

**Event-chain algorithm for the Heisenberg model: Evidence for  $z \simeq 1$  dynamic scaling**Yoshihiko Nishikawa,<sup>1,\*</sup> Manon Michel,<sup>2,†</sup> Werner Krauth,<sup>2,‡</sup> and Koji Hukushima<sup>1,3,§</sup><sup>1</sup>*Department of Basic Science, University of Tokyo, 3-8-1 Komaba, Meguro, Tokyo 153-8902, Japan*<sup>2</sup>*Laboratoire de Physique Statistique, Ecole Normale Supérieure, PSL Research University, UPMC, Université Paris Diderot, CNRS, 24 Rue Lhomond, 75005 Paris, France*<sup>3</sup>*Center for Materials Research by Information Integration, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan*

(Received 5 October 2015; published 14 December 2015)

We apply the event-chain Monte Carlo algorithm to the three-dimensional ferromagnetic Heisenberg model. The algorithm is rejection-free and also realizes an irreversible Markov chain that satisfies global balance. The autocorrelation functions of the magnetic susceptibility and the energy indicate a dynamical critical exponent  $z \approx 1$  at the critical temperature, while that of the magnetization does not measure the performance of the algorithm. We show that the event-chain Monte Carlo algorithm substantially reduces the dynamical critical exponent from the conventional value of  $z \simeq 2$ .

DOI: [10.1103/PhysRevE.92.063306](https://doi.org/10.1103/PhysRevE.92.063306)

PACS number(s): 02.70.Tt, 75.10.Hk, 75.10.Nr, 05.10.—a

**I. INTRODUCTION**

Ever since the advent of the local Metropolis Monte Carlo algorithm (LMC) [1], Monte Carlo simulations of systems with many degrees of freedom have played an important role in statistical physics. Near phase transitions, the LMC is severely hampered by dynamical arrest phenomena such as critical slowing down for second-order transitions, nucleation and coarsening for first-order transitions, and glassy behavior in disordered systems. A number of specialized algorithms then allow one to speed up the sampling of configuration space, namely, the Swendsen-Wang [2] and the Wolff [3] cluster algorithms, the multicanonical method [4], and the exchange Monte Carlo method [5] based on extended ensembles.

The above algorithms respect detailed balance, a sufficient condition for the convergence towards the equilibrium Boltzmann distribution. Recently, algorithms breaking detailed balance but satisfying the necessary global-balance condition have been discussed [6–9]. Among them, the event-chain Monte Carlo algorithm (ECMC) [9] has proven useful in hard-sphere [10,11] and more general particle systems [12,13], allowing one to equilibrate systems larger than previously possible [11,14]. It has also been applied to continuous spin systems [15]. The ECMC uses a factorized Metropolis filter [12] and relies on an additional lifting variable to augment configuration space [16]. It is rejection-free and realizes an irreversible Markov chain. So far, however, the speedup realized by the ECMC with respect to the LMC has always represented a constant factor in the thermodynamic limit, although larger gains are theoretically possible [16,17].

In this paper we apply the ECMC to the three-dimensional ferromagnetic Heisenberg model, defined by the energy

$$E(\{S_i\}) = \sum_{\langle i,j \rangle} E_{ij} = -J \sum_{\langle i,j \rangle} S_i \cdot S_j, \quad (1)$$

where  $J$  is the unit of the energy,  $S_i$  is a three-component unit vector, and the sum runs over all neighboring pairs of the  $N = L^3$  sites of a simple cubic lattice of linear extension  $L$ . In our simulations, we consider the critical inverse temperature  $\beta_c = J/T_c = 0.6930$  [18]. To describe the dynamics of the system, we compute the autocorrelation functions of the energy, the system magnetization  $M = \sum_k S_k$ , and the magnetic susceptibility

$$\chi = \frac{|M|^2}{N}.$$

Both the energy and the susceptibility are invariant under global rotations of the spins  $S_k$  around a common axis, whereas the magnetization follows the rotation. We will argue that the energy and the susceptibility are slow variables, that is, their slowest time constant describes the correlation (mixing) time of the underlying Markov chain. Under this hypothesis, we will present evidence that the ECMC for the three-dimensional Heisenberg model reduces the dynamical critical exponent from the LMC value of  $z \simeq 2$  to  $z \simeq 1$ . This considerable reduction of mixing times with respect to the LMC may be optimal within the lifting approach [17]. The observed reduction is all the more surprising as in the closely related  $XY$  model [15], where the spins are two-dimensional unit vectors, the ECMC realizes speedups by two orders of magnitude with respect to the LMC, but does not seem to lower the dynamical critical exponent.

