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General cluster Monte Carlo dynamics

Daniel Kandel and Eytan Domany*
Department of Electronics, Weizmann Institute of Science, Rehovot 76100, Israel
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Several cluster Monte Carlo methods were developed recently and proved to be very efficient in accelerating simulations of various models. We present a general cluster method for Monte Carlo simulations that unifies many of the previously developed algorithms. Our general scheme satisfies the detailed-balance condition, and may therefore serve as a framework for developing new cluster acceleration techniques.

I. INTRODUCTION

The rapid development of cluster Monte Carlo simulation techniques in the last few years[1-10] has attracted considerable attention. It is generally believed that such methods may solve problems of slowing down that arise when standard Monte Carlo procedures (e.g., the Metropolis algorithm[11]) are used. Cluster acceleration techniques are particularly important when standard procedures are prohibitively inefficient, as is the case, for example, near critical points and in models with frustration at low temperatures.

The pioneering work of Swendsen and Wang[1] (SW) on acceleration of simulations of ferromagnetic Potts models gave the first hints on the extraordinary efficiency that one may achieve using cluster algorithms. Their algorithm turns out to be very effective even near critical points, where standard simulations suffer from critical slowing down. For example, the dynamic critical exponent they obtain is $z_{SW} \approx 0.35$ for the two-dimensional Ising model and $z_{SW} \approx 0.75$ for the three-dimensional case, while $z \approx 2$ when the Metropolis algorithm is used. Heermann and Burkitt[12] claim that the actual exponent of the SW algorithm is even smaller, and that in the two-dimensional case the divergence of autocorrelation times with the correlation length is only logarithmic ($z = 0$).

The success of the SW procedure may be understood if one considers the reasons for critical slowing down in standard single-spin-flip simulations. Since near criticality the correlation length becomes very large, configurations with large correlated clusters of spins are probable. In order to induce transitions among such probable configurations that have large-scale differences, one has to perform *coherent* moves of large blocks of spins. Obviously, standard simulation techniques that flip single spins *incoherently,* tend to be very slow in such situations. To overcome this problem SW replace the original Potts system by one of decoupled, probabilistically determined clusters, each representing a block of Potts spins. In ferromagnetic Potts models these clusters turn out to be large enough to induce large-scale moves, but still smaller than the whole system, so that the proposed moves are nontrivial.

Other authors, encouraged by the success of the SW procedure, tried to generalize it. Success of such generalizations is by no means guaranteed. Naive generalizations may fail for two reasons. First, the clusters one generates may be too large; when nearly all spins belong to the same cluster, the resulting large-scale moves are trivial. Secondly, some of the generalizations introduce interactions between clusters. Simulations of the resulting system of interacting clusters turn out to be difficult in some cases, and suffer from slowing down. Keeping in mind that both of these problems have to be avoided, let us briefly mention several directions in which generalizations were attempted.

Kandel *et al.*[2] applied multigrid ideas to reduce the dynamic critical exponent of the SW procedure even further. They replaced the original system by a hierarchy of systems of interacting clusters. The first (finest) of these systems was the original one, while the last (coarsest) was the SW system of noninteracting clusters. Intermediate systems consisted of clusters smaller than those of SW, but with a ferromagnetic Potts interaction between clusters. Kandel *et al.* showed that by investing more work on coarser systems than on finer ones, critical slowing down was, apparently, eliminated.

Other researchers tried to devise cluster algorithms for systems with continuous degrees of freedom. Niedermayer[3] developed a scheme that may be used for such models, and so did Edwards and Sokal.[4] Both ideas fail when applied to the XY model. These algorithms are unable to simultaneously avoid the two problems mentioned above. Edwards and Sokal arrive at a model of interacting clusters with a Hamiltonian that is difficult to simulate. Niedermayer has parameters in his algorithm which can be tuned in order to minimize relaxation times. In a certain range of this parameter space he can avoid the problem of strong interactions between clusters, but then almost all the lattice ends up in a single cluster. By changing the parameters he may avoid the latter problem, but then the interactions between clusters get stronger and the simulation suffers from slowing down.

It is clear from the above discussion that naive application of cluster updating schemes in Monte Carlo simulations is not always efficient. One has to understand the essential large-scale physics, which is responsible for the slowing down of standard techniques, in order to devise an effective cluster algorithm. The definition of clusters

within such an algorithm should reflect the true physical correlations between degrees of freedom. For example, in order to accelerate simulations of the ferromagnetic XY model, one has to relax large-scale vortex and spin-wave excitations. Therefore, a cluster algorithm that tends to "freeze" all the spins around a vortex core into one cluster will not improve efficiency. Wolff[5] devised a cluster algorithm for ferromagnetic O(n) models that meets the above criterion. His algorithm breaks vortex and spin-wave excitations into several clusters and improves the efficiency of simulations by orders of magnitude. He succeeded in reducing critical slowing down significantly (and perhaps even eliminating it completely for the two-dimensional XY model). Brower and Tamayo[6] invented a similar method to reduce critical slowing down in the ϕ^4 theory. Their method breaks large-scale kinks into several clusters, thus taking into account the appropriate large-scale physics of the model.

So far we have mentioned cluster algorithms that successfully treat important large-scale excitations of the system. In some models, however, the low-temperature physics is further complicated by the fact that the ground state is highly degenerate. Single-spin-flip algorithms may be nonergodic at $T=0$ and extremely slow at low temperatures. Such degenerate ground states occur, for example, in antiferromagnetic Potts models. Wang, Swendsen, and Kotecky[7] invented a technique that samples all ground states of these models very efficiently even at low temperatures. Their method allows for accurate determination of zero-temperature entropies with modest amounts of computer time.

Highly degenerate ground states are encountered also in models with frustration. In some of these models (e.g., spin glasses) the nature of important excitations is extremely complicated as well, and severe slowing down is observed when standard simulation techniques are applied at low temperatures. The cluster algorithms that were mentioned above are unable to identify important large-scale degrees of freedom in frustrated systems, and do not accelerate the simulations.[13] The general question of efficient cluster algorithms for frustrated systems is an open problem, but some success was achieved for particular models. SW developed their "replica" Monte Carlo algorithm for Ising spin glasses[8] and demonstrated its efficiency in the two-dimensional case. Although their method may not be as useful in the three-dimensional case and for other models with competing interactions, it is certainly a step forward towards acceleration of simulations of frustrated systems. Kandel, Ben-Av, and Domany[9] found an extremely efficient cluster algorithm for the fully frustrated Ising model on the square lattice. Their algorithm does not suffer from noticeable slowing down even at $T=0$.

