New cluster method for the Ising model ⋆

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Abstract. We describe a cluster method for the Ising model. It is based on a new representation of the model in any dimension, which contains both the bond variables of the High-Temperature representation and those of the Fortuin-Kasteleyn clusters, and is similar to the representation in terms of spins and bond variables which underlies the Swendsen-Wang method. Magnetic fields can be included as well. The scaling properties of this cluster method are investigated.

1 Introduction

Different representations of the Ising model have been the basis for both theoretical and computational progress. The Fortuin-Kasteleyn (FK) random cluster representation [1] provides direct access to correlation functions. The corresponding joint Edwards-Sokal-Fortuin-Kasteleyn (ESFK) representation of spins and bonds [2] is the basis for the Swendsen-Wang cluster algorithm [3].

In this paper we will introduce two new joint representations that connect spins and FK-bonds with the bonds of the exact "High-Temperature"-representation of the Ising model. All the other representations in terms of spins and bonds then follow immediately by marginalization. Our bond-bond representation provides new insight into the FK cluster structure. It also implies a cluster algorithm, in the same way that the ESFK representation implies the Swendsen-Wang method, and allows the inclusion of a magnetic field, which is difficult with other schemes.

Existing representations: The Ising model on any graph Λ is expressed by the partition function

$$Z = \sum_{\{s\}} e^{\beta \sum_{\langle ij \rangle} s_i s_j} \ , \tag{1}$$

where $\langle ij \rangle$ are the edges in Λ, $s_i = \pm 1$, and $\beta = \frac{J}{k_b T}$. For each edge, one can use the simple algebraic identity [1,2]

$$\begin{aligned} e^{-\beta}\, e^{\beta s_i s_j} &= e^{-2\beta} + (1 - e^{-2\beta})\, \delta_{s_i s_j} \\ &= \sum_{f_{ij}=0,1} \left[\delta_{f_{ij},0}\, e^{-2\beta} + \delta_{f_{ij},1}\, (1 - e^{-2\beta})\, \delta_{s_i s_j} \right] \ , \end{aligned} \tag{2}$$

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which introduces new bond variables f_{ij}, and one obtains the ESFK representation

$$Z = e^{\beta V d} \sum_{\{f\}} \sum_{\{s\}} \prod_{\langle ij \rangle} \left[\delta_{f_{ij},0} \, (1-p) \; + \; \delta_{f_{ij},1} \, \delta_{s_i s_j} \, p \right] \; , \tag{3}$$

where Vd is the number of edges $\langle ij \rangle$ and $p = (1 - e^{-2\beta})$. Summing over spins then gives the Fortuin-Kasteleyn random bond representation

$$Z \; = \; e^{-\beta V d} \sum_{\{f\}} (e^{2\beta} - 1)^{n_f} \;\; 2^{\#clusters} \; , \tag{4}$$

where n_f is the number of bond variables that are "on" ($f_{ij} = 1$), and $\#clusters$ is the number of connected clusters of such bonds. This representation is also the basis for rigorous studies.

Observables can be written purely in bond-representation (so called "improved estimators" in computational language), e.g.

$$\langle s_i s_j \rangle \;\; = \;\; \langle \; \delta(\text{i and j are in the same cluster}) \; \rangle \; . \tag{5}$$

As pointed out by Edwards and Sokal [2], the joint representation (3) immediately implies the Swendsen-Wang cluster algorithm: Given a configuration $\{s_i\}$ of spins, on can generate bond variables f_{ij} with the conditional probabilities following from (3), namely $s_i = s_j$ implies that $f_{ij} = 1$ with probability $\frac{p}{(1-p)+p} = p$, and $s_i \neq s_j$ implies $f_{ij} = 0$, because then only the first term of (3) contributes. Conversely, given a configuration of bond variables $\{f_{ij}\}$, (3) implies that for $f_{ij} = 1$ we have $s_i = s_j$, i.e., all sites in a cluster have a common spin value; whereas $f_{ij} = 0$ does not imply any constraints on the product $s_i s_j$, i.e., the spin values of different clusters are independent of each other.

