# Critical Clusters and Efficient Dynamics for Frustrated Spin Models

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A general method to find, in a systematic way, efficient Monte Carlo cluster dynamics among the vast class of dynamics introduced by Kandel *et al.* [Phys. Rev. Lett. **65**, 941 (1990)] is proposed. The method is successfully applied to a class of frustrated two-dimensional Ising systems. In the case of the fully frustrated model, we also find the intriguing result that critical clusters consist of self-avoiding walk at the $\theta$ point.

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Since the pioneering work of Swendsen and Wang (SW) [1] on Monte Carlo (MC) cluster dynamics there have been many developments [2–9]. Nevertheless, a general scheme to implement an efficient cluster dynamics for general frustrated systems is still missing.

The original idea of SW is based on a cluster approach to spin systems introduced by Fortuin and Kasteleyn (FK) [10] and developed by Coniglio and Klein (CK) [11]. In the FK approach the clusters are defined in an annealed model equivalent to the original one. In the CK approach, instead, the clusters are defined directly in the original system. In particular, in the nearest neighbors (nn) ferromagnetic Ising model, for a given configuration of spin $\{S_i\}$, the CK clusters are defined as maximal sets of nn parallel spins connected by bonds. The probability of a bond being present between a nn parallel pair of spins is given by $p = 1 - e^{-2J\beta}$ where $J$ is the nn Ising spin interaction and $\beta = 1/k_BT$. Note that the bonds are fictitious; they do not affect the interaction energy, but only the cluster definition.

The clusters so defined have the property of percolating at the Ising critical point. In fact it can be shown that [10,12]

$$\langle S_iS_j\rangle = \langle \gamma_{ij}\rangle, \tag{1}$$

where $\langle S_iS_j\rangle$ is the spin-spin pair correlation function and $\langle\gamma_{ij}\rangle$ is the probability that $i$ and $j$ are in the same cluster. Here the indicator $\gamma_{ij}$ is 1 or 0 depending on whether or not sites $i$ and $j$ belong to the same cluster. The average, $\langle\cdot\rangle$, is over all the spins and bond configurations. These clusters have been extensively studied. In particular it has been shown that they have a fractal structure made of links and blobs [13] in a manner similar to the well known structure of percolation clusters.

The SW dynamics is generated by flipping in one step all the spins in the same cluster with probability 1/2 and the main reason for its efficiency stems from the equality (1) which relates the clusters to regions of correlated spins.

The generalization of CK clusters to Ising systems with positive and negative nn quenched interactions, $J_{ij} = \pm J$, with the Hamiltonian

$$H = -\sum_{\langle ij\rangle}(J_{ij}S_iS_j - J) \tag{2}$$

is straightforward. In this case the bonds can be present only between spins $i$ and $j$ satisfying the interaction, i.e., $\epsilon_{ij}S_iS_j = 1$ ($\epsilon_{ij} = J_{ij}/J$ is the sign of the interaction), with probability given by

$$P = (1 - e^{-2J\beta})\delta_{\epsilon_{ij}S_iS_j,1}. \tag{3}$$

The Kronecker delta $\delta_{\epsilon_{ij}S_iS_j,1}$ takes into account the fact that the probability is zero if the spins do not satisfy the interaction. For a given configuration of interaction $\{J_{ij}\}$, *without frustration*, Eq. (1) takes the form [14,15]

$$\langle S_iS_j\rangle = \langle\gamma_{ij}^{\parallel}\rangle \quad \text{if} \quad \langle S_iS_j\rangle > 0, \tag{4}$$

$$\langle S_iS_j\rangle = -\langle\gamma_{ij}^{\nparallel}\rangle \quad \text{if} \quad \langle S_iS_j\rangle < 0, \tag{5}$$

where $\gamma_{ij}^{\parallel}$ ($\gamma_{ij}^{\nparallel}$) is 1 or 0 depending on whether or not spins $i$ and $j$ are in the same cluster and parallel (antiparallel). Equations (4) and (5) are equivalent to

$$|\langle S_iS_j\rangle| = \langle\gamma_{ij}\rangle, \tag{6}$$

where $\gamma_{ij} = \gamma_{ij}^{\parallel} + \gamma_{ij}^{\nparallel}$. Equation (6) implies that, for configurations of interaction $\{J_{ij}\}$ without frustration, the clusters still percolate at the critical temperature and the related SW dynamics is still efficient. For systems *with frustration*, instead, relation (1) is replaced by [14]

