(\beta))/\partial\beta \cong 6 - 3\beta - 3\beta^2/4. \quad (13)$$

Noticing that $s = \beta(u - f)$, the "entropy" per site can be computed as

$$s(\beta) = S(\beta)N^{-3}N_t^{-1} \cong 4\ln 3 - 3\beta^2/2 - \beta^3/2. \quad (14)$$

Due to the self-duality of the system, the physics at high β can be related with that at low β. At a dual point $\tilde{\beta}$ of β,

$$\tilde{\beta}(\beta) = \tfrac{2}{3}\ln\{[1 + 2\exp(-3\beta/2)]/[1 - \exp(-3\beta/2)]\}, \quad (15)$$

which moves from ∞ to 0 as β goes from 0 to ∞, the "free energy" is given by

$$\tilde{\beta}f(\tilde{\beta}) = \beta f(\beta) + 6K(\beta) - 3\ln 3, \tag{16}$$

where

$$K(\beta) = \ln[1 + 2\exp(-3\beta/2)]. \tag{17}$$

The "internal energy" per site can be computed as follows:

$$u(\tilde{\beta}) = \partial[\tilde{\beta}f(\tilde{\beta})]/\partial\tilde{\beta}$$

$$= (\partial\beta/\partial\tilde{\beta})\partial[\tilde{\beta}f(\tilde{\beta})]/\partial\beta. \tag{18}$$

Substituting the series in eq. (12) into eq. (16), we obtain the approximants for $f(\beta)$ and $u(\beta)$ at the high-β region. The "entropy" $s(\tilde{\beta})$ can also be computed from eq. (7).

Results from Monte Carlo simulation. Now, let us present our MC results. In fig. 1 $u(\beta)$ and $|\langle L\rangle|$ for $H = 0.0$ are plotted against β with the third-order results for $u(\beta)$: eqs. (13) and (18). We did simulations after thermalization with disordered initialization in the region $0.0 \leqslant \beta \leqslant 0.75$ and with ordered initialization in the region $0.6 \leqslant \beta \leqslant 1.5$. A clear bistability (hysteresis) is seen in a narrow region $0.65 \lesssim \beta \lesssim 0.695$, indicating a discontinuous (first-order) transition near the self-dual point $\beta_{sd} = \frac{2}{3}\ln(1+\sqrt{3}) \cong 0.67$, which has already been seen in the pioneering MC work [5] on an $8^3 \times 20$ lattice. The two phases are regarded as the confinement phase ($\beta < \beta_{sd}$, $\langle L\rangle = 0.0$) and the deconfinement phase ($\beta > \beta_{sd}$, $\langle L\rangle$ = finite).

From the MC data for the distribution functions $P(A, \beta)$ we obtained the "free energy", applying the method explained in the last section. The thermal equilibrium was realized fairly well; the errors in $\Delta(\beta f)$ appeared of the order 10^{-4} at each step $\Delta\beta = 0.1$. In the high-β region ($\beta \gtrsim 1.2$), since the $\Delta(\beta f)$ are hidden within the errors, we started the computation downward from $\beta = 1.5$ with the boundary condition $(\beta f)(\beta = 1.5) = -\ln$ (gauge degrees of freedom per site) $= -\ln 3$, instead of starting from $\beta = \infty$. We did the procedure also in the confining region starting from $\beta = 0.0$ with the condition $(\beta f)(\beta = 0.0) = -\ln$ (number of configurations per site) $= -4\ln 3$. Generally speaking in the case where a first-order transition separates two phases, we need two boundary values; one in each phase. Otherwise we cannot go beyond the transition point, since the distribution functions of the two phases never overlap at the bistable region.

In fig. 2 we see a clear change in the slope of $\beta f(\beta)$ and meta-stability near the self-dual point β_{sd}, which again indicates a discontinuous transition. It should be noted here that $u(\beta)$ and $\beta f(\beta)$ from the MC data and the results from the third-order series agree unexpectedly well, except in the narrow region $0.6 \lesssim \beta \lesssim 0.75$.

In fig. 3 the "entropy" per site is plotted with the third-order results. The "entropy" decreases discontinuously when the $Z(3)$ system undergoes the phase transition from the confined to the deconfined phase, in other words, from the glueball phase to the frozen phase with only the freedom of gauge transformations.