The Swendsen-Wang algorithm iterates these steps [2] and drastically reduces critical slowing down [4] in simulations of the Ising and related models.

In the present paper, we will connect representations (1), (3), and (4) with the exact "High Temperature Representation" of the Ising model. That representation follows from the simple algebraic identity

$$\begin{aligned} e^{\beta s_i s_j} &= \cosh\beta \qquad\quad [\;\; 1 \;\; + \qquad (\tanh\beta)\, s_i s_j] \\ &= \cosh\beta \sum_{b_{ij}=0,1} \left[\delta_{b_{ij},0} \; + \; \delta_{b_{ij},1} (\tanh\beta)\, s_i s_j \right] \; , \end{aligned} \tag{6}$$

which introduces another, different, set $\{b_{ij}\}$ of bond-variables. Inserting (6) into (1) results in the joint representation

$$Z = (\cosh\beta)^{Vd} \sum_{\{s\}} \sum_{\{b\}} \prod_{\langle ij \rangle} \left[\delta_{b_{ij},0} \; + \; \delta_{b_{ij},1} \, (\tanh\beta) s_i s_j \right] \; . \tag{7}$$

Note that a cluster algorithm using the conditional probabilities of this representation would be possible, but would have a bad sign problem, since due to $s_i s_j = \pm 1$ the conditional probability for $b_{ij} = 1$ could be negative.

Summing over spins in (7), one notes that at each site i only *even* powers of s_i survive, which means that an even number of bonds $b_{ij} = 1$ must meet at each site. Writing this constraint as "$\partial b = 0$", we obtain the high temperature (HT) representation

$$Z = (\cosh\beta)^{Vd}\ 2^V \sum_{\{b\};\partial b=0} \prod_{\langle ij\rangle} \left[\delta_{b_{ij},0}\ +\ \delta_{b_{ij},1}\,(\tanh\beta)\right] \tag{8}$$

(with V the number of sites in the graph), which is an exact representation, and can be used as the basis for the high temperature expansion in powers of $\tanh\beta$. The bonds of the FK representation (4) and the high temperature representation (8) have up to now been completely unrelated.

2 New joint representation

We start again from a simple algebraic identity,

$$1 + O\,t = \sum_{b=0,1} \delta_{b,0}\ +\ \delta_{b,1}\,O\,t \tag{9a}$$

$$= \sum_{f=0,1} \sum_{b=0,1} \left[\delta_{f,1}\,(\delta_{b,0} + \delta_{b,1}\,O)\,t\ +\ \delta_{f,0}\,\delta_{b,0}\,(1-t)\right]\ , \tag{9b}$$

which introduces two auxiliary variables b and f. This transformation can, e.g., separate some operator O from its weight t. By applying (9b), with $O = s_i s_j$, $t = \tanh\beta$, to the joint representation (7) of spins and high-temperature bonds b_{ij}, we obtain our new representation for the partition function of the Ising model

$$\boxed{Z = (\cosh\beta)^{Vd} \sum_{\{s\}} \sum_{\{f\}} \sum_{\{b\}} \prod_{\langle ij\rangle} \Big[\ \delta_{f_{ij},1}\,(\delta_{b_{ij},0}\ +\ \delta_{b_{ij},1}\,s_i s_j)\,t \\ +\ \delta_{f_{ij},0}\ \ \delta_{b_{ij},0}\,(1-t)\Big]\ .} \tag{10}$$