Another open question is that of simulations of lattice gauge models. So far only the simplest gauge model can be simulated efficiently with a cluster algorithm. We refer here to the work of Ben-Av *et al.*[10] who invented a cluster technique to simulate the three-dimensional $\mathbb{Z}_2$ gauge model. They reduced critical slowing down significantly ($z\approx 0.73$ as compared with $z>2$ for standard simulation techniques).

Since as we have seen above, for each physical system we have to develop a new cluster algorithm that takes into account the appropriate large-scale physics, it is desirable to have a general scheme that will serve as a framework for devising new cluster algorithms. In this work we propose such a general scheme which unifies many previously developed cluster algorithms. A detailed description of the method is given in Sec. II, where we also give several important examples. In Sec. III we show that our scheme is a legitimate Monte Carlo procedure (i.e., satisfies the detailed balance condition). Ergodicity cannot be proven in general and has to be shown in each specific application explicitly. Finally, we demonstrate in Sec. III that many previously developed cluster algorithms[1,3–6,9] can be viewed as particular cases of our general scheme.

II. DESCRIPTION OF THE PROCEDURE

Consider a model Hamiltonian $\mathcal{H}$ that can be written as a sum of the form

$$\mathcal{H}=\sum_l V_l \ . \tag{2.1}$$

For example, one can write the nearest-neighbor Ising Hamiltonian on the square lattice as a sum of single-bond energies, or as a sum over elementary plaquettes, l, with each V_l consisting of four bonds. The aim of our Monte Carlo scheme is to generate a move from any initial point u in configuration space to another configuration, u', which involves some large-scale changes.

The first step of our general Monte Carlo procedure is to make independent decisions on each of the terms, V_l, of the Hamiltonian. To each V_l we assign one of n possible integers i. The decision which assigns an integer i to a V_l is stochastic, and may depend on the configuration of the system, u. That is, the probability of assigning i to l is written as $P_i^l=P_i^l(u)$. These $i=1,2,\ldots,n$ possibilities represent generalizations of the freeze-delete operations which are used in many cluster algorithms. Their probabilities are normalized, i.e.,

$$\sum_i P_i^l(u)=1 \tag{2.2}$$

for any term l and configuration u. Having generated $\{i(l)\}$, a particular assignment of an i to each l, we construct a new Hamiltonian,

$$\tilde{\mathcal{H}}_{\{i\}}=\sum_l \tilde{V}^{\,l}_{i(l)} \ , \tag{2.3}$$

where (for any $\tilde{u}$) we have

$$\tilde{V}_i^{\,l}(\tilde{u})=V_l(\tilde{u})-\frac{1}{\beta}\ln[P_i^l(\tilde{u})]+C_i^l \ . \tag{2.4}$$

The free parameters C_i^l are configuration independent; β is the inverse temperature.

The second step consists of a simulation of the model, which takes the system to a new configuration u'. To do this, we may use any procedure whose transition probabilities, $\tilde{T}_{\{i\}}(u\to u')$ satisfy the detailed balance condition *with respect to the new Hamiltonian,* i.e.,

$$e^{-\beta\tilde{\mathcal{H}}_{\{i\}}(u)}\tilde{T}_{\{i\}}(u\to u')=e^{-\beta\tilde{\mathcal{H}}_{\{i\}}(u')}\tilde{T}_{\{i\}}(u'\to u)\ . \tag{2.5}$$

These two steps define a cycle of the procedure; after completing the cycle we restore the original Hamiltonian and repeat the cycle, starting from the new configuration u'. Equation (2.4) is most important since it ensures that transitions generated by (2.5) satisfy the detailed balance condition *with respect to the original* $\mathcal{H}$ (see below).

In order to develop an intuitive understanding of the general procedure outlined above it is useful to investigate some of the possible modified interactions and their respective probabilities. To do this let us examine Eq. (2.4) more closely. Note first that the constants C_i^l do not depend on the configuration, and are therefore redundant. The reason for including them in expression (2.4) is purely aesthetic. They enable us to eliminate terms of the modified energies that have complex dependence on temperature and on coupling constants, but do not depend on the configuration.

As a first and important example, consider a term $V_l(u)$ of the Hamiltonian that can take m distinct energy values E_i, $i=1,2,\ldots,m$. Let us define m of the n possibilities to modify the interaction term. Let the probability to change the interaction according to the ith possibility be

$$P_i^l(u)=\begin{cases}p_i & \text{if } V_l(u)=E_i\\ 0 & \text{otherwise,}\end{cases} \tag{2.6}$$

and let us choose the constants

$$C_i^l=\frac{1}{\beta}\ln(p_i)-E_i\ . \tag{2.7}$$

The modified interaction now takes the form [see Eq. (2.4)]

$$\tilde{V}_i^{\,l}(\tilde{u})=\begin{cases}0 & \text{if } V_l(\tilde{u})=E_i\\ \infty & \text{otherwise}\ .\end{cases} \tag{2.8}$$

As explained above the second step of our procedure consists of Monte Carlo simulations that satisfy the detailed balance condition with respect to $\tilde{\mathcal{H}}$, the modified Hamiltonian. Say for a particular interaction term, l_1, the initial configuration was such that $V_{l_1}(u)=E_1$, and indeed $i=1$ was assigned (with probability p_1) to l_1. Then the modified interaction, $\tilde{V}_1^{\,l_1}(\tilde{u})$, assigns infinite energy to any $\tilde{u}$ for which $V_{l_1}\neq E_1$. Hence no such $\tilde{u}$ can be obtained in the simulation that uses $\tilde{\mathcal{H}}$ as its Hamiltonian. Thus, the ensuing simulations obviously conserve or *freeze* the energy of any term of the Hamiltonian that was modified according to one of the possibilities $i=1,2,\ldots,m$. We therefore call such a modification of the Hamiltonian a *freezing operation*. If the term V_l of the original Hamiltonian is frozen, all moves that conserve its energy are allowed in the ensuing simulations and occur with equal probabilities, but those moves that change its energy are forbidden. Note that the only restriction on the parameters p_i of Eq. (2.6) are $0\le p_i\le 1$. Thus any term of the Hamiltonian can always be frozen with arbitrary probability without violating the detailed balance condition.

The freezing operation becomes very simple in the case of the Ising model when the Hamiltonian is viewed as a sum of single-bond energies. If a bond that connects two spins is frozen, the relative orientation of the spins cannot change during the ensuing simulation, and they can be viewed as a cluster of spins. We therefore see that the freezing operation allows us to define clusters in the modified system. It is this fact that permits us to view our scheme as a generalized cluster algorithm. Freezing operations define clusters in the general case as well; degrees of freedom that interact via a frozen interaction are considered to be in the same cluster.