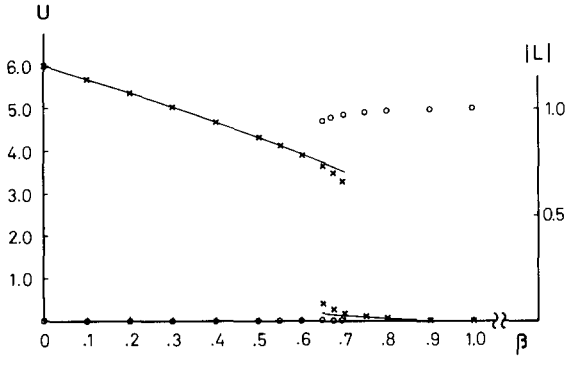

Fig. 1. The "internal energy" per site (×) and the absolute value of the Wilson line (○) for $H = 0.0$. The solid lines are from the third-order expansions.

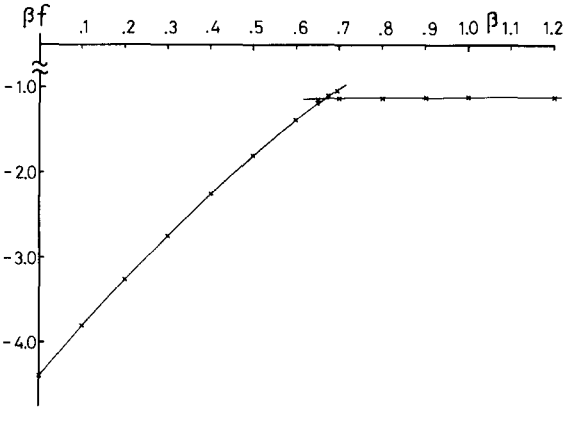

Fig. 2. The "free energy" times β per site (×). The solid lines are from the third-order expansions.

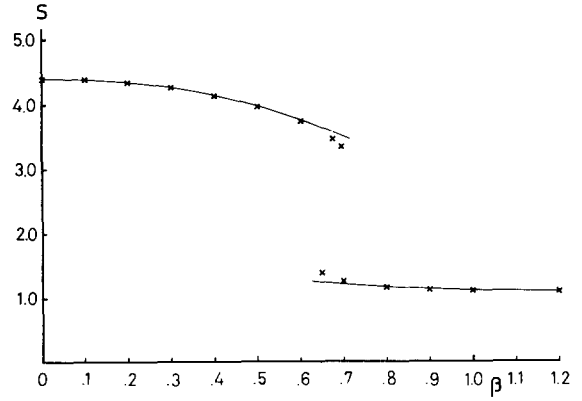

Fig. 3. The "entropy" per site (X). The solid lines are from the third-order expansions.

Finally the effective potential was computed by introducing an external field H, as explained in section 2. When H is increased, the critical coupling β_c of the first-order deconfining transition decreases; at $H = 0.7$, $\beta_c \cong 0.61$ for instance. The jump in $\langle \mathrm{Re}\, L \rangle$ and $u(\beta)$ at the transition decreases also for increasing H; we show in fig. 4 the internal energy and Wilson line at $H = 0.7$. The jump value $\Delta u(\beta_c)$, however, changes only slightly when H is changed, reflecting the fact that the external field in eq. (9) forces only the Wilson lines to align and allows the plaquette variables to fluctuate as in the $H = 0.0$ case. We employed boundary conditions for the effective potential such as $(\beta V)(\beta = \infty)N^{-3}N_t^{-1} = -\ln 3$ and $(\beta V)(\beta = 0.0)N^{-3}N_t^{-1} = -4 \ln 3$.

In fig. 5 the resultant effective potential per site $v = V(\beta)N^{-3}N_t^{-1}$ for several β values are depicted. Near the critical value β_{sd} one might expect two minima in the potential corresponding to bistability. However, since our present method is based on the distribution functions in quasi-equilibrium states, we can compute the potential only in the thermodynamically quasi-stable regions (right sides of the basins). With this understanding, we hope, the readers could imagine and interpolate the lacking (unstable) parts of the potential. In order to compute the effective potential in the unstable region, another new technique is required and this will be left for future work. When β is reduced from 0.695, which is the highest value that shows bistability, the minimal value of the potential at small $\langle \mathrm{Re}\, L \rangle$ decreases. And below $\beta = 0.6$, the unstable region disappears, leaving only one big potential well.