**II. THE ECMC ALGORITHM FOR THE HEISENBERG MODEL**

In the LMC, finite local moves are proposed randomly and a move from a configuration  $a$  to a configuration  $b$  is accepted with the notorious Metropolis filter

$$p^{\text{Met}}(a \rightarrow b) = \min[1, \exp(-\beta \Delta E)], \quad (2)$$

where  $\Delta E = E_b - E_a$  is the change of the system energy. For Heisenberg spins, as for any system with pairwise interactions,

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we may write Eq. (2) as

$$p^{\text{Met}}(a \rightarrow b) = \min \left[ 1, \prod_{(i,j)} \exp(-\beta \Delta E_{ij}) \right],$$

with the pair energies  $\Delta E_{ij} = E_{ij}^b - E_{ij}^a$  [see Eq. (1)]. If the move  $b \rightarrow a$  is proposed with the same probability as  $a \rightarrow b$ , the detailed-balance condition

$$\pi_a p^{\text{Met}}(a \rightarrow b) = \pi_b p^{\text{Met}}(b \rightarrow a) \quad (3)$$

is satisfied with the Boltzmann weights  $\pi_a = \exp(-\beta E_a)$  and  $\pi_b = \exp(-\beta E_b)$ . The LMC dynamics is diffusive and detailed balance is enforced through the rejections in the Metropolis filter of Eq. (2).

In contrast to the LMC, the ECMC produces persistent infinitesimal moves that nevertheless amount to finite displacements. Specifically, in the Heisenberg model, it augments the physical space of spin configurations by a lifting variable  $(k, \mathbf{v})$  that defines the considered infinitesimal counterclockwise rotation of spin  $k$  about the axis  $\mathbf{v}$ . This rotation is accepted according to a consensus based on all individual pair energies, namely, the factorized Metropolis filter [12]

$$p^{\text{fact}}(a \rightarrow b) = \prod_{(i,j)} \min[1, \exp(-\beta \Delta E_{ij})]. \quad (4)$$

For infinitesimal rotations and by virtue of the factorized Metropolis filter, this physical move can only be rejected by a single neighboring spin  $l$  and the lifting variable will then be moved as  $(k, \mathbf{v}) \rightarrow (l, \mathbf{v})$ , keeping the sense of rotation, but passing it on to the spin responsible for the rejection. In the augmented space, the rejections are thus supplanted by events, namely, the lifting moves for arrested physical states. As there are no clockwise moves, obviously  $p^{\text{fact}}(b \rightarrow a)$  is zero if  $p^{\text{fact}}(a \rightarrow b) > 0$ , so the detailed balance condition of Eq. (3) is broken. Nevertheless, it is easy to show for infinitesimal moves that the more general global balance condition

$$\sum_a \pi_a p^{\text{fact}}(a \rightarrow b) = \sum_c \pi_b p^{\text{fact}}(b \rightarrow c) \quad (5)$$

is satisfied [12,15], with the stationary Boltzmann weights. Equation (5) describes equality between the global probability flow into the configuration  $b$  (on the left-hand side) and the flow out of it (on the right-hand side). In contrast to Eq. (3),  $a, b, c, \dots$  now comprise the lifting variable and there are no rejections in this augmented space (see Ref. [15]).

Practically, while the spin  $\mathbf{S}_k$  rotates around  $\mathbf{v}$ , the azimuthal angle  $\phi_{v,k}$  increases from its initial value  $\phi_0$  until one of its neighbors  $l$  triggers a lifting  $(k, \mathbf{v}) \rightarrow (l, \mathbf{v})$  at  $\phi_{v,k} = \phi_{l,\text{event}}$ . One no longer samples the acceptance of each infinitesimal rotation of  $\mathbf{S}_k$ , but directly samples the event angle  $\phi_{l,\text{event}}$ . It is sampled with a single random number in the event-driven approach [12,13]. Precisely,  $\phi_{l,\text{event}}$  is given by the sampling of the positive pair energy increase

$$\Delta E_l = -[\ln \mathcal{R}(0,1)]/\beta, \quad (6)$$

where  $\mathcal{R}(0,1)$  is a uniform random number between 0 and 1.