Freezing operations generate clusters, but they do not determine the interactions between clusters. These interactions are determined by those modifications of the Hamiltonian which are not freezing operations [such as the $i=m+1,\ldots,n$ yet undefined modifications in our example (2.6)]. To demonstrate this, we now show how a noninteracting system can be generated by supplementing freezing by an operation that eliminates completely the interaction between clusters. This new type of modification of the Hamiltonian is termed a *deletion operation*. It replaces the interaction $V_l(\tilde{u})$ by the modified interaction

$$\tilde{V}_d^{\,l}(\tilde{u})=0 \tag{2.9}$$

for any configuration $\tilde{u}$. As opposed to the freezing case, here the probability to delete a term of the Hamiltonian is not arbitrary. Its dependence on the configuration is completely determined by Eq. (2.4):

$$P_d^l(u)=e^{\beta[V_l(u)+C_d^l]}\ . \tag{2.10}$$

The constant C_d^l must be chosen so that the relation $P_d^l(u)\le 1$ is satisfied for any configuration u. The deletion operation is simpler than freezing in the sense that it describes a single possibilty to modify the interaction, whereas the freezing operation consists of m distinct such possibilities.

If, for example, the term considered is a bond of a ferromagnetic Ising Hamiltonian, i.e., $l\leftrightarrow(jk)$ and $V_l(u)=-JS_jS_k$, the deletion probability (2.10) takes the form

$$P_d=e^{-\beta(JS_jS_k-C)},\quad \text{with } C\le -J\ . \tag{2.11}$$

Thus an unsatisfied bond can be deleted with probability $P_d=1$ (if $C=-J$ is chosen), whereas the probability to delete a satisfied bond is smaller: $P_d\le e^{-2\beta J}$.

Assume now that the new Hamiltonian $\tilde{\mathcal{H}}$ is generated by a procedure that uses only freezing and deletion operations. According to the definition of these operations, only frozen interactions that restrict the phase space appear in $\tilde{\mathcal{H}}$. In the ensuing simulation all the configurations that satisfy these restrictions should appear with the same probability. Since, by definition, restrictions occur only within clusters, the configuration of each cluster may be chosen independently, and the modified model is therefore a system of noninteracting clusters.

Freezing and deletion operations turn out to be important, and are used very frequently in cluster algorithms (see Sec. IV). Equation (2.4) is, however, much more gen-

eral, and allows for many other modifications of the Hamiltonian. Some other possibilities will be demonstrated in Sec. IV, but the generality of the procedure is certainly not exhausted by existing cluster algorithms.

III. PROOF OF DETAILED BALANCE

In this section we prove that our algorithm is a legitimate Monte Carlo procedure that takes the system to equilibrium (defined by the Hamiltonian $\mathcal{H}$) in the long time limit. In particular, we show that our general scheme satisfies the detailed balance condition. In principle, we have to supplement this condition by a proof of ergodicity, which unfortunately cannot be shown in general; it has to be proven anew for each application of the general scheme. Nevertheless, this situation does not limit usage of the method, since one can always incorporate in any simulation scheme additional sweeps, performed with a procedure that is known to be ergodic (e.g., Metropolis sweeps in finite-temperature simulations). One may think that the performance of the whole algorithm will be destroyed due to slowing down of the procedure used for these additional sweeps. This, however, need not be the case, as demonstrated by the examples of the ϕ^4 cluster algorithm[6] and the algorithm used by Kandel, Ben-Av, and Domany[9] to simulate the fully frustrated Ising model on the square lattice.

We turn now to prove the detailed-balance relation

$$e^{-\beta\mathcal{H}(u)}T(u\to u')=e^{-\beta\mathcal{H}(u')}T(u'\to u) \tag{3.1}$$

for any two configurations u and u', where $T(u\to u')$ is the transition probability per unit time from the state u to the state u'. In the second step of our procedure we perform simulations that satisfy condition (3.1) with respect to a modified Hamiltonian $\tilde{\mathcal{H}}$, and not with respect to $\mathcal{H}$ [see Eq. (2.5)]. However, the modified Hamiltonian is chosen in a probabilistic manner, and we have to show that when the probability to reach each modified Hamiltonian is taken into account, the transition rates satisfy the detailed balance condition with respect to the original Hamiltonian $\mathcal{H}$. To that end we write the transition rates in the form

$$T(u\to u')=\sum_{\{i\}}\tilde{T}_{\{i\}}(u\to u')P(\{i\}|u)\ , \tag{3.2}$$

where the sum is over all possible modification assignments $\{i(l)\}$. Here $P(\{i\}|u)$ is the (conditional) probability to obtain assignment $\{i\}$ for given configuration u, and $\tilde{T}_{\{i\}}(u\to u')$ are transition probabilities that satisfy the detailed balance condition with respect to the modified Hamiltonian $\tilde{\mathcal{H}}_{\{i\}}$. The decisions that led to $\{i(l)\}$ were taken *independently* for each interaction term l, and hence one has

$$P(\{i\}|u)=\left[\prod_l P^l_{i(l)}(u)\right]\ . \tag{3.3}$$

To prove (3.1) we first express $\tilde{T}_{\{i\}}(u\to u')$ in terms of $\tilde{T}_{\{i\}}(u'\to u)$ using Eq. (2.5):

$$\tilde{T}_{\{i\}}(u\to u')=e^{\beta\tilde{\mathcal{H}}_{\{i\}}(u)-\beta\tilde{\mathcal{H}}_{\{i\}}(u')}\tilde{T}_{\{i\}}(u'\to u)\ .$$

This can be rewritten [see Eqs. (2.3) and (2.4)] as

$$\tilde{T}_{\{i\}}(u\to u')=\left[\prod_l e^{\beta V_l(u)-\beta V_l(u')}\frac{P^l_{i(l)}(u')}{P^l_{i(l)}(u)}\right]\tilde{T}_{\{i\}}(u'\to u)\ . \tag{3.4}$$

Now substitute (3.4) and (3.3) into (3.2); the factor $\prod_l P^l_{i(l)}(u)$ cancels and we obtain

$$T(u\to u')=\sum_{\{i\}}\left[\prod_l e^{\beta V_l(u)-\beta V_l(u')}P^l_{i(l)}(u')\right]\tilde{T}_{\{i\}}(u'\to u)\ . \tag{3.5}$$

But from (2.1) and (3.3) we see that

$$\prod_l e^{\beta V_l(u)-\beta V_l(u')}P^l_{i(l)}(u')=e^{\beta\mathcal{H}(u)-\beta\mathcal{H}(u')}P(\{i\}|u')\ .$$

Substituting this into Eq. (3.5) we find

$$T(u\to u')=e^{\beta\mathcal{H}(u)-\beta\mathcal{H}(u')}\sum_{\{i\}}\tilde{T}_{\{i\}}(u'\to u)P(\{i\}|u')\ . \tag{3.6}$$

By (3.2), however, we have

$$\sum_{\{i\}}\tilde{T}_{\{i\}}(u'\to u)P(\{i\}|u')=T(u'\to u)\ ,$$

and hence (3.6) has the form

$$T(u\to u')=e^{\beta\mathcal{H}(u)-\beta\mathcal{H}(u')}T(u'\to u)\ ,$$

which proves that detailed balance is indeed satisfied by our two-step procedure.

