Phase transition and dynamical-parameter method in U(1) gauge theory

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Abstract

Monte Carlo simulations of the 4-dimensional compact U(1) lattice gauge theory in the neighborhood of the transition point are made difficult by the suppression of tunneling between the phases, which becomes very strong as soon as the volume of the lattice grows to any appreciable size. This problem can be avoided by making the monopole coupling a dynamical variable. In this manner one can circumvent the tunneling barrier by effectively riding on top of the peaks in the energy distribution which meet for sufficiently large monopole coupling. Here we present an efficient method for determining the parameters needed for this procedure, which can thus be implemented at low computational cost also on large lattices. This is particularly important for a reliable determination of the transition point. We demonstrate the working of our method on a $16^4$ lattice. We obtain an equidistribution of configurations across the phase transition even for such a relatively large lattice size.
1. Introduction

Recent investigations \cite{1, 2} of the compact U(1) lattice gauge theory in 4 dimensions have produced energy histograms indicative of a first-order transition. In the corresponding Monte Carlo simulations, however, the tunneling between the phases is strongly suppressed. In order to overcome the difficulties due to the lack of transitions the authors of \cite{1} introduce an iterative reweighting for different $\beta$, while the authors of \cite{2} use a matching of hot and cold start results. The problem is that on larger lattices conventional algorithms are not able to induce transitions at all. Therefore, we have looked for algorithmic alternatives.

To reduce the slowing down of the Monte Carlo algorithm in systems with a rough free-energy landscape the method of simulated tempering \cite{3} has been proposed and applied to the random-field Ising model. In this method the inverse temperature $\beta$ is promoted to the status of dynamical variable, taking values which range over some definite set. In this manner one tries to utilize the fact that at lower $\beta$ the free-energy barriers are lower. In an application of this procedure to spin-glass simulations \cite{4} it has turned out, however, that adjusting the set of temperatures and handling the corresponding probability distribution in an efficient way is far from straightforward. Nevertheless it has been possible to develop a procedure \cite{4} leading to a reduction of slowing down comparable to the one obtained with the multicanonical method \cite{5}, and with the additional advantages of allowing full vectorization of the code and of providing the canonical ensemble directly.

In the Potts model in 2 dimensions, the strength of the first-order transition decreases with the number of the degrees of freedom $q$ of the spins, the transition becoming of second order for $q < 5$. This has been used to set up an algorithm \cite{6} in which $q$ becomes a dynamical variable: by opening the easier pathway along the mountains of the joint probability distribution of $q$ and energy, one avoids the need of relying, for large $q$, on the strongly suppressed tunneling for equilibrating the configurations. To implement transitions between different $q$ cluster steps \cite{7} have been inserted. It turns out that by this algorithm one gains large factors in the autocorrelation times also in comparison to the multicanonical algorithm \cite{8}.

Proceeding along similar lines, we have obtained an efficient algorithm for the U(1) gauge theory \cite{9}. We start from the Wilson action supplemented by a monopole term \cite{10},

$$S = \beta \sum_{\mu > \nu, x} (1 - \cos \Theta_{\mu\nu, x}) + \lambda \sum_{\rho, x} |M_{\rho, x}|, \quad (1.1)$$

where $M_{\rho, x}$ is the monopole content of 3 dimensional cubes \cite{11}. One finds that the strength of the first order transition decreases with $\lambda$, the transition ultimately
becoming of second order. Thus, by making $\lambda$ a dynamical variable, we can again dispose of the tunneling transitions and proceed instead along the much easier pathway running over the top of the joint probability distribution $P(E, \lambda)$, $E$ being the average plaquette energy. With the use of appropriate Metropolis steps for the link variables as well as $\lambda$, moreover, one can make the algorithm fully vectorizable and parallelizable.

Before running the dynamical-parameter algorithm one has to determine the position of the phase transition as function of $\lambda$ and some parameters in the generalized action, which serve to enforce the prescribed $\lambda$ distribution. On lattices of moderate size (e.g. $8^4$) this is relatively easy because there is still some overlap between the peaks. On larger lattices determining these quantities is much more difficult and it becomes then crucial to perform the calculation without excessive computational cost. In the present paper we develop a method to achieve this goal. We demonstrate its effectiveness illustrating results obtained for a $16^4$ lattice. We will see that our method enables us to observe transitions also on large lattices, which is very important for a reliable determination of the transition point.