For a fixed rotation axis  $\mathbf{v}$ , the ECMC for the Heisenberg model reduces to the one of the XY model: With  $(\phi_{v,k}, \theta_{v,k})$  the spherical coordinates of a spin  $k$  in a system where the

$z$  axis is aligned with  $\mathbf{v}$ , the pair energy  $E_{kl}$  between spins  $k$  and  $l$  is

$$E_{kl} = -J' \cos(\phi_{v,k} - \phi_{v,l}) + K, \quad (7)$$

with

$$J' = J \sin \theta_{v,k} \sin \theta_{v,l}, \\ K = -J \cos \theta_{v,k} \cos \theta_{v,l}.$$

Both  $J'$  and  $K$  depend only on the polar angles  $\theta_v$  and remain unchanged along the event chain. The azimuthal-angle dependence in Eq. (7) is proportional to  $\cos(\phi_{v,k} - \phi_{v,l})$ , as in the XY model. The positive pair energy increase of Eq. (6) then becomes

$$\Delta E_l = -J' \int_{\phi_0}^{\phi_{l,\text{event}}} \max \left( 0, \frac{d \cos(\phi_{v,k} - \phi_{v,l})}{d \phi_{v,k}} \right) d \phi_{v,k}. \quad (8)$$

To solve Eq. (8) for  $\phi_{l,\text{event}}$ , one first slices off any full rotations (these  $n$  rotations by  $2\pi$  yield an energy increase of  $2nJ'$ ), leaving a value  $\Delta E_l^f$ ,

$$E_{\text{init}}^* + \Delta E_l^f = -J' \cos(\phi_{l,\text{event}} - \phi_{v,l} - 2n\pi), \quad (9)$$

where

$$E_{\text{init}}^* = \begin{cases} E_{kl} & \text{if the initial pair energy derivative is positive} \\ -J' & \text{otherwise.} \end{cases}$$

The true lifting event corresponds to the earliest of the independent event times sampled for all the neighbors of the spin  $k$ . In the ECMC, the Monte Carlo time is continuous and proportional to the total displacement of the spins.

The ECMC creates then chains of successive and consistent finite displacements of different spins. The choice of the length  $\ell$  of a chain, defined as the cumulative rotation angles about  $\mathbf{v}$  of the chain, is free. For the XY model of planar rotators,  $\mathbf{v}$  is uniquely defined as the axis perpendicular to the sense of rotation. For this reason, the ECMC around this axis is irreducible and the chain length  $\ell$  in this model is best taken equal to the simulation time [15]. For the Heisenberg model, spin rotations must be about at least two axes in order to reach the entire configuration space. The resampling of the rotation axis is performed after the chain length  $\ell$  is reached. All configurations of the chain sample the equilibrium distribution and any uniform subset of them yields valid observable averages. Observables may be integrated during the continuous evolution or, e.g., retrieved at regular intervals independent of the lifting events.

We have checked the correctness of the ECMC and obtained perfect agreement for the mean energy, the specific heat, and the susceptibility with the heat-bath algorithm [19,20] modified with the exchange Monte Carlo method (or parallel tempering) [5] (see Fig. 1).

### III. DYNAMICAL SCALING EXPONENT

At the critical temperature  $T_c$ , the correlation length  $\xi$  of a model undergoing a second-order phase transition equals the system size  $L$  and the autocorrelation time of slow variables  $\tau$  diverges as  $\tau \sim L^z$ , where  $z$  is the dynamical critical exponent. We define time in terms of sweeps: One ECMC sweep corresponds, on average, to  $N$  lifting events and one

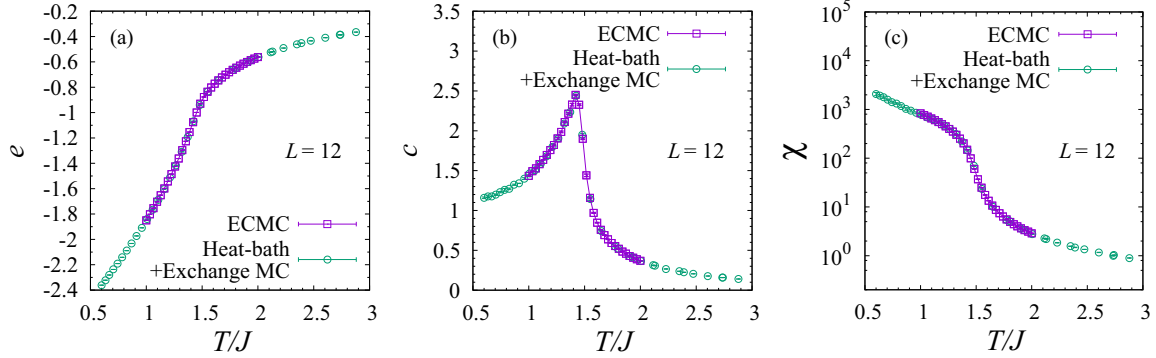


FIG. 1. (Color online) Temperature dependence of (a) the energy density  $e = E/N$ , (b) the specific heat  $c$ , and (c) the magnetic susceptibility  $\chi$  of the three-dimensional Heisenberg model with  $L = 12$ . A chain length  $\ell = N\pi/10$  is used.

