Ising embedding for cluster algorithms in finite-temperature SU(2) gauge theory

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To extend cluster algorithms also to continuous gauge theories is highly desirable. So far in the very special case of $N_\tau = 1$ in SU(2) lattice-gauge theory at finite temperature an embedding of an Ising model with variable couplings has been successful. We get an improvement in this case by using a different flipping rule for the cluster spins. Looking for a generalization to the case $N_\tau > 1$, we find that, by appropriate gauge transformations, one can trade field effects for frustration but not get a net improvement.

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In the case of the Ising model the cluster algorithm of Swendsen and Wang [1] reduces critical slowing down in Monte Carlo simulations considerably. Embedding of an Ising dynamics in models with continuous variables such as the O(n) model [2] and φ^4 theory [3] also leads to efficient algorithms. For gauge theories there are cluster algorithms for the discrete groups $Z(2)$ and $Z(3)$ in three dimensions [4,5]. However, so far there is no cluster algorithm for continuous gauge theories. Only in the very special case of $N_\tau = 1$ in finite-temperature SU(2) lattice-gauge theory [6] has an Ising embedding been successful.

Because critical slowing down increases when one approaches the region of physical interest in continuous gauge theories, any effort is justified to find a cluster algorithm for these theories, too. To consider SU(2) lattice-gauge theory at finite temperature in four dimensions for this purpose appears favorable because there are the mentioned achievements for $N_\tau = 1$ [6]. To study the possibilities in this case more thoroughly is the purpose of the present paper.

Ben-Av *et al.* [6] propose the embedding of an Ising model with variable couplings. For this embedding we achieve some improvement for $N_\tau = 1$ by exploiting the freedom in the choice of flipping rules for the cluster spins. Considering generalizations to $N_\tau > 1$ we look for ways to overcome the problems of treating frustration and external magnetic fields. In this context we use the fact that the update procedure can be changed by gauge transformations. It turns out that in this way one can trade magnetic field effects for frustration, but, not get a net improvement.

In [6] for the action

$$S = -\frac{\beta}{2}\sum_p \mathrm{tr}U_p, \qquad (1)$$

the relation to the signs σ_x of the Polyakov loops $P_x = \frac{1}{2}\mathrm{tr}U_x$ with $U_x = \prod_{t=1}^{N_\tau} U_{(x,t),0}$ has been established by noting that for $N_\tau = 1$ one has

$$\frac{1}{2}\mathrm{tr}U_p = P_x P_y + \mathrm{const} \qquad (2)$$

for the timelike plaquettes. We would like to point out that for general N_τ without imposing a particular gauge the action can be cast into the form

$$S = -\sum_{x,y} J_{x,y}(U)\sigma_x\sigma_y - \sum_x m_x(U)\sigma_x + R(U), \qquad (3)$$

where x and y are nearest neighbors on the three-dimensional spatial sublattice and $R(U)$ is independent of σ_x. With respect to σ_x one thus has an Ising model with variable couplings $J_{x,y}(U)$, which take positive and negative values, and variable magnetic fields $m_x(U)$.

Equation (3) follows from (1) after inserting the quantities $U_{x,2}U_{x,2}^\dagger$ and $U_{y,2}U_{y,2}^\dagger$ with $U_{x,2} = \prod_{t=2}^{N_\tau} U_{(x,t),0}$ into the timelike plaquettes of the first time slice. The contribution to S of such a plaquette (after absorbing the factors $U_{x,2}^\dagger$ and $U_{y,2}$) takes the form $\frac{1}{2}\mathrm{tr}(U_a U_x U_b^\dagger U_y^\dagger)$, where U_a and U_b are matrices on the spacelike links. In the Pauli-representation the Polyakov loops P_x and P_y are the zeroth components of U_x and U_y and (3) is obtained by explicitly calculating $\frac{1}{2}\mathrm{tr}U_p$ in this representation.

For $N_\tau = 1$ (3) simplifies drastically. The couplings $J_{x,y}$ become $\beta|P_x P_y|$ and thus are positive and the magnetic fields m_x vanish identically, such that the cluster algorithm works in the usual way. To update the remaining degrees of freedom and to ensure ergodicity, in addition to the cluster sweeps, local sweeps (Metropolis or heat bath) must be performed too. In [6] the clusters have been grown according to Wolff [2] (WO) and n cluster sweeps per local sweep have been done keeping the ratio $R = n\langle M\rangle/N_\sigma^3$, where M is the cluster size, constant. The latter implies a redefinition of the time scale which corresponds to the use of an effective autocorrelation time [7]. This is appropriate only if the cluster labeling takes most of the CPU time and if, with respect to different clusters, it is done in a purely sequential way [8]. It thus is not justified for our programs.