In Section 2 we outline the general features of the dynamical-parameter method. In Section 3 we derive relations among transition probabilities on which we will base the determination of the quantities required for the implementation of the algorithm. The detailed procedure followed for their calculation is described in Section 4. In Section 5 we will present some numerical results.

### 2. Outline of method

Conventional methods simulate the probability distribution

$$
\mu_\lambda(\Theta) = \exp(-S_\lambda(\Theta))/Z_\lambda
$$

where $\lambda$ is a fixed parameter. In order to make $\lambda$ a dynamical variable we consider $\mu_\lambda(\Theta)$ as the conditioned probability to get a configuration $\Theta$ given a value of $\lambda$ and prescribe a probability distribution $f(\lambda)$ to get the joint probability distribution $\mu(\Theta, \lambda) = f(\lambda)\mu_\lambda(\Theta)$. To simulate $\mu(\Theta, \lambda)$ we need it in the form

$$
\mu(\Theta, \lambda) = \exp(-S(\Theta, \lambda))/Z
$$

where

$$
S(\Theta, \lambda) = S_\lambda(\Theta) + g(\lambda)
$$
and
\[ g(\lambda) = -\log(f(\lambda)Z/Z_\lambda). \] (2.4)

Eventually we will require that the values of \( \lambda \) be approximately equidistributed, i.e. \( f(\lambda) \approx \text{const} \), which then gives \( g(\lambda) \approx \log Z_\lambda + \text{const} \).

In our application of the algorithm each update of the link variables \( \Theta_{\mu,x} \) is followed by an update of \( \lambda \), which can take values from a discrete, ordered set \( \lambda_q \) with \( q = 1, \ldots, n \). The individual update steps are Metropolis steps in both cases. For the \( \lambda \) update we use a proposal matrix \( \frac{1}{2}(\delta_{q+1,q'} + \delta_{q,q'+1} + \delta_{q,1}\delta_{q',1} + \delta_{q,n}\delta_{q',n}) \) and an acceptance probability \( \min(1, \exp(S(\Theta, \lambda_q) - S(\Theta, \lambda_{q'}))) \). The above form of the proposal matrix implies that, if the current value \( \lambda_q \) is not extremal, then we choose as new candidate value for \( \lambda \) one of the two neighboring values, \( \lambda_{q-1} \) or \( \lambda_{q+1} \), with equal probability, whereas, if \( \lambda_q \) lies at the boundary of the set of possible values, we preselect either its (only) neighboring value or \( \lambda_q \) itself, again with equal probability.

In order to implement the simulation, one must fix \( \beta(\lambda_q) \) (cfr. (1.1)) and \( g(\lambda_q) \) (cfr. (2.2) and (2.3)), for all values of \( q \). We demand \( \beta(\lambda_q) \approx \beta_w(\lambda_q) \), where \( \beta_w \) is the value of \( \beta \) which makes both phases equally probable. Our condition for fixing \( g(\lambda_q) \) is \( f(\lambda) \approx \text{const} \). In order to determine \( \beta(\lambda_q) \) and \( g(\lambda_q) \), we will use the fact that in a simulation the transition probabilities between neighboring values of \( \lambda \) are very sensitive to these quantities.

### 3. Transition Probabilities

To derive relations which can be used for the envisaged determination of \( \beta(\lambda_q) \) and \( g(\lambda_q) \) we use the probability for the transition from a value \( \lambda_q \) to a neighboring value \( \lambda_{q'} \)
\[ W(\Theta, q; q') = \frac{1}{2} \min(1, \exp(S(\Theta, \lambda_q) - S(\Theta, \lambda_{q'}))) \] (3.1)
and note that detailed balance implies
\[ f(\lambda_{q-1})\mu_{\lambda_{q-1}}(\Theta)W(\Theta, q - 1; q) = f(\lambda_q)\mu_{\lambda_q}(\Theta)W(\Theta, q; q - 1) . \] (3.2)