LMC sweep to  $N$  attempted moves. For both algorithms, the complexity of one sweep is  $O(N)$  and the CPU times used per sweep are roughly the same. Time autocorrelation functions are defined by

$$C_{O(t)} = \frac{\langle O(t'+t)O(t') \rangle - \langle O(t') \rangle^2}{\langle O^2(t') \rangle - \langle O(t') \rangle^2}, \quad (10)$$

where the angular brackets indicate the thermal average and  $t'$  is set sufficiently large for equilibration. The dynamical critical exponent of the LMC for the three-dimensional Heisenberg model was estimated from the autocorrelation function of the magnetization  $\mathbf{M}$  as  $z = 1.96(6)$  [21]. The overrelaxation algorithm [22,23] seems to give  $z \simeq 1.10$  [21], which was obtained from the autocorrelation function of the magnetization, and the Wolff algorithm is believed to yield a value close to zero:  $z \gtrsim 0$ , a value obtained from the susceptibility autocorrelation function [24].

To evaluate the correlation time and the dynamical critical exponent for the ECMC, one must pay attention to the irreversible nature of the underlying Markov chain. During one event chain, spins all rotate in the same sense and the system undergoes global rotations with taking into account the thermal fluctuation. This results in fast oscillations of the magnetization  $\mathbf{M}$  and a quick decay of its autocorrelation

function that is insensitive to the system size (see Fig. 2) and even to the temperature. However, this effect is also visible for a trivial algorithm, which simply performs global rotations (see the inset of Fig. 2). The trivial algorithm satisfies global balance, but its correlation time is infinite, as it does not relax the energy. A similar effect appears in the ECMC for particle systems [9], which likewise is not characterized by the mean net displacement of particles. To characterize the speed of the ECMC, we consider the energy density and the susceptibility that we conjecture to be slow variables at the critical temperature. Both  $\chi$  and  $e$  are insensitive to global rotations and do not oscillate.

As shown in Fig. 3, the autocorrelation functions both of the energy density and of the susceptibility are well approximated as a single exponential decay

$$C_{\chi}(t) = \exp(-t/\tau) \quad (11)$$

on essentially the same time scales. Furthermore, the finite-size behavior of the autocorrelation times indicates  $z \simeq 1$  dynamical scaling. This  $z$  value is significantly less than for the LMC and very similar to the one obtained for overrelaxation methods, although the  $z \simeq 0$  value of the cluster algorithm is not reached.

#### IV. DISCUSSION AND SUMMARY

The earliest application of lifting [16], the motion of a particle on a one-dimensional  $N$ -site lattice with periodic boundary conditions, already featured the decrease of the dynamical scaling exponent from  $z = 2$  to  $z = 1$  (the reduction of the mixing time from proportional to  $N^2$  to proportional to  $N$ ). To reach such reductions, the Markov chain must be irreversible. It was pointed out that the square-root decrease of the critical exponent was the optimal improvement [17]. The concepts of factorized Metropolis filters and of infinitesimal moves brought irreversible lifting algorithms to general  $N$ -body systems, although only finite speed-ups were realized in the  $N \rightarrow \infty$  limit. The three-dimensional Heisenberg model however seems to be an ECMC application with a lowered critical dynamical exponent. Our observation relies on the hypotheses that the energy and the susceptibility are indeed slow variables and that the observed decay of the autocorrelation function continues for larger times. However, in Fig. 3, a crossover from  $z = 1$  back to  $z = 2$  as it was

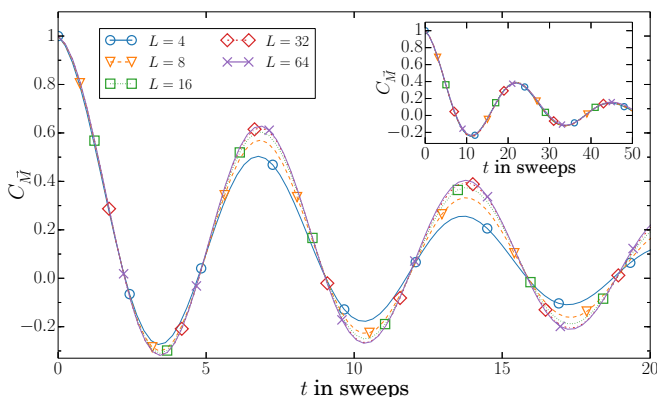


FIG. 2. (Color online) Autocorrelation function of magnetization  $C_M(t)$  at the critical temperature for various system sizes. The inset shows the spin autocorrelation function of a trivial algorithm that only performs global rotations in spin space along the two axes.