Now we note that by summing over the bond variables b_{ij} and using $(1 + s_i s_j) \equiv 2\delta_{s_i s_j}$, we obtain

$$Z = (\cosh\beta)^{Vd} \sum_{\{s\}} \sum_{\{f\}} \prod_{\langle ij\rangle} \left[\delta_{f_{ij},1}\,\delta_{s_i s_j}\,(2t)\ +\ \delta_{f_{ij},0}\,(1-t)\right] \tag{11}$$

$$\equiv e^{\beta V d} \sum_{\{s\}} \sum_{\{f\}} \prod_{\langle ij\rangle} \left[\delta_{f_{ij},1}\,\delta_{s_i s_j}\ \ p\ \ +\ \delta_{f_{ij},0}\,(1-p)\right]\ ,$$

i.e., (9b) contains the identity (2), and we reproduce, bond by bond, the ESFK representation (3). Thus the bond variables f_{ij} in (10) are the *same* as the FK bond variables in (3,4) and, *equation (10) provides a new joint representation of the Ising model in terms of spins s_i, FK-bonds f_{ij} and high-temperature bonds b_{ij}.*

We obtain another new representation by summing over spins s_i in (10). Again this leads to the constraint $\partial b = 0$, giving

$$\boxed{Z = (\cosh\beta)^{Vd}\, 2^V \sum_{\{f\}} \sum_{\{b\};\partial b=0} \prod_{\langle ij\rangle} \left[\delta_{f_{ij},1}\, t \;+\; \delta_{f_{ij},0}\; \delta_{b_{ij},0}\, (1-t)\right] \;,} \tag{12}$$

a joint representation in terms of FK-*bonds* f_{ij} and high-temperature *bonds* b_{ij}. This will be the basis for a new cluster method, introduced below.

Eq. (10), in terms of variables s, f, b, contains all the other representations we have mentioned. They can be obtained simply by marginalization, i.e. by summing over the unneeded, so-called "nuisance" variables. Thus (10) contains the representation (1) in terms of spins s_i, the FK representation (4) in bonds f_{ij}, the high temperature representation (8) in bonds b_{ij}, the ESFK representation (3) in spins s_i and bonds f_{ij}, the joint representation (7) in spins s_i and bonds b_{ij}, and the new representation (12) in bonds f_{ij} and bonds b_{ij}.

3 Some consequences

The representations (10),(12) imply new relations between Fortuin-Kasteleyn clusters and High-Temperature clusters.

To start, having representations in terms of different variables means that thermodynamic quantities can be expressed in several ways. For example, eqs. (1),(4),(5),(8) imply the known relations (with i, j being neighboring sites)

$$E = -Vd\,\langle s_i s_j\rangle \tag{13a}$$

$$= Vd \;-\; \frac{2}{1-e^{-2\beta}}\,\langle n_f\rangle \tag{13b}$$

$$= -\sum_{\langle ij\rangle} \langle\, \delta(i,j \text{ in same cluster})\,\rangle \tag{13c}$$

$$= -Vd\tanh\beta \;-\; (\frac{1}{\tanh\beta} - \tanh\beta)\,\langle n_b\rangle\;, \tag{13d}$$

and thus

$$\langle n_b\rangle \;=\; \frac{e^{2\beta}+1}{2}\,\langle n_f\rangle \;-\; Vd\,(e^{2\beta}-1)\;, \tag{14}$$

where n_f, n_b are the number of bonds $f_{ij}=1$, resp. $b_{ij}=1$. Similar relations follow from other derivatives of Z.

We can obtain new relations between the two kinds of bond clusters by considering the *conditional probabilities* between $\{f\}$ and $\{b\}$ which follow from (12):
Given a configuration of FK-bonds $\{f\}$:

$$\text{if } f_{ij}=0,\;\text{ then } b_{ij}=0 \text{ with probability } \tfrac{1-t}{1-t}=1; \tag{15}$$

$$\text{if } f_{ij}=1,\;\text{ then any } \{b\} \text{ that satisfies } \partial b=0 \text{ is equally probable.} \tag{16}$$

Given a configuration of HT-bonds $\{b\}$

$$\text{if } b_{ij} = 0, \text{ then } f_{ij} = 1 \text{ with probability } \frac{t}{1+(1-t)} = t \; ; \tag{17}$$

$$\text{if } b_{ij} = 1, \text{ then } f_{ij} = 1 \text{ with probability } \frac{t}{t} = 1. \tag{18}$$

These relations imply that *high-temperature-clusters are strictly contained within Fortuin-Kasteleyn clusters*. This appears to be a new result connecting the previously unrelated FK-clusters (corresponding to subsets of regions of "flipped spins" of the low-temperature expansion) and the clusters of the High-Temperature representation, in any dimension and at any temperature. It implies, e.g., that the size of HT-clusters cannot grow faster than that of FK-clusters.