$$\langle S_iS_j\rangle = \langle\gamma_{ij}^{\parallel}\rangle - \langle\gamma_{ij}^{\nparallel}\rangle \tag{7}$$

and consequently

$$|\langle S_iS_j\rangle| \le \langle\gamma_{ij}\rangle, \tag{8}$$

implying, in general, that the clusters percolate at temperatures higher than the critical temperature as numerically shown in the 2D [16] and 3D [17] spin glasses and other frustrated systems [18]. In this case the clusters represent interfering fluctuations. Two spins can be parallel in one cluster and antiparallel in another, giving rise to a net correlation which is smaller than the cluster size [14]. Although the SW dynamics still satisfies the detailed balance, it is not efficient anymore due to the fact that the clusters no longer represent correlated spins.

A method to generate a vast class of cluster dynamics which satisfy detailed balance has been suggested by Kandel, Ben-Av, and Domany (KBD) [5,6]. Although for the particular case of the fully frustrated model they

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have been able to choose an efficient dynamics, in general the method does not identify those dynamics which will indeed lead to a reduction of the slowing down.

The aim of this Letter is to develop a method to choose, in a systematic way, efficient dynamics in the class of the KBD dynamics. We will be guided by the idea that the better Eq. (6) is satisfied the more efficient would be the cluster dynamics associated with it. Before going into the details of the method we give the procedure to define the clusters which lead to the KBD dynamics.

Following Refs. [5,6] we partition the lattice into basic units labeled by an index $l$ so that the Hamiltonian (2) can be decomposed into $H = \sum_l H_l$. $H_l$, for example, can be the Hamiltonian of a single pair, a plaquette, or larger units [Figs. 1(a)–1(c)]. To fix the ideas we consider the case in which $H_l$ is restricted to a single plaquette. We decompose the Hamiltonian $H_l$ into a set of new Hamiltonians. Each of them is obtained replacing each interaction $J_{ij}$ with a new interaction $\hat{J}_{ij}$ with the same sign of $J_{ij}$ and with strength $|\hat{J}_{ij}|$ which can be either 0 or $J' \mapsto \infty$. In this way we obtain 16 configurations of interaction which we label by the index $\alpha$. They correspond to the 16 Hamiltonians $\hat{H}_l(\alpha, \{S_i\}) = -\sum_{\text{plaq}}[\hat{J}_{ij}(\alpha) S_i S_j - |\hat{J}_{ij}(\alpha)|]$ where the sum is over nn spin pairs on the plaquette and $\hat{J}_{ij}(\alpha)$ is the value of the interaction between the spin pair $(ij)$ in the configuration $\alpha$. We assign to each interaction configuration $\alpha$ a weight $W_\alpha$ in such a way that the new partition function is equivalent to the original one:

$$\sum_{\{\alpha\}} W_\alpha e^{-\beta \hat{H}_l(\alpha, \{S_i\})} = e^{-\beta H_l(\{S_i\})}. \tag{9}$$

Each term of the left hand side of Eq. (9) divided by the normalizing factor $e^{-\beta H_l(\{S_i\})}$ gives the probability that in the plaquette $l$, given the spin configuration $\{S_i\}$, the interaction configuration $\alpha$ occurs:

$$P_\alpha(\{S_i\}) = \frac{W_\alpha e^{-\beta \hat{H}_l(\alpha, \{S_i\})}}{e^{-\beta H_l(\{S_i\})}}. \tag{10}$$

This equation generalizes Eq. (3). More precisely the procedure to construct clusters in the original spin system (2) interacting via $\{J_{ij}\}$ is the following. Given a spin configuration, $\{S_i\}$, we assign to each plaquette $l$ a bond configuration $\alpha$ with a probability $P_\alpha(\{S_i\})$ [19]. Once a realization of bonds is obtained on each plaquette, two spins in the entire lattice are said to be in the same cluster if they are connected by at least one chain of bonds. The factor $e^{-\beta \hat{H}_l(\alpha, \{S_i\})}$ in Eq. (10) assures that bonds can only be present between spins satisfying the interaction [20]. It can be shown that the SW cluster dynamics related to these clusters satisfies detailed balance [6] and that Eq. (7) still holds [15].