IV. EXAMPLES

We turn now to show that our general procedure unifies many previously developed cluster algorithms, starting with the SW algorithm[1] for ferromagnetic Potts models. Our second example is the Niedermayer generalization,[3] while in the third part of the section we examine the cluster scheme proposed by Edwards and Sokal.[4] Next we show that Wolff's algorithm[5] for O(n) models and the ϕ^4 cluster algorithm[6] can also be viewed as particular cases of our method. Lastly, we examine the more complicated case of the recently developed algorithm[9] for the fully frustrated Ising model on the square lattice. In each case we find the appropriate modified energies $\tilde{V}^l_i(u)$ (see above for definition), the probabilities $P^l_i(u)$, and the constants C^l_i.

A. The Swendsen-Wang algorithm

We restrict ourselves here to the case of the Ising model, but generalization for other Potts models is straightforward. According to the prescription of our general procedure we should first write the Hamiltonian as a sum of the form (2.1). This is done most naturally in the case of the nearest-neighbor ferromagnetic Ising model by writing the Hamiltonian as a sum of single-bond energies; each nearest-neighbor pair plays the role of a V_l, and

$$\mathcal{H}=-J\sum_{\langle j,k\rangle}S_jS_k\ . \tag{4.1}$$

The next step is to modify each term of the Hamiltonian in a probabilistic manner in order to create a system of noninteracting clusters. As was explained in Sec. II, freezing operations must be supplemented by deletion operations in order to eliminate the interactions between clusters. SW use expression (2.11) with $C=-J$ for the deletion probability of the bond that connects the spins S_j and S_k, which becomes

$$P_d = e^{-\beta J(S_j S_k + 1)} , \tag{4.2}$$

while the probability to freeze the bond is $P_f = 1 - P_d$. Therefore all unsatisfied bonds are deleted with probability $P_d = 1$, while some of the satisfied bonds are frozen, giving rise to clusters of aligned spins. The fact that only freezing and deletion operations are used here implies that frozen clusters do not interact (see Sec. II). A possible outcome of the SW procedure is depicted in Fig. 1. Frozen bonds are denoted by double lines, and deleted bonds are not marked. Note that all unsatisfied bonds are deleted, while some of the satisfied ones are frozen.

As we have shown (see Sec. II), an operation with the probability (4.2) when used in (2.4) indeed yields deletion. We have also shown that freezing operations with arbitrary probabilities are consistent with Eq. (2.4). Therefore our proof of detailed balance holds for the SW procedure, provided the new configuration is obtained by means of a Monte Carlo simulation that satisfies the detailed-balance condition with respect to the modified Hamiltonian. But since this is a Hamiltonian of noninteracting clusters, the "simulation" is realized by flipping each cluster with probability $\frac{1}{2}$, as done by SW.

B. The Niedermayer generalization

In many cases (e.g., models with frustration) the clusters generated by the SW algorithm are too large. Niedermayer[3] proposed a way to interpolate between the single-spin-flip Metropolis rule and the SW cluster algorithm, in order to control cluster sizes. Let us first consider the simple case of the Ising model, leaving the discussion of Niedermayer's more general idea for a later stage. Since cluster sizes are determined by the freezing probability P_f, we may be able to reduce the average cluster size by choosing smaller values for P_f. The compelentary operation is not deletion anymore, but is still determined by Eq. (2.4). Thus Niedermayer's proposal is to freeze the bond between the spins S_j and S_k with probability

$$P_f = \begin{cases} 1 - e^{-\beta(JS_jS_k - E_0)} & \text{if } JS_jS_k > E_0 \\ 0 \quad \text{otherwise} , \end{cases} \tag{4.3}$$

with E_0 as a free parameter. The complementary operation is performed with probability $P_{\text{comp}} = 1 - P_f$ and the modified energy, which is deduced from Eq. (2.4), depends on the constant E_0. If $E_0 < -J$ the condition $JS_jS_k > E_0$ is always satisfied, and the complementary operation has probability $P^{jk}_{\text{comp}} = e^{-\beta(JS_jS_k - E_0)}$. Substitution into (2.4) yields $\tilde{V}(S_j, S_k) = \text{const}$, independent of S_j, S_k; therefore the complementary operation is still deletion. On the other hand, if $E_0 \geq J$ no freezing operations occur (the complementary operation has $P_{\text{comp}} = 1$), and we end up with single spin "clusters" interacting via the original Ising interaction with the coupling constant J. When, however, E_0 is chosen to be in the range $-J \leq E_0 < J$, only aligned spins can be frozen, but the probability to freeze can be reduced by increasing E_0. We now note that when E_0 is in this range, the probability $P^{jk}_{\text{comp}}(u)$ to choose the complementary operation for a particular bond jk is given by

$$P^{jk}_{\text{comp}} = \begin{cases} e^{-\beta(J - E_0)} & \text{if } S_j = S_k \\ 1 \quad \text{if } S_j \neq S_k . \end{cases} \tag{4.4}$$

Substituting this into (2.4) and choosing $C^{jk}_{\text{comp}} = \frac{1}{2}(E_0 - J)$, we find that

$$\tilde{V}_{\text{comp}}(S_j, S_k) = -\tilde{J} S_j S_k , \quad \tilde{J} = \tfrac{1}{2}(J + E_0) , \tag{4.5}$$

and hence the complementary operation *weakens* the bond rather than deleting it.