Most interestingly, we obtain a physical meaning for the geometric classification of bonds in FK-clusters. Specifically, the HT bonds $\{b\}$ turn out to be the "black" and "red" bonds in the classification of Caselle and Gliozzi [5]. This provides a physical framework to understand why, indeed, just the black and red bonds suffice to provide the very interesting geometric estimator for a thermodynamic quantity, the specific heat, which was constructed by Caselle and Gliozzi [5].

4 Cluster algorithm

The Swendsen-Wang algorithm implements the conditional probabilities following from the ESFK joint representation (3), as explained in the introduction. In the same way, the new joint bond-bond representation (12) implies a different cluster algorithm, which switches back and forth between configurations $\{b\}$ of HT-bonds and configurations $\{f\}$ of FK-bonds, with the conditional probabilities given in (15–18).

For a specific case, an equivalent cluster-algorithm has been found before, namely the method which Ben-Av et al. [6] developed for 3-dimensional Z(2) lattice gauge theory. In fact, that algorithm was the starting point (with M. Marcu) for our investigation. We noted that it could be seen as a procedure for the dual of 3d Z(2) gauge theory, namely the high-temperature-representation of the 3d Ising model, and could then be generalized to any dimension. Eventually this led us to the new representation (10).

Ben-Av et al. provided an ingenious way to satisfy eq. (16), i.e., to generate a random bond configuration $\{b_{ij}\}$ with constraint $\partial b = 0$, and with equal probability for each allowed configuration. For completeness we provide our version of this procedure here, with an example in fig. 1.

Since b-clusters are strictly contained within f-clusters (see above), the construction can be done for each f-cluster separately.

(1) Given an f-cluster (fig. 1a), construct any "spanning tree" (fig. 1b), i.e. a set of connected bonds reaching all sites of the cluster, without loops. For the present construction, all spanning trees are equivalent. To construct a

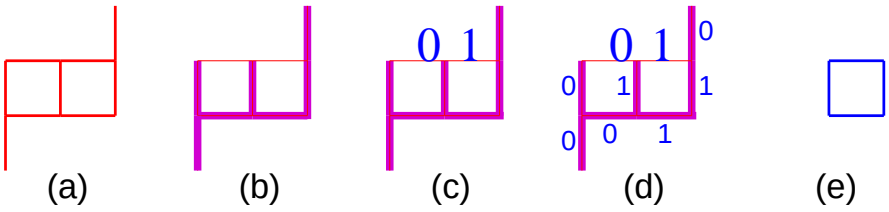

Fig. 1. Example for generating a divergence-free configuration of bonds b_{ij}.

spanning tree, start from any site (called the *root* of the tree), and perform a breadth-first-search ([7]): Put the initial site into a list. Iterate:
Go through all neighbors of the current site (in any order).
If the neighbor is in the f-cluster and is already contained in the list, use the bond towards that neighbor for step (2).
If the neighbor is in the f-cluster and is not yet in the list, add it to the end of the list. (The bond towards that neighbor belongs to the spanning tree, but we do not actually need to store it now). Mark the site as being in the list.
Take the next site from the list. Stop when there is no more next site.

(2) The bonds of the f-cluster which are not contained in the spanning tree correspond to loops of the f-cluster. On each of these bonds, choose $b_{ij} = 0$ or $b_{ij} = 1$ at random with equal probability (fig. 1c). In practice this can already be done during construction of the spanning tree, step (1). If there are n_l such bonds, then 2^{n_l} different choices are possible.