In general Eq. (9), beside the standard solution [21], has many other solutions. How can we choose the solution which leads to a cluster dynamics able to reduce the critical slowing down? In simple cases, like the fully frustrated (FF) model, one might be guided by intuition [5]. For more complex cases like the asymmetric fully frustrated (AFF) model, which we will consider later, or when one goes beyond the single plaquette [see, for instance, Fig. 1(c)], the choice becomes extremely difficult and one needs a systematic procedure. Our proposal is to choose the solution, $W_\alpha$, which satisfies Eq. (6) for all pairs $ij$ on a subsystem made by a single isolated unit, namely,

$$|\langle S_i S_j \rangle_l| = \langle \gamma_{ij} \rangle_l \tag{11}$$

for each $ij$ on the unit $l$ [22]. Here

$$\langle \cdots \rangle_l = \frac{\sum_{\alpha, \{S_i\}} \cdots P_\alpha(\{S_i\}) e^{-\beta H_l(\{S_i\})}}{\sum_{\{S_i\}} e^{-\beta H_l(\{S_i\})}}. \tag{12}$$

To check whether this scheme works we consider the 2D AFF model where each plaquette contains three equal ferromagnetic bonds $J$ and one antiferromagnetic bond $-XJ$ $(0 \le X \le 1)$ [Fig. 1(d)]. This model interpolates between the FF model $(X = 1)$ and the diluted ferromagnetic Ising model $(X = 0)$. According to the scheme outlined the system is divided into plaquettes in a checkerboard manner and for the $l$th plaquette we identify the configurations as shown in Fig. 2. Because of the symmetry the number of independent weights reduces to nine [23]. From Eq. (9) and condition (11) we get a set of equations whose solution is given by

$$W_1 = u^3, \quad W_2 = u^2(u^X - u), \tag{13}$$

$$W_4 = u(1 + u^2 - 2u^{X+1}) \tag{14}$$

and

$$2W_6 = \begin{cases} (1-u^2)(u^X - u), & u > u^*, \\ 2W_4, & u < u^*, \end{cases} \tag{15}$$

$$2W_5 = \begin{cases} u(3+u^2) - u^X(1+3u^2), & u > u^*, \\ 0, & u < u^*, \end{cases} \tag{16}$$

$$W_8 = \begin{cases} 0, & u > u^*, \\ u^X - u^3 - 3u + 3u^{X+2}, & u < u^*, \end{cases} \tag{17}$$

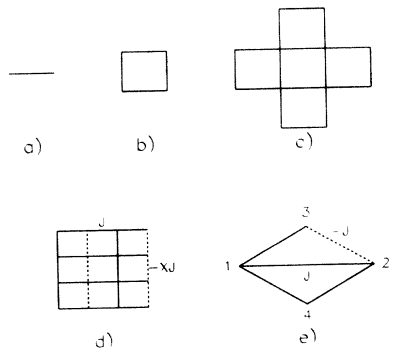


FIG. 1. (a)–(c) Basic units giving three possible partitions of a square lattice; (d) the AFF lattice; (e) the basic cell of a decorated Ising model where each spin pair of the square lattice (1,2) is decorated with two extra spins (3,4). In (d) and (e) ferromagnetic (antiferromagnetic) interactions are shown as solid (dashed) lines.

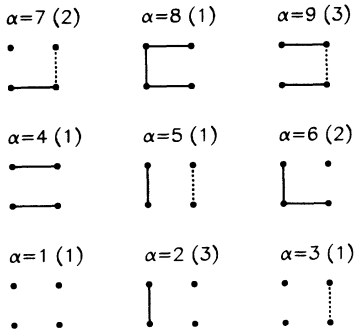


FIG. 2. Nine of the sixteen interaction configurations, labeled by $\alpha$, in which a plaquette of the AFF model can be decomposed. The infinite strength ferromagnetic bonds (antiferromagnetic) are shown as solid (dashed) lines; no line means zero strength interaction. The integers in brackets give the number of interaction configurations to which we assign the same weight. The configuration $\alpha = 16$, made of four infinite strength interactions, is irrelevant since the associated weight, $W_{16}$, always enters in the combination $W_{16}e^{-\beta \hat{H}_l(\alpha=16,\{S_i\})}$ which is 0 for any spin configuration.

