Comment on "Cluster Monte Carlo study of the antiferromagnetic $Z(q)$ model"

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It is shown that a recently proposed cluster-update Monte Carlo update for the general $Z(q)$ symmetric class of models [A. Benyoussef *et al.*, Phys. Rev. B **67**, 094415 (2003)] is in general not a valid Monte Carlo algorithm. As soon as coupling terms differing from that of the planar clock model are introduced, the proposed algorithm violates detailed balance. Independent of the choice of couplings the update is seen to be non-ergodic for models with an even number of states q. The latter deficiency can be easily amended and it is shown that the resulting algorithm for the case of the planar clock model with arbitrary number of states q is just a special case of the embedded cluster algorithm for the XY model introduced by Wolff.

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In Ref. 1, Benyoussef, Loulidi and Rachadi (henceforth denoted as BLR) present a cluster-update Monte Carlo algorithm for general, nearest-neighbor $Z(q)$ symmetric models with Hamiltonian

$$\mathcal{H} = -\sum_{\langle i,j\rangle}\sum_{m=1}^{\lfloor q/2\rfloor} J_m \cos\left[\frac{2\pi}{q}m(k_i-k_j)\right], \qquad (1)$$

where the state variables $k_i \in \{0,\ldots,q-1\}$. The $m=1$ term in Eq. (1) corresponds to the Hamiltonian of the planar clock model, to which the $Z(q)$ class reduces for $J_m = 0$, $m \geq 2$. In constructing their algorithm, they build upon the idea of embedding Ising spins into state variables of higher symmetry originally introduced by Wolff to formulate a cluster update algorithm for the $O(n)$ spin models[2]. These effective Ising variables can then be updated according to the cluster algorithm of Swendsen and Wang[3] (or its single-cluster variant due to Wolff[2]). An application of the same idea has been used to formulate a cluster update for the antiferromagnetic standard Potts model[4].

BLR's ansatz for constructing a cluster algorithm proceeds by splitting the Hamiltonian (1) with respect to one state $n \in \{0,\ldots,q-1\}$ according to the identity $\cos(a-b) = \cos a\cos b + \sin a \sin b$ in two parts, $\mathcal{H} = \mathcal{H}_1(n) + \mathcal{H}_2(n)$, where

$$\mathcal{H}_1(n) = -\sum_{\langle i,j\rangle}\sum_{m=1}^{\lfloor q/2\rfloor} J_m \cos[\delta(mk_i-n)]\cos[\delta(mk_j-n)], \qquad (2)$$

and

$$\mathcal{H}_2(n) = -\sum_{\langle i,j\rangle}\sum_{m=1}^{\lfloor q/2\rfloor} J_m \sin[\delta(mk_i-n)]\sin[\delta(mk_j-n)], \qquad (3)$$

with $\delta = 2\pi/q$. Defining effective Ising variables (i.e., signs) as

$$\epsilon_i(n) = \mathrm{sign}\{\sin[\delta(k_i-n)]\}, \qquad (4)$$

they recast $\mathcal{H}_2(n)$ in an Ising language as

$$\mathcal{H}_2(n) = -\sum_{\langle i,j\rangle} \tilde{J}_{ij}(n)\epsilon_i(n)\epsilon_j(n), \qquad (5)$$

with effective couplings $\tilde{J}_{ij}(n) = A_{ij}(n) + B_{ij}(n)$, where

$$\begin{aligned} A_{ij}(n) &= J_1|\sin[\delta(k_i-n)]\sin[\delta(k_j-n)]|, \\ B_{ij}(n) &= \sum_{m=2}^{\lfloor q/2\rfloor} J_m \frac{\sin[\delta(mk_i-n)]\sin[\delta(mk_j-n)]}{\epsilon_i(n)\epsilon_j(n)}. \end{aligned} \qquad (6)$$