(3) The "zero divergence condition" $\partial b = 0$ now uniquely fixes the value of all other b_{ij} in this cluster. To evaluate them, work backwards through the list of sites in the spanning tree, and at each site evaluate b_{ij} for the (one !) bond of the spanning tree which leads to its parent site. (See fig. 1d).

(4) The result is a new b-cluster (fig. 1e). Each choice in step (2) results in a different b-cluster.

Since this cluster algorithm, based on (12), contains the FK clusters, one can use the same improved estimators (i.e. observables represented in bonds f_{ij}) as for Swendsen-Wang. Similar to the Swendsen-Wang method, our algorithm can also be used in a single-cluster version [8]. For single-cluster algorithms in general, we showed recently that *infinite lattices* can be simulated directly [9], by making use of the improved estimator (5). Our new method can also be used with embeddings of the Ising model in other systems, like the $O(N)$ model [8,10].

5 Dynamical critical exponent

We have investigated the dynamical properties of the new algorithm on hypercubic lattices L^d with periodic boundary conditions, in $d = 2$, 3, and 4 dimensions at the critical temperature T_c [11]. We used the regular multi-cluster version of the algorithm, with 10^5 – 10^6 sweeps per lattice size.

For the observables energy, magnetization, susceptibility, and spatial correlation function at distance $L/2$, we measured the autocorrelation functions [10] via FFT, and determined their statistical errors by the jackknife procedure [12]. We fitted the asymptotic behavior as $\exp(-t_{MC}/\tau_{exp})$, where t_{MC} is the time separation in units of Monte-Carlo sweeps. In the fits we neglected the covariances of different distances in the respective autocorrelation function; thus our error-bars will be somewhat underestimated.

We found straight exponential decays (except at very small distances for observables other than the energy). The decay rate τ_{exp} was the same for all observables, within statistical errors. We determined the dynamical critical exponent z_{exp} from fits to $\tau_{exp} \sim L^{z_{exp}}$. Our main aim was to compare the HT algorithm to Swendsen-Wang, and we employed only moderate system sizes and statistics. The results for z_{exp} include the statistical errors from the fits, but no extrapolation of their dependence on the size of the largest lattice used.

Our results for z_{exp} with the Swendsen-Wang algorithm differ slightly from the apparently best measurements available for z in the literature [4]. For $d = 3$ and 4 these measurements are, however, for the exponent of the *integrated* autocorrelation times for the energy. They are $z_{exp} = z_{int} = 0.26(1)$ in $d = 2$; $z_{int,E} = 0.54(2)$ in $d = 3$; and $z_{int,E} = 0.86(2)$ in $d = 4$.

In $d = 2$ dimensions we found autocorrelation functions indistinguishable from those of the Swendsen-Wang procedure, apparently due to the self-duality of the model. As is already known for Swendsen-Wang, they are also compatible with a logarithmic dependence on L.

In $d = 3$ dimensions we found a critical exponent compatible with that of Swendsen-Wang, (and somewhat lower than measured by Ben-Av et al [6]), with a marginally larger prefactor for autocorrelation times.

In $d = 4$ dimensions the dynamical critical exponent is close to unity, noticeably higher than that of Swendsen-Wang, but still far below the value $z \approx 2$ of local updates.

We also used the pure high-temperature representation (8) to perform *local* updates, in which we proposed flips of b_{ij} on elementary plaquettes. (Note that with periodic boundary conditions, such local updates suffer from lack of ergodicity on finite systems, since they cannot generate b-clusters that completely wind around the lattice.) As expected, we found $z \approx 2$, with autocorrelation times far larger than those of the HT clusters (e.g. $\tau_{exp} \approx 45$ instead of ≈ 3.2 for a 16^2 lattice).