It is clear [from Eq. (4.3)] that Niedermayer can reduce the average cluster size by choosing appropriate values for the constant E_0, but he has to pay a price. The noninteracting SW clusters are replaced by clusters that interact via a modified Ising coupling. The strength of the bond between two clusters can be found in the following way. Since only satisfied bonds may be frozen according to the algorithm, each cluster consists of spins which are either all + or all −. Therefore, one can associate a "coarse" Ising degree of freedom with each cluster that was generated by the frozen interaction. There is a one-to-one correspondence between configurations of the system of coarse Ising spins and configurations of the original system, which are allowed by the modified Hamiltonian (ie., have finite modified energies). To find the effective bonds of the coarse system, consider any two

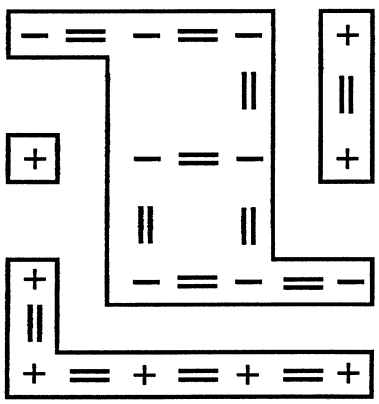

FIG. 1. Demonstration of the SW procedure. The ± signs represent a particular configuration u of the spins. The figure describes a possible outcome of the freeze-delete decisions. Double lines denote frozen bonds, while deleted bonds are not marked. The original system is replaced by one of noninteracting clusters.

clusters. Let us denote these two coarse spins by $\tilde{S}_j$ and $\tilde{S}_k$. Any bond that connects two of the original spins, that belong one to $\tilde{S}_j$ and the other to $\tilde{S}_k$, has been weakened by the procedure that generates the clusters. Its general strength J was replaced by $\tilde{J}$ [see Eq. (4.5)]. Therefore, the strength of the bond between $\tilde{S}_j$ and $\tilde{S}_k$ is $\mathcal{N}_{jk}\tilde{J}$, where $\mathcal{N}_{jk}$ is the number of nearest-neighbor pairs of original spins, such that one of the spins of each pair belongs to $\tilde{S}_j$ and the other to $\tilde{S}_k$. To illustrate this point consider Fig. 2. Figure 2(a) presents one possible outcome of the probabilistic decisions made on bonds according to Niedermayer's prescription with $-J < E_0 < J$. Some of the bonds are frozen and are denoted by double lines, while others are weakened and are denoted by zigzag lines. In Fig. 2(b), clusters, generated by frozen bonds, are replaced by coarse Ising spins that interact via two-body interactions. Bonds of the coarse system are denoted by heavy lines. Numerals $\mathcal{N}_{jk}$ near the lines denote strengths of coarse bonds in units of the modified coupling $\tilde{J}$.

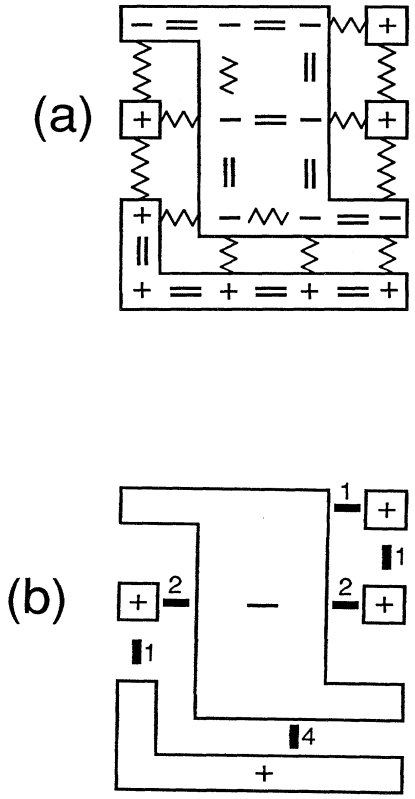

FIG. 2. Demonstration of Niedermayer's procedure. (a) A possible outcome of the algorithm. Double lines denote frozen bonds, while weakened bonds are denoted by zigzag lines. The original system is replaced by one of interacting clusters. (b) Each cluster of frozen spins is replaced by a coarse Ising spin. The coarse spins j and k interact via a ferromagnetic interaction with a modified coupling constant $\mathcal{N}_{jk}\tilde{J}$ (see text). Modified bonds are denoted by heavy lines with numerals near them to indicate their strengths in units of $\tilde{J}$.

More generally, Niedermayer proposes to freeze the interaction term $V_l(u)$ with probability $P_f[V_l(u)]$ while performing a complementary operation with probability $1-P_f[V_l(u)]$. The modified interaction, $\tilde{V}_{\text{comp}}(u)$, generated after the complementary operation was carried out is given by Eq. (2.4). As was emphasized earlier, the simulation of the resulting system of interacting clusters may suffer from slowing down, and therefore the freezing probability has to be chosen in a clever way to avoid this. Moreover, in the general case the moves allowed by the freezing operation may become difficult to perform. In the case of the Ising model each cluster has only two states, since the relative orientation of spins within a cluster cannot be changed. In the general case, however, the number of configurations of a cluster with a fixed original internal energy may be very large, and the problem of choosing one of them at random may become nontrivial.

C. The Edwards-Sokal generalization

We turn now to discuss the generalization of Edwards and Sokal, which is conceptually different from the examples considered above. So far we have discussed algorithms with a finite number of possibilities to modify each term of the Hamiltonian. The variable i that we used to differentiate between the possibilities to modify the interactions was thus discrete and took the values $i=1,2,\ldots,n$. We may however choose to work with a continuum of possibilities, in which case we change notation and replace the discrete variable i by the continuous variable x. The probability $P_i^l(u)$ is replaced by $P^l(x,u)dx$, and the normalization condition takes the form $\int P^l(x,u)dx=1$ for any term l and configuration u. The constants C_i^l become functions of x as well, and the new Hamiltonian can be written as $\tilde{\mathcal{H}}_{\{x\}}(u)=\sum_l \tilde{V}^l(x(l),u)$. Condition (2.4) is replaced by

$$\tilde{V}^l(x,u)=V_l(u)-\frac{1}{\beta}\ln[P^l(x,u)]+C^l(x)\ . \tag{4.6}$$

Edwards and Sokal[4] shift the energy scale so that $V_l(u)\geq 0$ for any configuration u. They also confine x to the interval [0,1]. Within the framework of our scheme their procedure is equivalent to choosing $C^l(x)=0$ for any x, and for given configuration u choosing the modification index x stochastically according to the probability density

$$P^l(x,u)=\begin{cases} e^{\beta V_l(u)} & \text{if } 0\leq x\leq e^{-\beta V_l(u)} \\ 0 & \text{if } e^{-\beta V_l(u)}<x\leq 1\ . \end{cases} \tag{4.7}$$

Note that the normalization condition is satisfied by (4.7). In effect, values of x in the range $0\leq x\leq e^{-\beta V_l(u)}$ are selected with equal probability for each l. According to (4.6) their modified interaction takes the form

$$\tilde{V}^l(x,u)=\begin{cases} 0 & \text{if } 0\leq x\leq e^{-\beta V_l(u)} \\ \infty & \text{if } e^{-\beta V_l(u)}<x\leq 1\ . \end{cases} \tag{4.8}$$

Thus the original system is replaced by a system with constraints, restricting the available configuration space. Some of the configurations have infinite energy and are

therefore forbidden, while all other configurations have zero energy and appear with equal probability. Such a modified system may be viewed as a model with a degenerate ground state at zero temperature.