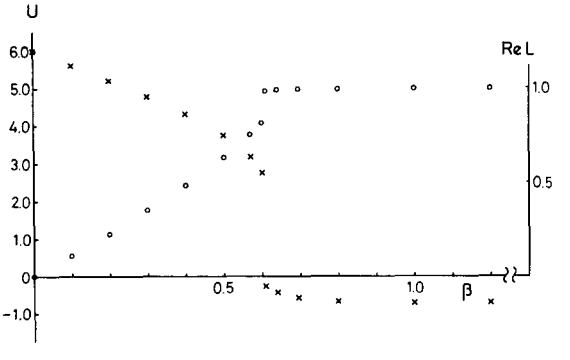

Fig. 4. The "internal energy" per site (X) and the real part of the Wilson line (○) for $H = 0.7$.

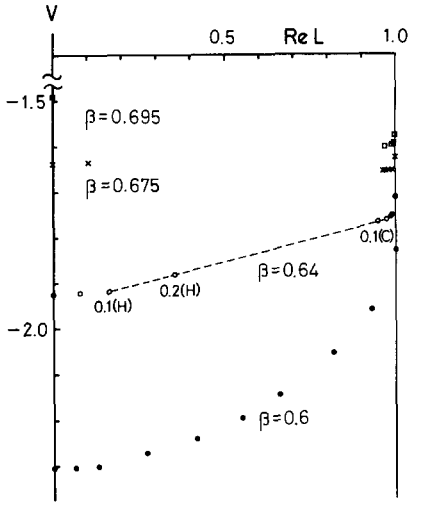

Fig. 5. The effective potential per site for several β's. The numbers with (H or C) imply the value of H with a hot (disordered) start or a cold (ordered) start. The points at Re $L = 1.0$ are given by $-\ln 3/\beta$.

4. Conclusion and discussions

A method to compute probability-sum type quantities, which uses MC data for (energy) distribution functions, was applied to the four-dimensional Z(3) lattice gauge model. The obtained free energy and the entropy indicate clear evidence for a discontinuous transition near the self-dual point. The effective potential with respect to the Wilson line was also computed in the same way.

Let us give some comparisons of our method with others [6] which compute the entropy and the effective potential. These methods measure first a response, in a sense, to some perturbation (temperature or field) and then compute the entropy or the effective potential by an integration of such a response. However, such procedures have two practical defects: firstly, the measurement of the response, which is equal to some fluctuation, contains statistical errors as a usual consequence of MC simulations, secondly, the integration needs to sum up infinitely many infinitesimal terms. On the other hand, our method avoids such difficulties, because firstly it allows a finite step in β without spoiling the computational accuracy as far as the overlap in the $P(A, \beta)$ exists, and secondly the accuracy of simulation can be assured by checking the A-independence of eq. (5).

Quantities which we call "entropy", "internal energy" and "free energy" in this note do not have such meaning in the truly thermodynamical sense; we have given these names according to the analogy of β with the inverse temperature. For instance, the "internal energy" in this note actually implies the average of action/β at zero temperature. Then how can we compute true thermodynamical quantities at finite temperature? For this purpose we have to vary the size N_t to change the temperature and measure not only the action but also the energy at the same time in each MC sweep. We have recently discussed some problems related to such an internal energy measurement [7]. Such simulations will give us the distribution function $P(A, \beta, T)$, the free energy $F(\beta, T)$ and the internal energy $U(\beta, T)$ from which we can compute lastly the entropy $S(\beta, T)$ by the method explained in section 2 with a trifling modification. The application of such a method to U(1) and SU(2) lattice gauge theories is in progress and will be reported on in future publications

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References

[1] J.P. Valleau and D.N. Card, J. Chem. Phys. 57 (1972) 5457.
[2] K. Sogo and N. Kimura, Phys. Lett. A 115 (1986) 221.
[3] T. Yoneya, Nucl. Phys. B 144 (1978) 195;
C.P. Korthals Altes, Nucl. Phys. B 142 (1978) 315.
[4] R. Balian, J.M. Drouffe and C. Itzykson, Phys. Rev. D19 (1979) 72.
[5] M. Creutz, L. Jacobs and C. Rebbi, Phys. Rev. D 20 (1979) 1915.
[6] S. Kirkpatrick, in: Ill-condensed matter, eds. R. Balian, R. Maynard and G. Toulouse (Les Houches 31, 1978) (North-Holland, Amsterdam) p. 321;
M. Creutz and B. Freedman, Ann. Phys. (NY) 132 (1981) 427;
D.J.E. Callaway and D.J. Maloof, Phys. Rev. D 27 (1983) 406;
L. O'Raifeartaigh, A. Wipf and H. Yoneyama, preprint DIAS-STP-85-29, Nucl. Phys. B, to be published.
[7] N. Kimura and K. Sogo, preprint INS-Rep.-583 (1986).