Obviously, a similar transformation could be performed with the part $\mathcal{H}_1(n)$ instead. The cluster update should now proceed in the usual way, setting bonds between spins whose "Ising part" of the energy is negative, i.e., for which

$$-\tilde{J}_{ij}(n)\epsilon_i(n)\epsilon_j(n) < 0, \qquad (7)$$

according to the probability

$$p_{ij}(n) = 1 - \exp(-2\beta|\tilde{J}_{ij}(n)|), \qquad (8)$$

where β denotes inverse temperature. The spins in the resulting clusters are probabilistically flipped with respect to their signs $\epsilon_i(n)$, which amounts to the operation

$$k_i \to (-k_i + 2n + q) \bmod q. \qquad (9)$$

The validity of this procedure rests on a couple of assumptions. First, the disregarded part $\mathcal{H}_1(n)$ of the Hamiltonian has to be invariant under the transformation (9) applied. It is apparent from inspection that this is only the case for the term with $m = 1$, whereas for $m \geq 2$ the cosines are not even under the transformation (9). Hence, the embedding of the Ising variables is incomplete and the algorithm will not work for the general case of terms with $m \geq 2$ included in (1). Disregarding this shortcoming for a moment, as a second condition the Hamiltonian (5) has to be that of an effective Ising model with variables $\epsilon_i(n)$. This, however, is in the general case $m \geq 2$ also not fulfilled, since the effective couplings $\tilde{J}_{ij}(n)$ depend on the configuration of the

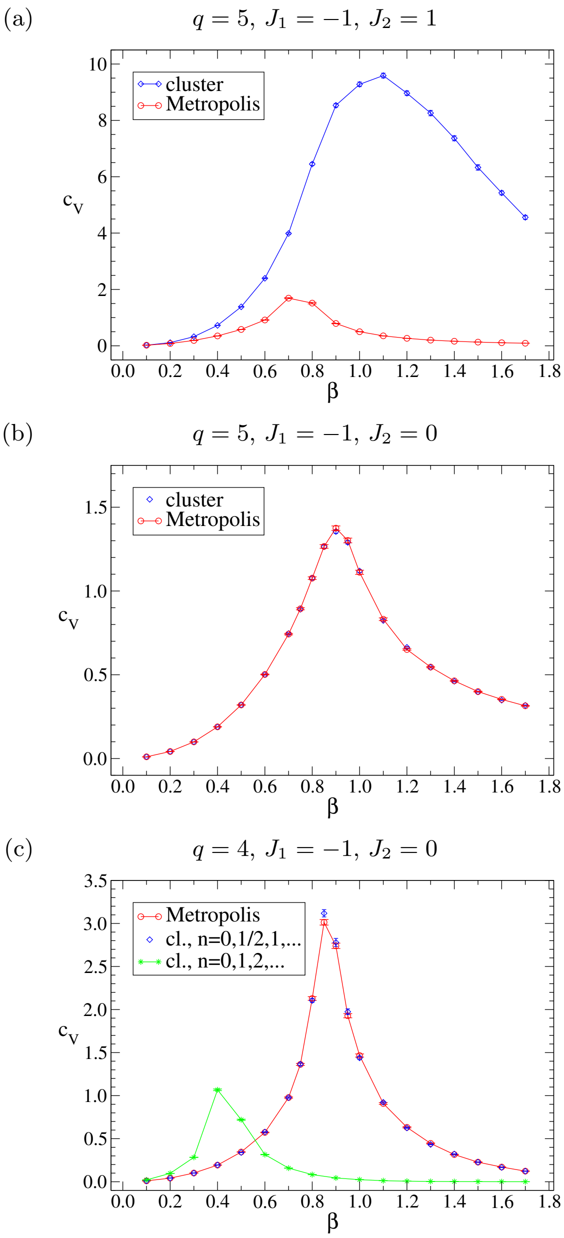

FIG. 1: Measured specific heat for the anti-ferromagnetic $Z(q)$ model with different parameters and algorithms for a 16^2 system with periodic boundary conditions. (a) The $q = 5$ model with coupling term $J_2 \neq 0$. The BLR cluster algorithm violates detailed balance. (b) For the $q = 5$ model with $J_2 = 0$, i.e., a clock model, detailed balance is satisfied. (c) For even q such as $q = 4$ the BLR cluster algorithm ("cl.") is non-ergodic for integer choices $n = 0, 1, 2, \ldots$ in Eq. (9). The inclusion of half-integer $n = 0, 1/2, 3/2, \ldots$ restores ergodicity. All error bars are evaluated by jackknifing[5].