Let us consider subsets \( K(q) \) of configurations \( \Theta \) with probability distributions proportional to \( \mu_{\lambda_q}(\Theta) \) and weight \( w_K(q) = \sum_{\Theta \in K(q)} \mu_{\lambda_q}(\Theta) \). If we introduce the average transition probability for the set \( K(q) \)
\[ p_K(q; q') = \frac{1}{w_K(q)} \sum_{\Theta \in K} \mu_{\lambda_q}(\Theta)W(\Theta, q; q') , \] (3.3)
by averaging (3.2) we obtain
\[ f(\lambda_{q-1}) w_K(q-1) p_K(q-1; q) = f(\lambda_q) w_K(q) p_K(q; q-1). \] (3.4)

We now apply (3.4) to sets \( K_c \) and \( K_h \) of configurations in the cold phase and in the hot phase separately. Because we are interested in cases where transitions between the phases are extremely rare, in practice it is easy to obtain sets of this type with numbers of configurations sufficient for the present purpose. Also, for the same reason, the corresponding equations can be considered to be independent. We assume that our two conditions, \( \beta(\lambda) = \beta_w(\lambda) \) and \( f(\lambda) = \text{const} \), are satisfied. The condition on \( \beta \) implies that the two phases are equally populated, i.e. \( w_{K_c} = w_{K_h} \). Moreover, since the two subsets \( K_h \) and \( K_c \) essentially exhaust the whole set of configurations (in the cases we are considering the overlap is extremely small), all of the weights are, to a very good approximation, equal to \( \frac{1}{2} \). Using this fact, the constancy of \( f(\lambda) \), and (3.4) for \( K = K_c \) and \( K = K_h \) separately, we get a pair of equations which simplifies to
\[
\begin{align*}
p_{K_c}(q-1; q) &= p_{K_c}(q; q-1) \\
p_{K_h}(q-1; q) &= p_{K_h}(q; q-1)
\end{align*}
\] (3.5)

This is what we will exploit to determine \( \beta(\lambda_q) \) and \( g(\lambda_q) \).

Our strategy will be to adjust \( \beta(\lambda_q) \) and \( g(\lambda_q) \), for known \( \beta(\lambda_{q-1}) \) and \( g(\lambda_{q-1}) \), in such a way that (3.3) holds. Starting from given \( \beta(\lambda_1) \) and arbitrarily chosen \( g(\lambda_1) \), in this manner we can obtain \( \beta(\lambda_q) \) and \( g(\lambda_q) \) for \( q = 2, \ldots, n \).

4. Determination of \( \beta(\lambda) \) and \( g(\lambda) \)

To begin our procedure we select a value for \( \lambda_1 \) in the region where the peaks of the probability distribution associated to the two phases strongly overlap so that tunneling occurs frequently and \( \beta(\lambda_1) \) can easily be obtained by a conventional simulation. Because only the differences \( g(\lambda_{q-1}) - g(\lambda_q) \) are relevant we can choose \( g(\lambda_1) \) arbitrarily. Then for \( q = 2, \ldots, n \) we consecutively determine \( \beta(\lambda_q) \) and \( g(\lambda_q) \) for known \( \beta(\lambda_{q-1}) \) and \( g(\lambda_{q-1}) \).

In order to proceed from \( q - 1 \) to \( q \) we choose a new \( \lambda_q \), approximately at the same distance from \( \lambda_{q-1} \) as in the previous steps. As a first rough approximation we obtain \( \beta(\lambda_q) \) by extrapolation from the former values. At this point we use the sets of cold and hot configurations \( K_c(q-1) \) and \( K_h(q-1) \) at \( \lambda_{q-1} \), available from
the previous step, and generate two new sets of Θ configurations $K_c(q)$ and $K_h(q)$ at $\lambda_q$ by short Monte Carlo runs with cold and hot start, respectively. For each set $K_i(q')$ we can easily calculate the quantity

$$\tilde{p}_{K_i}(q'; q'') = \frac{1}{N_{K_i}(q')} \sum_{\Theta \in K_i(q')} W(\Theta, q'; q'') ,$$

where $N_{K_i}(q')$ is the number of configurations in the set and $W(\Theta, q'; q'')$ is given by (3.1) (of course, the variables $q', q''$ stand for $q - 1, q$ or $q, q - 1$, as appropriate).