Edwards and Sokal consider the ferromagnetic XY model as an example. Their algorithm replaces the XY Hamiltonian,

$$\mathcal{H}=-J\sum_{\langle j,k\rangle}(\mathbf{S}_j\cdot\mathbf{S}_k-1)$$
$$=-J\sum_{\langle j,k\rangle}[\cos(\theta_j-\theta_k)-1]\ , \tag{4.9}$$

by a model where the difference of phases between nearest-neighbor spins takes values in a restricted range. This range is determined probabilistically and independently for each nearest-neighbor bond. The modified energy of a bond is infinite if the phase difference is outside the chosen range, or zero if the phase difference is within the range. In this particular case, Eq. (4.7) for the probability $P^{jk}(x;\theta_j,\theta_k)$ to modify the energy of the bond connecting the spins $\mathbf{S}_j$ and $\mathbf{S}_k$, according to the possibility denoted by the index $x\in[0,1]$ takes the form

$$P^{jk}(x;\theta_j,\theta_k)=P(x_{jk};\theta_j-\theta_k)=\begin{cases}e^{-\beta J[\cos(\theta_j-\theta_k)-1]} & \text{if } 0\le x_{jk}\le e^{\beta J[\cos(\theta_j-\theta_k)-1]}\\ 0 & \text{if } e^{\beta J[\cos(\theta_j-\theta_k)-1]}<x_{jk}\le 1\ .\end{cases} \tag{4.10}$$

The modified energy (4.8) can now be expressed as

$$\tilde{V}^{l}(x_{jk},\theta_j,\theta_k)=\begin{cases}0 & \text{if } |\theta_j-\theta_k|\le\Delta(x_{jk})\\ \infty & \text{if } |\theta_j-\theta_k|>\Delta(x_{jk}),\end{cases} \tag{4.11}$$

where the allowed range of the phase difference Δ is given by

$$\Delta(x)=\begin{cases}\arccos\left[1+\dfrac{1}{\beta J}\ln x\right] & \text{if } x>e^{-2\beta J}\\ \pi & \text{otherwise.}\end{cases} \tag{4.12}$$

The resulting modified Hamiltonian (4.11) assigns to each bond an interaction $\tilde{V}$, which either vanishes or takes an infinite value, if the angle difference exceeds a (bond-dependent) threshold. This can be viewed as a zero-temperature step model with bond disorder. Simulations of this model are far from trivial and suffer from slowing down. This is an example of the general case, mentioned in the Introduction, where it may be difficult to simulate the model defined by the modified Hamiltonian. In some cases, however, there may be a way to perform efficient simulations of the resulting model. Only then can such a generalization be useful.

D. The O(n) and ϕ^4 cluster algorithms

We turn now to a different approach, which does succeed in accelerating simulations of the XY model—Wolff's algorithm[5] for ferromagnetic O(n) models. This method has some similarities to the SW algorithm for Potts models, but differs from the latter technique in two aspects. First, rather than *flipping* blocks of spins, Wolff proposes to *reflect* clusters of spins with respect to a randomly chosen hyperplane in spin space. Secondly, Wolff builds one cluster at a time and reflects all of its spins rather than dividing the whole system into clusters and reflecting each cluster with probability $\frac{1}{2}$. This second aspect may be implemented in the SW algorithm for Potts models as well, and the resulting single-cluster algorithm turns out to be more efficient than the original SW scheme.[14] Here we do not deal with single-cluster algorithms although they, as well, may be represented as particular cases of our procedure. For the sake of simplicity we consider a many-cluster version of Wolff's algorithm for O(n) models.

As in the SW procedure we may write the ferromagnetic nearest-neighbor O(n) Hamiltonian as a sum of bond energies

$$\mathcal{H}=-J\sum_{\langle j,k\rangle}\mathbf{S}_j\cdot\mathbf{S}_k\ . \tag{4.13}$$

Now we choose a random direction $\hat{\mathbf{s}}$ in spin space, and express each O(n) spin as a sum of two vectors parallel and perpendicular to the unit vector $\hat{\mathbf{s}}$:

$$\mathbf{S}_j^{\parallel}=(\mathbf{S}_j\cdot\hat{\mathbf{s}})\hat{\mathbf{s}},\quad S_j^{\perp}=\mathbf{S}_j-\mathbf{S}_j^{\parallel}\ . \tag{4.14}$$

Next, we write the Hamiltonian as a sum of two terms

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_1\ , \tag{4.15a}$$

with

$$\mathcal{H}_0=-J\sum_{\langle j,k\rangle}\mathbf{S}_j^{\perp}\mathbf{S}_k^{\perp}\ ,$$
$$\mathcal{H}_1=-\sum_{\langle i,j\rangle}J_{jk}\sigma_j\sigma_k\ , \tag{4.15b}$$

and

$$\sigma_j=\mathrm{sgn}(\mathbf{S}_j\cdot\hat{\mathbf{s}}),\quad J_{jk}=J|\mathbf{S}_j^{\parallel}|\,|\mathbf{S}_k^{\parallel}|\ . \tag{4.15c}$$

Wolff proposes moves that reflect O(n) spins with respect to a hyperplane perpendicular to the unit vector $\hat{\mathbf{s}}$. Such moves change the signs of the Ising spins σ_j, but leave the couplings J_{jk} and the first part of the Hamiltonian $\mathcal{H}_0$ invariant. Since the new couplings J_{jk} are ferromagnetic we can use the SW algorithm for ferromagnetic Potts models to generate clusters of σ spins in order to effectively simulate the $\mathcal{H}_1$ system. Note that since such a procedure does not change $\mathcal{H}_0$ and satisfies the detailed balance condition with respect to $\mathcal{H}_1$, it also satisfies detailed balance with respect to the original Hamiltonian

$\mathcal{H}$. The description in terms of our general scheme is therefore similar to the description of the SW procedure, with the slight modification that in the present case the probabilities $P_i^l(u)$ and the constants C_i^l depend explicitly on l through the inhomogeneous couplings J_{jk}. A new random vector $\hat{\mathbf{s}}$ has to be chosen each sweep. Thus, in each sweep we apply the SW algorithm to a different Ising model.

The essential ingredients for the success of Wolff's algorithm is the type of global move that he has chosen. Our general procedure does not give hints on how to choose correct global moves that will take into account the large-scale physics of a given model. However, once the move is chosen, our method tells us how to maintain detailed balance, which may be a nontrivial issue in complicated cases such as frustrated systems (see below).

