Erratum: Cluster Monte Carlo study of the antiferromagnetic $Z(q)$ model [Phys. Rev. B 67, 094415 (2003)]

A. Benyoussef, M. Loulidi, and A. Rachadi

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A misprint error was found which conssits of a parenthesis that was not inserted in the right place. So the equations (3)–(5) and (7) should read

$$H_1^{(n)} = -\sum_{\langle ij\rangle}\sum_{\langle m=1\rangle}^{[q/2]} J_m \cos[um(\sigma_i - n)]\cos[um(\sigma_j - n)] \tag{3}$$

$$H_2^{(n)} = -\sum_{\langle ij\rangle}\sum_{\langle m=1\rangle}^{[q/2]} J_m \sin[um(\sigma_i - n)]\sin[um(\sigma_j - n)] \tag{4}$$

$$\alpha_{i,m}^{(n)} = \mathrm{sgn}(\sin[um(\sigma_i - n)]) \tag{5}$$

and

$$J_{ij}^{(n)} = J_1|\sin[u(\sigma_i - n)]\sin[u(\sigma_j - n)]| + \sum_{\langle m=2\rangle}^{[q/2]} J_m \frac{\sin[um(\sigma_i - n)]\sin[um(\sigma_j - n)]}{\alpha_{i,1}^{(n)}\alpha_{j,1}^{(n)}}. \tag{7}$$

In addition, the algorithm in its original form is not ergodic for even values of the number of states q. This anomaly can be corrected simply by allowing n in the above equations, to take half-integer values in the case where q is even. Indeed, the transformation $\sigma_i \rightarrow 2n - \sigma_i \mathrm{mod}q$ preserves the state parity for even values of q. So when a cluster is updated, some configurations have no chance to be reached because the system is trapped in some regions of the configurational space thus preventing ergodicity. In contrast, when n can take integer and half-integer values, the state parity is broken and ergodicity is easily restored.

On the other hand, we estimate that some points need to be clarified so that the reader can better understand our conclusions. First, let us review some symmetry aspects of the problem. We consider that the states σ_i are represented in space by points equally distributed on a circle of radius 1.

(i) The set $\{\sigma_i\}$ is invariant under the symmetry group of rotations of angles $(2\pi/q)l$ with $l=0,\ldots,q$ with $l=q$ representing the identity.

(ii) The set $\{\sigma_i\}$ is also invariant under the operations of reflections with respect to any symmetry axis. This is given by the operation

$$R^{(n)}(\sigma_i) = 2n - \sigma_i \mathrm{mod}q.$$

Here n represents an integer between 1 and q for odd values of q. For q even, n can take integer or half-integer values. There are q such symmetry axes (for q even, $q/2$ axes are added by allowing n to be half-integer).

(iii) Moreover, from operation symmetries of Hamiltonian (1), we can see that all the terms of order m can be obtained from the term of order $m=1$, by performing the following operation:

$$M(\sigma_i) = m\sigma_i \mathrm{mod}q.$$

mod$q$ here, reflects the invariance under the symmetry group of rotations and ensures that $M(\sigma_i)$ is a state between 1 and q. This operator can take us from the first term $(m=1)$ of the Hamiltonian (1) to the term of order m.

Now we will examine the action of the reflection $R^{(n)}$ after applying the M operator both on σ_i and on n (the mod$q$ is added when necessary to obtain a state in the range $1,\ldots,q$:

$$R^{(M(n))}(M(\sigma_i))\mathrm{mod}q = 2M(n) - M(\sigma_i)\mathrm{mod}q = 2mn - m\sigma_i \mathrm{mod}q = m(2n - \sigma_i \mathrm{mod}q)\mathrm{mod}q = M(R^{(n)}(\sigma_i)).$$

This is an important relation. What does it state? It implies that, when going from the first order term in the Hamiltonian $H_2^{(n)}$ to the term of order m, the reflection operation operates exactly the same way. In other terms, we need only one reflection operation for all the m terms. Figure 5 illustrates this result for $q=5$ and $n=4$ and for orders $m=1$ and $m=2$. We see, clearly, that the same reflection operation gives the expected results when performed on both the two terms, that is, the symmetry relations between the corresponding states are preserved.

As a result, when extracting the embedded Ising variables, we can choose any of the $\alpha_{i,m}^{(n)}$ to represent them in the Hamiltonian $H_2^{(n)}$. Our choice of $\alpha_{i,1}^{(n)}$ is founded on the fact the other values are directly deducible from them. And if we write Eq. (7) in the following form:

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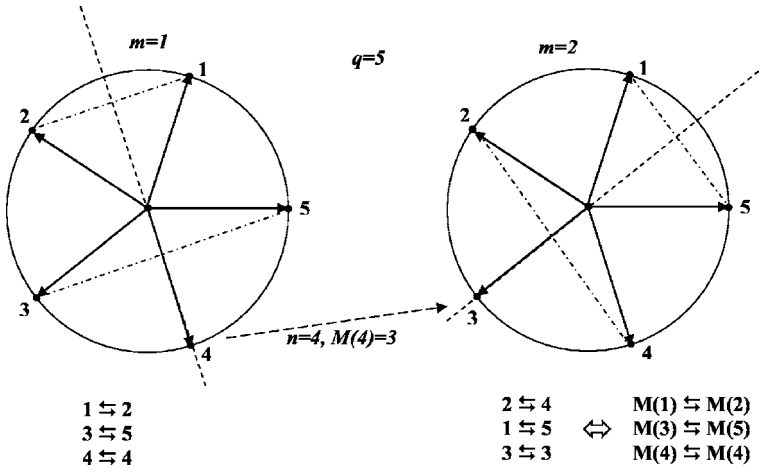

FIG. 5. The outcome of the reflection operation when going from the term $m=1$ to the term $m=2$ of the Hamiltonian $H_2^{(n)}$, for $q=5$ and $n=4$.

$$J_{ij}^{(n)} = \sum_{m=1}^{[q/2]} J_m |\sin[mu(\sigma_i - n)]\sin[mu(\sigma_j - n)]| \left(\frac{\alpha_{i,m}^{(n)}}{\alpha_{i,1}^{(n)}}\right)\left(\frac{\alpha_{j,m}^{(n)}}{\alpha_{j,1}^{(n)}}\right), \tag{8}$$

we can see that any change in the sign of the denominators affects automatically the sign of the numerators. Thus, $J_{ij}^{(n)}$ is invariant under the transformation of the sign variables, the fact that guarantees detailed balance.

We note also that there was a paper[1] which was published in the subject prior to our work. We were not aware of this by the time we published our article. In that paper, the authors derived some cluster algorithms from graphical representations of discrete spin systems. Their approach is similar to Fortuin-Kasteleyn (FK) representation where they transform the lattice into interconnected clusters constituted with bonds of different "colors" depending on their energies. And it can be applied for a large class of spin models including the $Z(q)$ model. One can easily see that this algorithm is very different from ours by ramarking that in our approach, a bond can take only two states depending on the ising states of the ending sites, while in Chayes and Machta's algorithm,[1] there are as many possible colors for a bond as there are energy values.

Finally, We would like to thank Martin Weigel for bringing to our attention the fact that the original form of the algorithm does not satisfy detailed balance and that n must be allowed to take half-integer values in order to ensure ergodicity for even values of q and also for suggesting to us the paper of Chayes and Machta (Ref. 1).

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[1] L. Chayes and J. Machta, Physica A **239**, 542 (1997).