Ising-type variables $\epsilon_i(n)$ via the denominators of $B_{ij}(n)$ in Eq. (6). Thus, a flip of one of the Ising spins connected by the coupling $\tilde{J}_{ij}(n)$ *changes* this effective coupling, such that the resulting effective model cannot be considered as an Ising model in the usual sense. Especially, the bond energy $-\tilde{J}_{ij}(n)\epsilon_i(n)\epsilon_j(n)$ is in general not antisymmetric with respect to a flip of one of the spins $\epsilon_i(n)$ or $\epsilon_j(n)$, which is assumed in constructing the bond-setting probability of Eqs. (7) and (8). As a consequence, the proposed algorithm *does not satisfy detailed balance* in the enlarged space of spin and graph (i.e., bond) variables (cf. the general treatment of cluster algorithms in Refs. 6). To be specific, consider the energy cost of breaking a single bond. According to the construction of the Swendsen-Wang cluster algorithm for the Ising model[3], this should appear in the exponential of the bond setting probability (8), i.e., it should equal

$$\Delta E_{ij}(n) = 2|\tilde{J}_{ij}(n)|. \tag{10}$$

However, according to the Hamiltonian (5) with the couplings from (6) it is given by

$$\begin{aligned} \Delta E_{ij}(n) &= -\tilde{J}'_{ij}(n)\epsilon'_i(n)\epsilon_j(n) + \tilde{J}_{ij}(n)\epsilon_i(n)\epsilon_j(n) \\ &= 2[\tilde{J}_{ij}(n) - B_{ij}(n)]\epsilon_i\epsilon_j, \end{aligned} \tag{11}$$

where the primed variables correspond to the flipped spin $\epsilon'_i(n) = -\epsilon_i(n)$. Obviously, Eq. (10) is in contradiction with Eq. (11) unless $B_{ij}(n) \equiv 0$. Hence, the algorithm presented by BLR is not valid unless one restricts the Hamiltonian (1) to that of the planar clock model with $m = 1$. This is demonstrated in Fig. 1. Figure 1(a) shows a temperature scan of the specific heat for the $q = 5$ model with $J_1 = -1$ and $J_2 = 1$, i.e., with non-vanishing couplings $B_{ij}(n)$ in Eq. (6), for a 16^2 square lattice with periodic boundary conditions[7]. The deviation of the BLR cluster result from the outcome of a local Metropolis update is apparent[8]. In Fig. 1(b) the outcome of a similar simulation for couplings $J_1 = -1$ and $J_2 = 0$, i.e., for an antiferromagnetic clock model, is depicted, showing that for this case the problem of detailed balance violation does not occur since $B_{ij}(n) \equiv 0$.

A third assumption for the formulation of the cluster algorithm of BLR to be valid is that the transformations of the spins defined by Eq. (9) are ergodic in the sense that any state $0, \ldots, q-1$ can be generated out of any other state by a series of such "flips". An inspection of the prescription (9) shows that it amounts to a reflection of the spins $\boldsymbol{\sigma}_i = (\cos[\delta k_i], \sin[\delta k_i])^{\mathrm{T}}$ at the line defined by the vector $\boldsymbol{n} = (\cos[\delta n], \sin[\delta n])^{\mathrm{T}}$, cf. Fig. 2. From this picture it is also obvious that BLR's prescription to disregard spins of value n completely in the process of building clusters is not strictly necessary since these spins are anyway an invariant of the transformation (9) and a bond involving such a spin is never set due to the condition (7). From Fig. 2 it is easy to convince oneself that for an odd number of states q any two states are connected to each other by a series of flips with respect to different axes $n \in \{0, 1, \ldots, q-1\}$. For q even, however, such flips never transform a spin with an odd label k to a spin with an even label and vice versa, such that the proposed dynamics is not ergodic. An ergodic set of moves can be constructed noting that for the transformation (9) to yield a valid new state k_i it is only necessary for $2n$ to

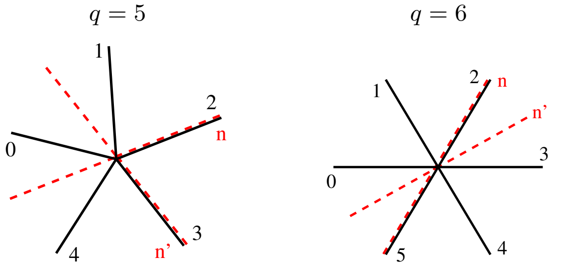

FIG. 2: Possible transitions between clock model states by reflections along an axis n. For an odd number of states q (left) the set of directions n parallel to the states generate an ergodic update. For q even (right), the transitions with n parallel to one of the states do not mix states with odd and even labels. Including the intermediate axes n' as reflection lines restores ergodicity.