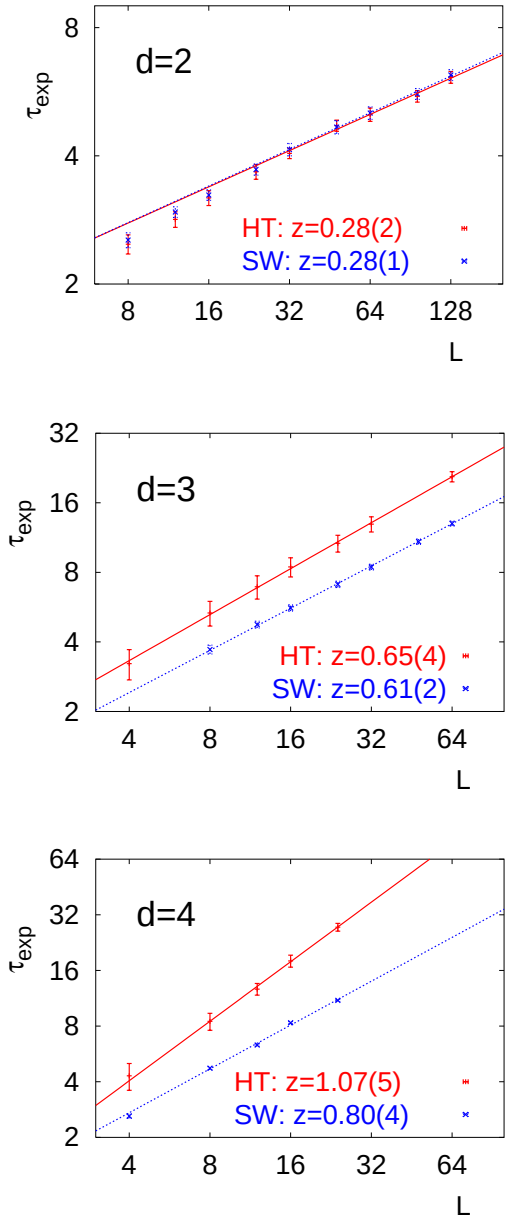

Fig. 2. Autocorrelation times and critical exponents z for the magnetization in the HT cluster algorithm, compared to those for the Swendsen-Wang method. The HT cluster algorithm corresponds to the upper curves, the SW algorithm to the lower ones. See text for interpretation of fitted critical exponents z.

6 Including a magnetic field

The same approach that led to (12) can also be used to include a magnetic field h. The partition function then contains a term $\exp(\beta h s_i)$ for each site, which we expand similar to the high-temperature representation (6), and to which we apply (9b):

$$e^{\beta h s_i} = c\,[1 + \eta s_i] \tag{19a}$$

$$= c \sum_{q_i=0,1} [\delta_{q_i,0} \,+\, \delta_{q_i,1}\, s_i\, \eta] \tag{19b}$$

$$= c \sum_{r_i=0,1} \sum_{q_i=0,1} [\delta_{r_i,1}\,(\delta_{q_i,0} + \delta_{q_i,1}\, s_i)\,\eta \;+\; \delta_{r_i,0}\,\delta_{q_i,0}\,(1-\eta)\,] \;, \tag{19c}$$

with $c = \cosh(\beta h)$ and $\eta = \tanh(\beta h)$. We have introduced two sets of sources $\{q_i\}$ and $\{r_i\}$. If we use (19b) with (6) then we obtain the high temperature representation with magnetic fields, in which lines of $b_{ij} = 1$ are either sourceless, like before, or end in sources $q_i = 1$, i.e. the combined constraint on bonds $\{b\}$ and sources $\{q\}$ can be written as "$\partial b = q$".