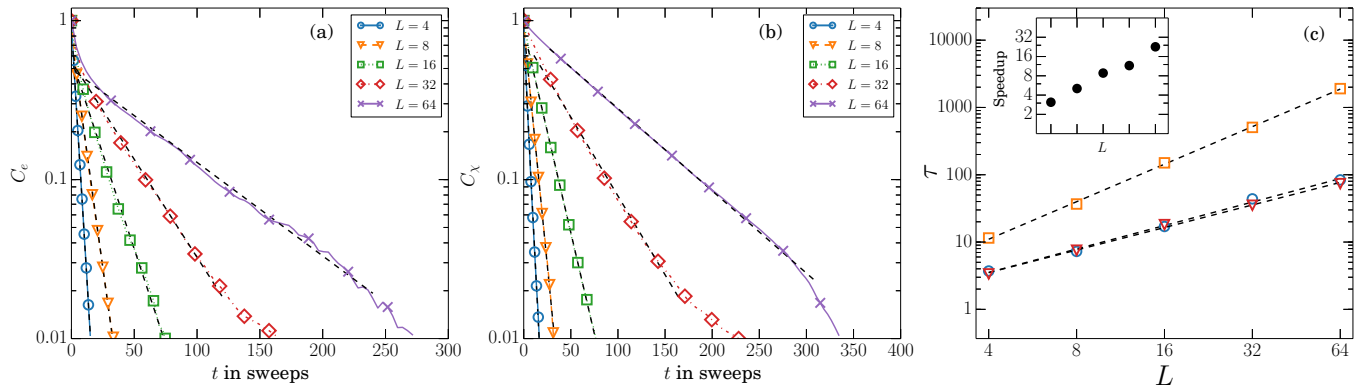


FIG. 3. (Color online) Autocorrelation functions and time constants of the ECMC for the three-dimensional Heisenberg model at its critical point  $\beta = 0.693$ : (a) energy density autocorrelation function  $C_e$  for system sizes  $4^3, 8^3, \dots, 64^3$ , (b) susceptibility autocorrelation function  $C_\chi$  for the ECMC for the three-dimensional Heisenberg system sizes  $4^3, 8^3, \dots, 64^3$ , and (c) scaling of the autocorrelation time  $\tau_\chi$  ( $\tau_e$ ) of the susceptibility  $\chi$  (energy density  $e$ ) with system size  $L$  for the ECMC [blue circles (red triangles)] and of the autocorrelation time of the susceptibility for the LMC (yellow squares). Error bars are smaller than the markers size. The inset shows the speedup for the susceptibility  $\chi$  in comparison to the LMC for system sizes  $4^3, 8^3, \dots, 64^3$ .

observed in the XY model after approximately five sweeps [15] appears unlikely to arise after hundreds of sweeps. The dynamical critical exponent  $z \approx 1$  represents a maximal improvement with respect to the  $z \approx 2$  of the LMC, supposing again that the theorems of Ref. [17] apply to infinitesimal Markov chains.

In summary, we have successfully applied the ECMC to the Heisenberg model in three dimensions. The ECMC shows considerable promise for spin models and the numerical data presented in this paper allow us to formulate the exciting conjecture that the dynamical critical exponent for the Heisenberg model is  $z \simeq 1$ . The ECMC is also applicable to frustrated magnets and spin glasses, which involve antiferromagnetic interactions and/or quenched disorder. Our preliminary study indicates that the ECMC algorithm is also useful for a Heisenberg spin glass model. The ECMC can be easily combined with other algorithms such as the exchange Monte Carlo method and the overrelaxation algorithm in the usual manner. This may allow the investigation of the three-dimensional Heisenberg

spin glass model in the low-temperature region. Large-scale simulations in this direction are currently in progress. It would be very interesting to understand why the ECMC is so much more successful in the Heisenberg model than both in hard and soft disks and in the XY model.

#### ACKNOWLEDGMENTS

Y.N. and K.H. thank S. Hoshino and M. J. Miyama for useful discussions and J. Takahashi and Y. Sakai for carefully reading the manuscript. This research was supported by Grants-in-Aid for Scientific Research from the JSPS, Japan (Grants No. 25120010 and No. 25610102) and JSPS Core-to-Core program “Nonequilibrium dynamics of soft matter and information.” This work was granted access to the HPC resources of MesopSL financed by the Region Ile de France and the project Equip@Meso (Reference No. ANR-10-EQPX-29-01) of the programme Investissements d’Avenir supervised by the Agence Nationale pour la Recherche.

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