where $u = e^{-2J\beta}$ and $u^*$ is the solution of the equation $(1 + 3u^2)u^X - u^3 - 3u = 0$. Furthermore, $W_3 = W_7 = W_9 = 0$. From the $W_\alpha$ using (10) we get the $P_\alpha$. For $X = 0$ (diluted ferromagnetic Ising model) it can be shown, after some algebra, that the solution factorizes and gives the standard solution [21] which, in this case, is extremely efficient. For $X = 1$ (FF model) we get $W_1 = u^3$ and $W_4 = W_5 = u(1 - u^2)$ while all the other weights vanish. The resulting cluster dynamics is different from that initially proposed in Ref. [5] and coincides with the one proposed later by the same authors, which gives very good results [7]. To check the efficiency for general $X$ we have calculated for various values of $X$ and lattice sizes $L$ up to $L = 120$ the magnetization $M$, and the autocorrelation function

$$\phi(t) = \frac{\langle |M(t)||M(0)| \rangle - \langle |M(t)| \rangle^2}{\langle M(0)^2 \rangle - \langle |M(0)| \rangle^2} \tag{18}$$

for various temperature ranges around the critical temperatures $T_c(X)$. The averages are taken over 50 000 MC sweeps after discarding the first 10 000. For the various values of $X$ studied we find, around the critical temperatures, a very strong reduction of the critical slowing down as shown in Fig. 3 for $X = 0.5$. We have also calculated the critical temperature $T_c(X)$, the susceptibility exponent $\gamma$, and the correlation exponent $\nu$ and found that the data agree, within the numerical errors, with the exact values [24,25] which are $T_c = 0$, $\gamma = 3/2$, and $\nu = 1$ for $X = 1$, while $T_c(X) \neq 0$, $\gamma = 7/2$, and $\nu = 1$ for $X \neq 1$. To check whether Eq. (6) is reasonably satisfied for the entire lattice we have calculated the percolation temperature $T_p(X)$, the mean cluster size exponent $\gamma_p$, and the correlation length exponent $\nu_p$, and we have found, within the numerical error, that $T_p(X) = T_c(X)$,

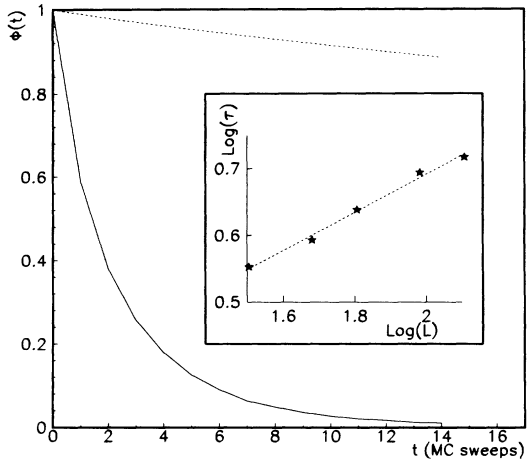


FIG. 3. The relaxation function $\phi(t)$ [see Eq. (18)] as a function of the time (MC steps) for the heat bath dynamics (dashed line) and for the cluster dynamic studied in this Letter (solid line) for the AFF model with $X = 0.5$. The system size is $L = 32$ and the temperature $T = 1.3$. Inset: The estimated value of the autocorrelation time $\tau = \sum_{t=0}^{\infty} \phi(t)$ as a function of the system size $L$ ($L = 32, 48, 64, 96, 128$) at the critical temperature $T_c = 1.23$. The estimated value of the dynamical exponent is $z \sim 0.3$.

$\nu_P = \nu$, and $\gamma_p = \gamma$. More details will be published in a forthcoming paper [15].

We have also investigated the geometrical structure of the critical clusters at $T_p(X)$ for $X = 0$ and $X = 1$ (Fig. 4). In the Ising case ($X = 0$) we find that a typical configuration of critical clusters is a fractal made of links and blobs as predicted theoretically [13]. For the FF case ($X = 1$), instead, we find a fractal structure made of a self-avoiding chain with fractal dimension $D = \frac{1}{2}(d + \gamma/\nu) = \frac{7}{4}$ which coincides with the fractal dimension of a 2D self-avoiding walk (SAW) at the $\theta$ point [26].