Here we use (19c). The product over sites of (19c) multiplies (10). Summing over spins s_i will now result in the additional constraint that there has to be an *even* number of sources $q_i = 1$ for each f-cluster. Eq. (12) then becomes

$$\begin{aligned} Z = (\cosh\beta)^{Vd}\, 2^V \sum_{\{f\}} \sum_{\{b\};\partial b=q} \prod_{\langle ij\rangle} \left[\delta_{f_{ij},1}\, t \,+\, \delta_{f_{ij},0}\, \delta_{b_{ij},0}\,(1-t)\right] \times \\ \times \cosh(\beta h)^V \sum_{\{r\}} \sum_{\{q \text{ even}\}} \prod_i \left[\delta_{r_i,1}\,\eta \,+\, \delta_{r_i,0}\,\delta_{q_i,0}\,(1-\eta)\,\right] \;, \end{aligned} \tag{20}$$

with an analogous generalization of (10). Eq. (20) can be used for a cluster update [13] analogous to the method above, with mappings between $\{f\}$ and $\{b\}$ and additionally with mappings between $\{r\}$ and $\{q\}$, using the conditional probabilities following from (20), which are analogous to those following from (12).

We note that our treatment of the magnetic field is equivalent to introducing a "ghost spin" $s_0 = +1$ in (10),(12), to which every other spin couples with strength h [3]. Then q_i could also be written as a "bond" variable b_{i0} and r_i as f_{i0}. Thus, if we sum over sources q_i in (19c) we recover the Swendsen-Wang algorithm with ghost spin, which performs well only in a very small magnetic field, since a single case of $q_i = 1$ in an FK-cluster suffices to freeze this cluster to the value $s_0 \equiv +1$.

However, in (20) we progress differently. There is no "freezing" of (f, r) clusters, since spins do not appear in (20), and sources r_i and q_i can fluctuate

even in a strong field. Note that summing over bonds $\{b_{ij}\}$ and sources $\{q_i, r_i\}$ in (20) must recover the FK-like representation

$$Z \;=\; e^{-\beta V d} \sum_{\{f\}} \left(e^{2\beta}-1\right)^{n_f} \prod_{\text{clusters}} \left(e^{\beta h V_{cluster}} + e^{-\beta h V_{cluster}}\right) \;, \qquad (21)$$

where $V_{cluster}$ is the number of sites in a cluster. This expression follows directly from multiplying (3) with $\prod_i \exp(\beta h s_i)$ and summing over spins. Thus our approach (20) is an auxiliary-variable method to implicitly reweight the size of clusters.

7 Generic formalism for models with constraints

We can see (9b) as a formalization for "tentative updates" (including situations with global constraints), i.e., Monte Carlo steps in which some state $b = 1$ is *proposed* ($f = 1$) with a certain probability t, and performed with another probability depending on O.

More specifically, we use (9b) to write

$$\begin{aligned} &\mathrm{tr} \prod_i \left(1 + O_i t_i\right) \;= \\ &\mathrm{tr} \prod_i \sum_{f_i=0,1} \sum_{b_i=0,1} \left[\delta_{f_i,1} \left(\delta_{b_i,0} + \delta_{b_i,1}\, O_i\right) t_i \;+\; \delta_{f_i,0}\, \delta_{b_i,0} \left(1 - t_i\right)\right] \;. \end{aligned} \qquad (22)$$

We now view the $\{b_i\}$ as basic variables, with some trace over "spins" which may imply a global constraint. Then $f_i = 1$ can be seen as a *proposal* to *allow* $b_i = 1$, and Eq. (22) provides the conditional probabilities for generating $\{b\}$ given $\{f\}$ and vice versa.

One example where this procedure has implicitly been used is the paper by Ben-Av et al [6]. Another is the cluster method by Rieger and Kawashima [14] for the Ising model in a transverse field, where a set of sources q_i are proposed, and one realization of sources is later accepted subject to a constraint.

8 Conclusions

We have introduced a cluster algorithm for the Ising model (as well as for embeddings into other models). It corresponds to switching between configurations of Fortuin Kasteleyn bonds and High Temperature bonds in a new joint representation of the Ising model, which also sheds new light on the physical meaning of geometric properties of clusters. The dynamic critical exponent is as good as that of Swendsen and Wang in two and three dimensions, and slightly higher in four dimensions. Magnetic fields can be included in the procedure in a related way.

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