The ϕ^4 cluster algorithm[6] can be described in a similar manner. Each field ϕ_j can be expressed as a product of its sign σ_j and its magnitude. If we consider moves that change the signs but leave the magnitudes unchanged, we may describe the dynamics in terms of a Hamiltonian of a ferromagnetic Ising model. The rest of the description in terms of the general procedure is the same as for O(n) models. In the ϕ^4 case, however, cluster sweeps have to be supplemented by simulations that change also the magnitudes of the fields, in order to ensure ergodicity.

E. The fully frustrated Ising model on the square lattice

In all the examples we encountered so far the Hamiltonian was expressed as a sum of single-bond energies. Next, each bond was treated independently using information on the values of the two spins that it connects. Such a strategy is not always successful. For example, in models with competing ferromagnetic and antiferromagnetic nearest-neighbor interactions one has to consider information on more than two spins in order to determine the relative orientation of two neighboring spins in a ground state. Indeed when the SW algorithm is applied to such models at low temperatures it freezes the whole lattice into a single cluster allowing only trivial moves.

Kandel, Ben-Av, and Domany[9] showed that this problem may be overcome if one uses more general partitions of the Hamiltonian. They considered the fully frustrated nearest-neighbor Ising model on the square lattice with periodic boundary conditions. In this model each elementary plaquette has an odd number of antiferromagnetic bonds, so that at most three bonds of the plaquette may be satisfied simultaneously. Kandel, Ben-Av, and Domany checkerboard-partitioned the lattice, and randomly chose one of the two possible sets of plaquettes. Then they expressed the Hamiltonian as a sum of plaquette energies, where the sum is over all plaquettes that belong to the chosen set. When the Hamiltonian is expressed in this form each bond belongs to exactly one of the chosen plaquettes. Each plaquette may be in one of 16 possible spin configurations (since there are four spins at its corners), but its energy can take only two values because all the bonds were given the same strength $|J|$. If three bonds of a plaquette are satisfied and one is not, the energy of the plaquette is $E_p=-2|J|$, while if three of the four bonds are unsatisfied the energy takes the value $E_p=2|J|$. We will now specify the possible modifications of plaquette energies and show that the scheme used by Kandel, Ben-Av, and Domany fits into our general framework. In fact Kandel, Ben-Av, and Domany used the general scheme described in the present work to extend a physically desirable $T=0$ cluster algorithm to finite T, thus ensuring that their procedure satisfies the detailed balance condition.

We find it convenient to describe the modified interactions in terms of deletion and freezing operations on bonds as defined in Sec. II. If we apply the SW rules to each of the four bonds of a plaquette independently, there will be 16 possible modified interactions. For a number of reasons[9] Kandel, Ben-Av, and Domany are interested in generating a modification scheme that keeps only $n=7$ of these possibilities. They allow for the deletion of all four bonds (one possibility, $i=1$) or for the deletion of two bonds and freezing of the two remaining ones (six possibilities, $i=2,3,\ldots,7$). Figure 3 illustrates the seven possibilities. Frozen bonds are denoted by double lines, while deleted bonds are not marked. Modification $i=2$, for example, corresponds to freezing two horizontal bonds and deleting the two vertical ones, etc. Having decided on the desired modified interactions, one has to design, or "engineer," conditional probabilities $P_i^l(u)$ that will indeed produce them when used in Eq. (2.4).

We now show that the procedure of Kandel, Ben-Av, and Domany produces the modified interactions appropriate for the seven modifications described in Fig. 3. This is done in two steps: First, we define the probabilities $P_i^l(u)$ for all configurations u, and then use Eq. (2.4) to show that the modified interactions correspond to deletion and freezing operations as described above. Unfortunately, we have to use the terms freezing and deletion in the first step before actually proving that these are indeed the appropriate terms for the relevant modified interactions. This is done in order to avoid complications in terminology and cumbersome descriptions.

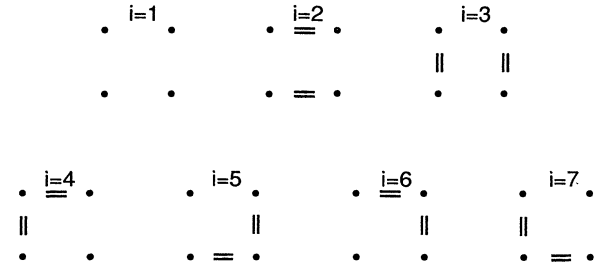

FIG. 3. Illustration of the seven possible modifications of plaquette energies. Double lines denote frozen bonds and deleted bonds are not marked. The first possibility, $i=1$, corresponds to deletion of all four bonds, while the six possibilities, $i=2,3,\ldots,7$, correspond to freezing two of the bonds and deletion of the two remaining ones.

As in previously described algorithms, the decision on the modified interaction depends on the configuration. In their algorithm Kandel, Ben-Av, and Domany require that only satisfied bonds may be frozen; unsatisfied bonds are always deleted. To satisfy this requirement, they choose $P_i^l(u)=0$ if modification i freezes a bond which is unsatisfied in configuration u. Consider, for example, modification $i=2$ which freezes the two horizontal bonds. Assume also that α, a horizontal bond of plaquette l, is unsatisfied in configuration u. If we start a cycle from configuration u, the bond α cannot be frozen, and therefore modification $i=2$ of the energy of plaquette l is forbidden; i.e., $P_2^l(u)=0$.

Next, we have to define the probabilities $P_i^l(u)$ which do not vanish in the scheme of Kandel, Ben-Av, and Domany. Since the number of frozen bonds in a plaquette must be even, the freezing rule described above implies that none of the bonds of a plaquette with three unsatisfied bonds can be frozen. Hence, if only one of the bonds of plaquette l is satisfied in configuration u, we have $P_1^l(u)=1$. On the other hand, if in configuration u our plaquette l has three satisfied bonds, the decision on it has four possible outcomes. First, we may choose $i=1$ with probability

$$P_1^l(u)=e^{-4\beta|J|} . \tag{4.16a}$$

In the three remaining cases two of the three satisfied bonds are frozen, while the third one and the unsatisfied bond are, as we will show, deleted. Kandel, Ben-Av, and Domany choose to delete the unsatisfied bond and the satisfied bond parallel to it (while freezing the other two bonds) with probability

$$p=(1-e^{-2\beta|J|})^2 . \tag{4.16b}$$

Lastly, with probability

$$p'=1-p-P_1^l(u)=2e^{-2\beta|J|}(1-e^{-2\beta|J|}) \tag{4.16c}$$

they randomly choose one of the two satisfied bonds which are perpendicular to the unsatisfied bond. This bond and the unsatisfied bond are deleted while the other two are frozen. The probabilities of all other possible modifications of the interaction vanish since they are incompatible with the rule that only satisfied bonds may be frozen.