Since $\tilde{p}$ approximates (3.3), this allows us to calculate the quantities $p_{K_i}$ which, for the correct choice of $\beta(\lambda_q)$ and $g(\lambda_q)$, should satisfy (3.5). We adjust then $\beta(\lambda_q)$ and $g(\lambda_q)$ until the equations (3.5) are satisfied. In practice this takes only a very small amount of computer time. We obtain good estimates for $\beta(\lambda_q)$ and $g(\lambda_q)$ though only approximate quantities enter (3.5) because the peaks related to the phases vary only little with $\beta$. In addition, the quantities $\tilde{p}_{K_i}(q'; q'')$ are used to adjust the distances between neighboring $\lambda$ values in such a way that one has roughly equal transition probabilities for all steps.

After a larger number of $q$ steps the errors may accumulate. Therefore we perform short runs of the dynamical-parameter algorithm to test whether the simulation does indeed travel along the mountains of the distribution in the hot as well as in the cold phase. If it gets stuck we slightly increase or decrease the couplings $\beta(\lambda_q)$ in the region of $\lambda$ where the transitions fail. We determine then the corresponding values $g(\lambda_q)$ from the conditions

$$\tilde{p}_{K_c}(q - 1; q) + \tilde{p}_{K_h}(q - 1; q) = \tilde{p}_{K_c}(q; q - 1) + \tilde{p}_{K_h}(q; q - 1)$$

and run the dynamical algorithm again. Typically one or two trials are sufficient.

After performing the simulations with dynamical $\lambda$, improved $\beta(\lambda_q)$ can be obtained by reweighting [12] the distribution at the values of $\lambda$ where deviations from the equidistribution of configurations in the cold and hot phase are seen to occur. Corresponding new values for $g(\lambda_q)$ are then obtained from (4.2). Alternatively improved values for $g(\lambda_q)$ can be obtained by replacing the current values with $g(\lambda_q) + \ln(f(\lambda_q))$.

5. Numerical results

Our method has made it possible to determine the phase transition region for a lattice as large as $16^4$ using only a moderate amount of computer time. We have used
approximately $2 \times 10^4$ sweeps per each value of $\lambda$ to get the sets of configurations $K_c$ and $K_h$ and approximately $4 \times 10^4$ sweeps, in total, in the short test runs with the dynamical algorithm. These preliminary calculations have been used to determine $\lambda_q$, $\beta(\lambda_q)$ and $g(\lambda_q)$ following the procedure described in Section 4. Our results for these parameters are reproduced in Table 1. Altogether we used 25 values for $\lambda$ ranging from $\lambda = 0.4$ (our starting point) down to $\lambda = 0$. In our simulations with dynamical $\lambda$ we performed approximately $10^6$ sweeps of the lattice and we observed a large number of transitions between the phases also on the $16^4$ lattice.

We define as location $\beta_C$ of the phase transition the maximum of the specific heat. We have used reweighting [12] in order to explore a range of $\beta$ in the neighborhood of the value $\beta(\lambda_q)$. As a matter of fact reweighting is necessary not only to find $\beta_C$, but also to determine accurately $\beta_w$ (the value of $\beta$ where the configurations are equidistributed between the phases) since in order to implement the procedure of Section 4 we only needed to make the areas under the peaks approximately equal.

Figure 1 shows $\beta_C$ as function of $\lambda$ for the $16^4$ lattice and also our earlier results [9] for the $8^4$ lattice. In particular, for the $16^4$ lattice at $\lambda = 0$, we obtain the value $\beta_C = 1.01084(5)$, where the error has been estimated from the fluctuation of different samples. This confirms the result $\beta_C = 1.01082(6)$ obtained in Ref. [2] by a matching procedure.

In Figure 2 we show the distribution $P(E, \lambda)$ at $\beta_w$ (for $\lambda = 0.6$ at $\beta_C$) which we got (after reweighting) from our simulations. The data have been obtained with the dynamical-parameter algorithm, except for $\lambda = 0.5$ and $\lambda = 0.6$ where the peaks overlap and the conventional Metropolis algorithm is adequate. Comparing with the corresponding figure for the $8^4$ lattice in [9] the much stronger suppression of tunneling in the transition region is obvious. In fact, on the $8^4$ lattice, because of the overlap between the peaks, there is still substantial tunneling. (For this reason, in our earlier simulations on the $8^4$ lattice we could determine $g(\lambda_q)$ following the less sophisticated procedure based on (4.2).)