The freedom in the choice of flipping rules for the cluster spins can be used to optimize the algorithm. Respective possibilities have been studied for the ferromagnetic Ising case [8] and analyzed in more detail later [9]. Here in addition to the WO rule also the rule of flipping the spin of the largest cluster (LC) [10] is considered.

Our simulations for $N_\tau = 1$ are for $\beta_c = 0.8730$ [6] and $N_\sigma = 4, 6, 8, 10, 12, 16, 24$. We compare the algorithms with the LC rule and one cluster sweep per local sweep, with the WO rule and one cluster sweep per local sweep (WO1), with the WO rule where n is scaled keeping $R \approx 0.28$ (WOn), and a local algorithm (Metropolis for spacelike links, heat bath for timelike links). The statistics collected is 5×10^5 to 1.5×10^6 sweeps in each of these cases. The measured observables are timelike plaquette W_τ, Polyakov loop $P = (1/N_\sigma^3)|\sum_x P_x|$, susceptibility thereof $\chi_P = (1/N_\sigma^3)(\sum_x P_x)^2$, and cluster size M. Our exponential autocorrelation times $\tau_{\rm exp}$ and integrated autocorrelation times $\tau_{\rm int}$ are determined as described in [8], fitting the autocorrelation function to $c\exp(-t/\tau)$.

Figure 1 shows typical fits of $\tau_{\rm exp}$ to kN_σ^z. It is seen that the LC rule leads to the smallest autocorrelations (for the WO rule we also give WOn results though for comparison actually only the WO1 ones are appropriate). We have determined exponential and integrated autocorrelation times for the observables W_τ, P, χ_P, M obtained by the local algorithm and by the algorithms with the rules WO1, WOn, and LC. All of the data we get for $\tau_{\rm exp}$ and $\tau_{\rm int}$ allow fits to the law kN_σ^z. Tables I to IV summarize our results for z and k. The exponential times are seen to be independent of the particular observable as they should. On larger lattices using the rule that requires flipping the largest cluster and those not in contact with it (SC rule) described in [8,9] further improvement is to be expected.

We have also investigated the dependence of the autocorrelation function on the numbers of local steps and of cluster steps within one total sweep. In particular, considering the case where s_c cluster sweeps using the LC rule are performed per local sweep, we find that there is only very little gain for $s_c > 1$ as compared to $s_c = 1$. On the other hand, in the case of the WO rule we see still some gain for $s_c > 1$, which is in agreement with observations in Ref. [6].

For $N_\tau > 1$ (3) no longer simplifies and one is confronted with external magnetic fields and frustration effects [11]. There are two ways to deal with the magnetic fields in the simulations.

The first way accounts for the magnetic fields not when growing the clusters but when flipping their spins [1,13]. The delete probabilities of the cluster growth then are

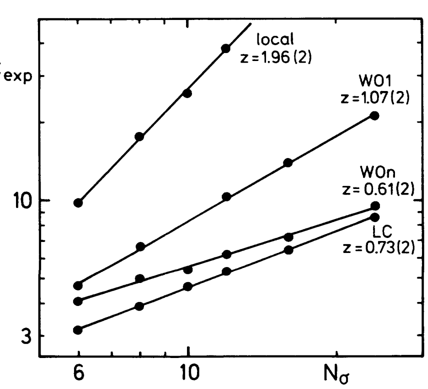

FIG. 1. Typical fits of $\tau_{\rm exp}$ to kN_σ^z (shown for the Polyakov loop) for various flipping rules (with errors smaller than symbols).

TABLE I. Fit results z for $\tau_{\rm exp} = kN_\sigma^z$.

Observable	Local	WO1	WOn	LC
W_τ	1.91(2)	1.06(4)	0.59(2)	0.75(2)
P	1.96(2)	1.09(3)	0.61(3)	0.73(2)
χ_P	1.92(2)	1.07(2)	0.61(3)	0.73(2)
M		1.05(2)	0.59(3)	0.74(2)

$$p_{xy,\rm del}(\sigma) = \exp(-J_{xy}\sigma_x\sigma_y - |J_{xy}|) \tag{4}$$

and the spin of a particular cluster is flipped with probability

$$p_C = \frac{\exp\left(-\sum_{x\in C} m_x\sigma_x\right)}{\exp\left(-\sum_{x\in C} m_x\sigma_x\right) + \exp\left(\sum_{x\in C} m_x\sigma_x\right)} \tag{5}$$

in order to respect detailed balance.