Now let us use Eq. (2.4) to calculate the modified energies $\tilde{V}_i^l(\tilde{u})$, and show that modification $i=1$ indeed deletes all four bonds of a plaquette, while modifications $i=2,3,\ldots,7$ freeze two bonds and delete the two remaining ones. Consider first modification $i=1$. If three of the bonds of plaquette l are unsatisfied in configuration $\tilde{u}$, we have $V_l(\tilde{u})=2|J|$ and $V_1^l(\tilde{u})=1$, and therefore

$$\tilde{V}_1^l(\tilde{u})=2|J|+C_1^l . \tag{4.17}$$

If, on the other hand, only one of the bonds of plaquette l is unsatisfied, we have to use Eq. (4.16a) together with $V_l(\tilde{u})=-2|J|$. Relation (4.16a) was so chosen that Eq. (4.17) for $\tilde{V}_1^l$ holds in this case as well. Thus the interaction obtained when modification $i=1$ is chosen is independent of the configuration $\tilde{u}$, as is the "interaction" obtained by deleting all bonds. We may now choose

$$C_1^l=-2|J| \tag{4.18}$$

to get $\tilde{V}_1^l=0$ for any configuration $\tilde{u}$.

To calculate the modified energies $\tilde{V}_i^l$ for $i\geq 2$, denote by α_1 and α_2 the two bonds that modification i freezes. Unless both α_1 and α_2 are satisfied in $\tilde{u}$, we have $P_i^l(\tilde{u})=0$ (see above) and hence $\tilde{V}_i^l(\tilde{u})=\infty$. Such a configuration $\tilde{u}$ is therefore forbidden in the ensuing simulation with the modified Hamiltonian. This ensures that modification i indeed *freezes* the bonds α_1 and α_2. For all configurations $\tilde{u}$ in which both bonds *are* satisfied, we use Eq. (2.4) to get

$$\tilde{V}_i^l(\tilde{u})=-2|J|-\frac{1}{\beta}\ln\bar{p}+C_i^l , \tag{4.19}$$

with either $\bar{p}=p$ or $\bar{p}=\frac{1}{2}p'$ depending on i. As in the case $i=1$ it is convenient to choose the constants C_i^l so that the modified energies vanish:

$$C_i^l=2|J|+\frac{1}{\beta}\ln\bar{p} . \tag{4.20}$$

This shows that for any $i\geq 2$ the modified energy $\tilde{V}_i^l(\tilde{u})$ can take two possible values: Either $\tilde{V}_i^l(\tilde{u})=\infty$ (when a bond frozen in i is not satisfied in $\tilde{u}$), or $\tilde{V}_i^l(\tilde{u})=0$. In other words, all configurations consistent with the freezing scheme i have the same energy, as indeed should be the case when bonds are frozen or deleted. Note that our conclusion holds for any value of p. The particular choice (4.16b) made by Kandel, Ben-Av, and Domany ensures that the clusters generated by the procedure are never too large. They showed that at least two large clusters are created even at $T=0$ and therefore the lattice never freezes into a single cluster.

Finally, let us mention that Kandel, Ben-Av, and Domany use only freezing and deletion operations, and therefore (see Sec. II) their procedure defines a modified system of noninteracting clusters, which is trivial to simulate. To ensure ergodicity they supplement their algorithm by Metropolis sweeps.

V. SUMMARY

We have devised a general scheme for Monte Carlo simulations which encompasses many recently developed, seemingly unrelated cluster Monte Carlo techniques as special cases. In addition to this aesthetically pleasing unifying aspect, our scheme is also of practical relevance. As we have indicated in Sec. IV, there are two important steps in devising efficient cluster Monte Carlo algorithms. First, one has to identify the relevant large-scale moves, and choose the type of clusters to be formed by the algorithm accordingly. The physical properties of the system, which are responsible for slowing down of standard simulation techniques, have to be taken into account at this first stage. For example, in ferromagnetic Ising models the appropriate moves are coherent flips of clusters of spins. Such large-scale flips, however, do not suffice in O(n) models, where the relevant moves are reflection of blocks of O(n) spins with respect to a randomly chosen

direction in spin space. Our general scheme does not improve our understanding of the large-scale physics of the system, and therefore does not determine the appropriate moves. Experience in using the scheme may, however, give hints on possible moves and types of clustering. Secondly, one has to incorporate the chosen moves within an ergodic Monte Carlo procedure that satisfies the detailed balance condition. This is where our scheme becomes most useful. One may use it to devise, on an engineering level, legitimate Monte Carlo procedures that perform the appropriate moves. This was demonstrated in detail in Sec. IV on the cluster algorithm for the fully frustrated Ising model.[9] Knowledge of the physical properties of the system allowed Kandel, Ben-Av, and Domany to put restrictions on the possible clustering and moves. They came to the conclusion that one has to deal with plaquettes rather than single bonds. At $T=0$ they wanted to either delete all four bonds of a plaquette or freeze two satisfied parallel bonds, while deleting the other two. Under these restrictions, our scheme completely determines their algorithm (even for $T\neq 0$).

Our general strategy is to modify the Hamiltonian of the system in a probabilistic manner, with the hope that the modified Hamiltonian may be simulated more efficiently. We have shown that our scheme satisfies the detailed balance condition, justifying its use as a legitimate Monte Carlo procedure. However, one has to be cautious; we have not proved that the method is ergodic. The condition of ergodicity cannot be proven in general, and has to be shown separately for each particular algorithm. In some cases the procedure has to be supplemented by sweeps of a different (sometimes less efficient) algorithm to ensure ergodicity. Even if the added procedure is very slow, the performance of the algorithm as a whole need not degrade as was emphasized in Sec. III.

As was shown in Sec. IV, most existing cluster Monte Carlo algorithms are special cases of our scheme. We have demonstrated that the SW procedure[1] for Potts models, the generalizations of Edwards and Sokal[4] and of Niedermayer,[3] Wolff's algorithm[5] for O(n) models, the ϕ^4 cluster algorithm,[6] and the simulation method of Kandel, Ben-Av, and Domany[9] for the fully frustrated Ising model on the square lattice can all be described in terms of our method. Clearly, our procedure contains many other possibilities and is far more general than any of the techniques mentioned above. It may therefore serve as a general framework for the development of new efficient simulation methods.

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*Present address: Department of Theoretical Physics, University of Oxford, Oxford OX1 3NP, England.

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