In regards to the efficiency of our algorithm versus conventional methods, the number of sweeps required to observe comparable numbers of tunnelings is greatly reduced already on an $8^4$ lattice. One must make here a distinction (cfr. the discussion in [9]) according to whether one is interested in all values of $\lambda$, in which case our method produces all of the results in one stroke, or in a single $\lambda$. In the latter case, since our method requires that one still simulates a whole range of $\lambda$ values, fairness requires that the the observed mean time between tunnelings be multiplied roughly by the number of $\lambda$ values considered. Even in this case, with an $8^4$ lattice there is still considerable gain, for example, for $\lambda = -0.3$, and some gain...
remains also for $\lambda = 0$ [4].

With a $16^4$ lattice a comparison is, as a matter of fact, impossible, simply because the separation between the phases is so strong that with conventional algorithms one does not observe any transition at all. With our algorithm, instead, on a $16^4$ lattice and for $\lambda = 0$, we observe average tunneling times of the order of $10^3$ (for tunneling time we follow the definition of [13]). If we were interested only in $\lambda = 0$, this number ought to be multiplied by 25, i.e. the number of $\lambda_q$ involved. This is certainly not a small time, however it is small as compared to infinity, which corresponds to observing no transition at all.

For a further reduction of the autocorrelation times, in addition to circumventing tunneling, one would have to replace the local Metropolis steps for $\Theta$ with more efficient ones. In the dynamical parameter algorithm for the Potts model [3] the cluster steps, which were originally introduced to implement the transitions between different $q$, have the additional advantage of reducing critical slowing down and, correspondingly, the autocorrelation time in the second order region. However, at this stage an implementation of cluster steps for gauge theories with continuous groups appears very problematic, if not plainly impossible [14]. A more promising direction to pursue might be along the lines of multi-scale algorithms [15], provided that these could be modified to account for the actual structure of the configurations.

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Table 1

$\beta(\lambda)$ and $g(\lambda)$ of simulations on $16^4$ lattice

| $\lambda$ | $\beta$       | $g(\lambda)$          |
|-----------|---------------|------------------------|
| 0.000     | 1.01078       | $0.0000000 \times 10^0$|
| 0.020     | 0.99941       | $1.3184682 \times 10^3$|
| 0.040     | 0.98800       | $2.6584643 \times 10^3$|
| 0.060     | 0.97656       | $4.0189975 \times 10^3$|
| 0.080     | 0.96509       | $5.4003278 \times 10^3$|
| 0.100     | 0.95358       | $6.8044118 \times 10^3$|
| 0.120     | 0.94206       | $8.2270033 \times 10^3$|
| 0.140     | 0.93049       | $9.6746392 \times 10^3$|
| 0.160     | 0.91888       | $1.1146171 \times 10^4$|
| 0.180     | 0.90722       | $1.2643661 \times 10^4$|
| 0.200     | 0.89551       | $1.4167621 \times 10^4$|
| 0.215     | 0.88670       | $1.5327348 \times 10^4$|
| 0.230     | 0.87785       | $1.6504340 \times 10^4$|
| 0.245     | 0.86897       | $1.7697237 \times 10^4$|
| 0.260     | 0.86006       | $1.8906291 \times 10^4$|
| 0.275     | 0.85111       | $2.0133296 \times 10^4$|
| 0.290     | 0.84211       | $2.1380201 \times 10^4$|
| 0.300     | 0.83610       | $2.2219762 \times 10^4$|
| 0.315     | 0.82701       | $2.3501546 \times 10^4$|
| 0.330     | 0.81790       | $2.4799088 \times 10^4$|
| 0.345     | 0.80870       | $2.6124186 \times 10^4$|
| 0.360     | 0.79945       | $2.7470739 \times 10^4$|
| 0.375     | 0.79015       | $2.8839072 \times 10^4$|
| 0.390     | 0.78080       | $3.0229562 \times 10^4$|
| 0.400     | 0.77455       | $3.1167136 \times 10^4$|
Figure 1: Location of phase transition as function of $\lambda$ for $8^4$ (circles) and $16^4$ (crosses) lattices.

Figure 2: Distribution $P(E, \lambda)$ at the phase transition line on $16^4$ lattice.