The second possibility is to account for the magnetic fields already when growing the clusters by defining a ghost spin [14]. In addition to the delete probability (4) related to neighboring spins one now introduces the probability

$$p^g_{x,\rm del}(\sigma) = \exp(-m_x\sigma_x - |m_x|), \tag{6}$$

referring to the relation between a spin and the ghost spin. The cluster spins then are flipped with probability 0.5 except for that of the ghost cluster, i.e., of the one which contains the ghost spin which must not be flipped.

In our simulations for $N_\tau = 2$ and $\beta_c = 1.873$ [15] on lattices with $N_\sigma = 6$, 8, 12, 16, using the first way to account for magnetic fields we obtain $\tau_{\rm exp} = 24.96(6)$, 44.7(2), 99(2), 185(4), and $\tau_{\rm int} = 24.5(2)$, 43.7(2), 98(1), 184(1), respectively, for the Polyakov loop and similar results for the other observables. This leads to the dynamical critical exponents $z_{\rm exp} = 2.02(3)$ and $z_{\rm int} = 2.04(2)$, which are of the magnitude characteristic for conventional algorithms. Thus the question arises if frustration or magnetic fields or both are responsible for this effect.

Our simulations indicate that frustration effects are small. Considering bond numbers as observables, on lattices with $N_\sigma = 6$ we find that about 7 out of 144 bonds are frustrated (i.e., related to antiparallel neighboring spins). For $N_\sigma = 8$ there are about 16 out of 331. Further, in a typical configuration the spatial mean of the magnetic fields turns out to be close to zero. Thus one may wonder why the algorithm nevertheless is not effective. The reason is that the values of the fields in different regions of space are not small: we obtain about 1.22 for $(1/N_\sigma^3)\langle\sum_x |m_x|\rangle$. This causes the spins to fol-

TABLE II. Fit results k for $\tau_{\rm exp} = kN_\sigma^z$.

Observable	Local	WO1	WOn	LC
W_τ	0.31(1)	0.72(7)	1.43(5)	0.82(3)
P	0.29(1)	0.68(3)	1.41(3)	0.87(2)
χ_P	0.31(1)	0.70(3)	1.38(3)	0.86(2)
M		0.73(4)	1.45(7)	0.83(2)

TABLE III. Fit results z for $\tau_{\text{int}} = kN_\sigma^z$.

Observable	Local	WO1	WOn	LC
W_τ	1.79(2)	1.08(2)	0.59(3)	0.75(2)
P	1.93(2)	1.04(3)	0.46(3)	0.65(2)
χ_P	1.90(2)	1.05(2)	0.48(2)	0.66(2)
M		0.30(4)	0.56(2)	0.67(2)

TABLE IV. Fit results k for $\tau_{\text{int}} = kN_\sigma^z$.

Observable	Local	WO1	WOn	LC
W_τ	0.31(1)	0.55(2)	1.29(4)	0.74(2)
P	0.31(1)	0.75(2)	1.84(5)	0.87(2)
χ_P	0.30(1)	0.72(2)	1.76(4)	0.93(2)
M		1.08(4)	0.69(3)	0.97(2)

low the fields. We confirm numerically that the magnetic fields are indeed correlated with the spins such that $m_x\sigma_x$ is positive in most cases. This causes the values of p_C for larger clusters to get too small.

We have also performed simulations for $N_\tau = 2$ using the second way to account for the magnetic fields, i.e., using a ghost spin. The results for τ and z are very similar to the ones above. The effect now is that the ghost cluster gets very large. For example, for $N_\sigma = 6$ its size is about 164 (out of 216). Thus only a small fraction of the spins is updated and the algorithm again becomes ineffective.

Looking for a possible way out we note that the value of $m_x\sigma_x$ can be reduced by appropriate gauge transformations. We therefore have investigated the effect of such a transformation, applying it before the cluster sweep is performed and transforming back to the temporal gauge afterwards. While the change of the sign of a Polyakov loop corresponds to the update $U \to -U^\dagger$ on the timelike links, this procedure amounts to $U \to -VU^\dagger V$. In practice the transformations have been chosen at random, accepting them for decreasing $m_x\sigma_x$. Typically, for $N_\sigma = 6$ and five gauge transformation steps per sweep we reduce the size of the largest cluster from 94 to 6, which on the average means a substantial increase of the probability p_C. In addition, also the p_C for the smaller clusters rise, e.g., from 0.043 to 0.100 for cluster size five, and still from 0.237 to 0.288 for cluster size two. However, at the same time the frustration effects become larger, the number of frustrated bonds rising to 30 out of 69. Thus it turns out that one can trade field effects for frustration. However, again determining autocorrelation times, we get similar numbers as before. This shows that by such transformations one does not get a general improvement.

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