be an integer, while n can be half-integer without problem. This amounts to using a reflection axis intermediate between two states as depicted by n' in the right panel of Fig. 2. As is easily seen, this enlargement of possible moves restores ergodicity for even choices of q. This is demonstrated in Fig. 1(c), where the BLR cluster algorithm for the $q = 4$ model with $J_1 = -1$, $J_2 = 0$ and $n \in \{0, \ldots, q-1\}$ is compared to a Metropolis update and a corrected version of the algorithm using directions $n \in \{0, 1/2, 1, \ldots, q-1/2\}$. Note that due to the non-mixing of even and odd labels of the original BLR algorithm and a start in the "all spins up" configuration, the corresponding simulation data depicted in Fig. 1(c) actually coincides with data of an anti-ferromagnetic Ising model on the square lattice[9].

Finally, I would like to point out that the BLR cluster algorithm, for the case $J_m = 0$, $m \geq 2$, i.e., the clock model, where it is applicable and with corrected choices $n \in \{0, 1/2, 1, \ldots, q-1\}$ for even values of q, is identical to the natural restriction of Wolff's embedded cluster algorithm for the XY model[2] to discrete values of the spins. Writing Eq. (1) for $J_m = 0$, $m \geq 2$ as an XY model with restricted values of the spins,

$$\mathcal{H} = -\sum_{\langle i,j\rangle} J_1 \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, \qquad (12)$$

Wolff's algorithm introduces a (random) projection vector $\boldsymbol{r}$, with respect to which (12) can be written as effective Ising model with variables ϵ_i,

$$\mathcal{H} = -\sum_{\langle i,j\rangle} \hat{J}_{ij}\epsilon_i\epsilon_j + \text{const}, \qquad (13)$$

where the effective couplings are given by

$$\hat{J}_{ij} = J_1 |\boldsymbol{\sigma}_i \cdot \boldsymbol{r}||\boldsymbol{\sigma}_j \cdot \boldsymbol{r}|, \qquad (14)$$

and the "const" part in Eq. (13) refers to the terms containing the spin components perpendicular to $\boldsymbol{r}$, which are invariant under flips of the Ising spins ϵ_i. Now, to accommodate for the discreteness of the spins $\boldsymbol{\sigma}_i = (\cos[\delta k_i], \sin[\delta k_i])^{\mathrm{T}}$ for the clock model as compared to the XY model, the projection vectors $\boldsymbol{r}$ have to be restricted to values compatible with the discrete spins,

$$\boldsymbol{r} = (\cos[\delta n + \pi/2], \sin[\delta n + \pi/2])^{\mathrm{T}}, \quad 2n \in \mathbb{N}, \qquad (15)$$

where the additional shifts of $\pi/2$ result from the fact that the lines of reflection are perpendicular to the vectors $\boldsymbol{r}$. Then, Eq. (14) becomes

$$\hat{J}_{ij} = J_1 |\sin[\delta(k_i - n)]\sin[\delta(k_j - n)]|, \qquad (16)$$

which is identical to the expression (6) for the part $A_{ij}(n)$ of the couplings for BLR's formulation.

In summary, BLR's cluster algorithm is not applicable to the general $Z(q)$ symmetric model due to a violation of detailed balance. To ensure ergodicity for even values of q, the choice of reflection vectors has to be enlarged. In the case where this corrected algorithm is applicable, namely the planar clock model, it is a simple restriction of Wolff's algorithm for the XY model to the case of discrete spins.

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[7] Note that the solid lines shown in all graphs have no physical significance and are merely drawn to guide the eye.

[8] In the present context, I ignore the question of whether the noticeable peaks in Figs. 1(a), (b) and (c) indicate the presence of phase transitions. I consider these curves merely as a check of the employed algorithms.

[9] Note that the *true* thermodynamic properties of the $q = 4$ clock model correspond to those of two independent $q = 2$ Potts or Ising models, such that the two curves in Fig. 1(c) are exactly related by a re-scaling of the axes.