We have also applied the same scheme to a ferromagnetic Ising model where each spin pair is decorated as in Fig. 1(e). Again our scheme, applied at a level of single spin pair (standard SW dynamics), does not reduce the slowing down while, applied to the set of spins formed by

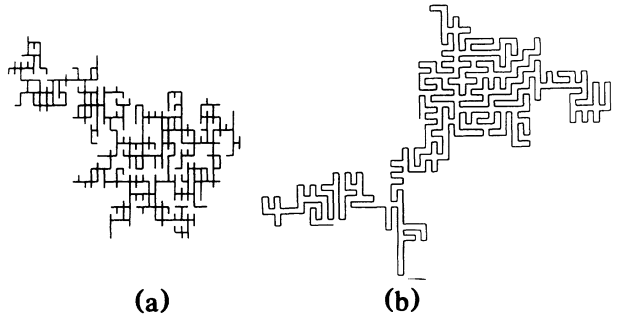


FIG. 4. Critical clusters at the critical temperature for systems with $L = 60$; (a) for the diluted ferromagnetic Ising model ($X = 0$); (b) for the FF model ($X = 1$).

a spin pair plus the two decorating spins, it restores the efficiency of the cluster algorithm [15].

It is natural to wonder if the same scheme can be used for the $\pm J$ Ising spin glass model. We have simulated the Ising spin glass model for different concentrations, $c$, of antiferromagnetic interactions with cluster dynamics based (1) on a pair unit [Fig. 1(a)] and (2) on a plaquette [Fig. 1(b)]. In the range $0 < c < 0.1$, we have found that in the first case the percolation temperature $T_p(c)$ is higher than that found in the second case. At the same time, as expected from the lowering of $T_p(c)$, the estimated relaxation time for the plaquette dynamics becomes smaller than the one for the dynamics based on a pair unit. Therefore we have registered an improvement passing from pair to plaquette dynamics [15]. These results suggest that going to dynamics based on larger units [Fig. 1(c)] would be possible to decrease the critical slowing down in a systematic way.

In conclusion, we have proposed a systematic way to improve the SW cluster algorithm for frustrated spin models. At the lowest level (pair) the algorithm coincides with the SW algorithm which is efficient for nonfrustrated systems. At the next level (plaquette) we find a cluster dynamics which efficiently applies to the AFF model for all values of the parameter $X$. For spin glass one has to go to higher levels by choosing larger units. This is currently being investigated. We have also found the intriguing result that the critical cluster in the FF model is a typical SAW configuration at the $\theta$ point. This means that correlations travel along a one-dimensional path consistently with the zero temperature transition.

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[19] To be precise the bonds now must be considered fictitious like in the CK clusters. We label the bond configurations by the same symbol $\alpha$ used to label the interaction configurations ($\infty$ interactions are mapped into present bonds).
[20] When $l$ corresponds to a single pair $(ij)$, Eq. (10) reproduces the standard solution (3). In fact, say $\alpha = 1$ ($\alpha = 2$) the configuration of an absent (present) bond between spins $i$ and $j$. The solution of Eq. (9) is $W_1 = e^{-2J\beta}$ and $W_2 = 1 - e^{-2J\beta}$ and $e^{-\beta\hat{H}(\alpha,\{S_i\})} = \delta_{\epsilon_{ij}S_iS_j,1}$. From Eq. (10) it follows that the probability of a bond being present, $P_2$, is given by Eq. (3) while the probability of it being absent is $P_1 = 1 - P_2$.
[21] By standard solution we mean that $P_\alpha$, written in terms of $W_\alpha$, can be factorized in terms of $P$ and $1 - P$ with $P$ given by Eq. (3). In this case the clusters coincide with the standard CK clusters.
[22] Note that the condition (11) is satisfied only on a single unit. This does not imply that Eq. (6) is necessarily satisfied on the entire lattice [Eq. (6)]. On the other hand, the larger the unit for which (11) holds, the better Eq. (6) is satisfied. However, for ferromagnetic or unfrustrated systems the solution which satisfies Eq. (11) on a single bond [Eq. (3)] satisfies Eq. (11) on any larger units. In fact it satisfies Eq. (6) on the entire lattice for any $i$ and $j$. This consideration gives a hint that in the more general case of frustrated systems it is enough to satisfy (11) on a smaller unit to ensure that Eq. (6) is well approximated.
[23] In the general case the number of equations introduced by (9) and (11) may be different from the number of unknowns $W_\alpha$. If the solution is not unique, we expect that any solution leads to improved dynamics and, going to larger and larger units, all of them will give the same result. On the other hand, when Eqs. (9) and (11) do not have solutions we can relax Eq. (11) by requiring only the equality of the moments $\sum r_{ij}^k \langle \gamma_{ij} \rangle = \sum r_{ij}^k \langle S_i S_j \rangle$ ($r_{ij}$ is the distance between sites $i$ and $j$) and choosing $k$ in such a way that, at least, a solution can be obtained.
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