# Generalized Kawasaki dynamics of the Heisenberg model

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Kawasaki spin-exchange dynamics is generalized to study ordering dynamics in the three-dimensional ferromagnetic Heisenberg model with a conserved vector order parameter. It is found, by using conventional temperature-quenching Monte Carlo simulations, that the generalized Kawasaki dynamics enables the system to reach thermodynamic equilibrium faster than the conventional Kawasaki dynamics does at lower temperatures, while both are similar at higher temperatures. With the generalized Kawasaki dynamics the domain size grows with time as $t^{1/4}$, in agreement with recent studies using Langevin-type dynamics. Evidence for the existence of spin waves is observed in the Monte Carlo simulations for the generalized Kawasaki dynamics. Its relation to domain growth is discussed.

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It is of current interest to understand the dynamics of ordering phenomena in systems with continuous symmetry [1–6]. Although there is no clear concept of a domain boundary in systems with continuous symmetry, which is crucial for understanding the ordering dynamics of systems with discrete symmetry [7,8], it was suggested that the ordering process in such systems can still be characterized by a correlation function $C(r,t)$ which obeys the scaling form [9]

$$C(r,t) = f(r/R(t)), \tag{1}$$

assuming the existence of a scaling regime and a dominant length scale $R(t)$. $R(t)$ is then an appropriate time-dependent measure of the coherence length of the evolving order ("domain"). In the case of conserved order parameters, both renormalization group analysis [1,2] and numerical studies [3,5], on the basis of Langevin equations, showed that $R(t) \sim t^n$ with $n = \frac{1}{4}$, where the growth exponent $n$ is independent of temperature. Most studies on the ordering dynamics of systems with continuous symmetry were focused on phenomenological models with Langevin dynamics [1–5,9]. This may be because of the convenience of this approach, believed to be valid within our current understanding of late-stage ordering dynamics. It is also believed that the growth exponent $n$ is determined by the nature of the conservation law for order parameters, but not by other system properties, such as the detailed dynamics by which systems approach to thermodynamic equilibrium. For microscopic models, however, the belief was formed by studying systems with scalar order parameters, such as the Ising system, but its validity has not been checked for systems with continuous symmetry, such as the Heisenberg magnetic system. Although a Monte Carlo study, based on statistical mechanical microscopic models, of the ordering dynamics in nonconserved order parameter systems with continuous symmetry was reported recently [6], so far, to our knowledge there has been no such study in the case of conserved order parameters.

In this paper, we report a Monte Carlo simulation study, using the three-dimensional ferromagnetic Heisenberg model, on ordering dynamics in systems with a conserved vector order parameter. The order parameter can be conserved in the Monte Carlo simulations by applying the spin-exchange dynamics that was introduced by Kawasaki to the Ising model for studying binary alloys [10]. In Kawasaki dynamics (KD), two neighboring spins on the lattice are chosen and they are interchanged with a probability dependent on the change in energy for the interchange. The conventional Kawasaki dynamics not only conserves the order parameter, defined as the average spin orientation, but also conserves the entire distribution of spin orientations. The ordering dynamics in an Ising-like model can be studied by conventional temperature-quenching Monte Carlo simulations [11,12], in which a system is initiated at a very high temperature and, therefore, has a flat distribution of spins. However, when one applies the method to the Heisenberg model, it is not clear whether the system with KD would ever evolve into its equilibrium state at low temperatures. Therefore, we argue that it is necessary in principle for Heisenberg magnetic systems to generalize the conventional Kawasaki dynamics.

The three-dimensional ferromagnetic Heisenberg model is defined by the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{2}$$

where $\mathbf{S}_i = (S_{xi}, S_{yi}, S_{zi})$ is a classical spin vector of unit length, and $J > 0$. The spin variables are arrayed on a simple cubic lattice. The Heisenberg model has a second-order phase transition from a paramagnetic phase to a ferromagnetic phase at $\mathrm{k_B}T_c/J = 1.44$ [13]. The order parameter of the Heisenberg model can be defined as $\mathbf{M} = L^{-3} \sum_i \mathbf{S}_i$, a macroscopic magnetic moment specified by a length (the magnetization) and a direction in space, where $L^3$ is the number of spins in a system of finite size $L$. The spins in the Heisenberg model do not correspond to different species, so KD is not the most natural way to conserve the order parameter. If one removes the constraint on the direction of each spin in KD, what is the simplest dynamics? In the Heisenberg model, each spin $\mathbf{S}_i$ has two degrees of freedom because of the

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fixed length of the spin; i.e., $|\mathbf{S}_i|=1$. So there are four degrees of freedom for a pair of such spins. If a pair of spins, $\mathbf{S}_i$ and $\mathbf{S}_j$, are changed to a new pair of spins, $\mathbf{S}_i'$ and $\mathbf{S}_j'$, there are three constraints on the degrees of freedom of the pair of spins, namely $\mathbf{S}_i + \mathbf{S}_j = \mathbf{S}_i' + \mathbf{S}_j'$, in order to conserve the vecter order parameter $\mathbf{M}$. The only one degree of freedom left is a rotation around the direction determined by the vector, $\mathbf{n}_{ij} = \mathbf{S}_i + \mathbf{S}_j$. It is obvious that such a rotation changes neither the value nor the direction of $\mathbf{n}_{ij}$; therefore, no change in the vector order parameter $\mathbf{M}$ occurs. Such a rotation, however, is not trivial in Monte Carlo simulations because it can change the directions of $\mathbf{S}_i$ and $\mathbf{S}_j$, respectively. A generalized Kawasaki dynamics (GKD) can then be described as follows. Choosing randomly a pair of the nearest-neighbor spins each time, one rotates them uniformly around the direction determined by their vector sum with a random angle, $\psi$, between 0° and 360° instead of exchanging their spatial positions. In fact, KD is a special case of the GKD with $\psi = 180°$ in the Heisenberg model.

We studied the ordering dynamics in the Heisenberg model using conventional temperature-quenching Monte Carlo simulations [11,12]. Although the stochastic processes bring the quenched system towards thermodynamic equilibrium in Monte Carlo simulations, they may not correspond to the real dynamics in the system. However, the dynamical interpretation of Monte Carlo simulation has been successfully applied to studying the ordering dynamics in systems with discrete symmetry [14]. The Heisenberg spin system, on simple cubic lattices subject to periodic boundary conditions, was initiated in a highly disordered phase ($T \sim \infty$) and instantly quenched to a temperature below the transition temperature, $T_c$. Therefore, $\mathbf{M} \approx \mathbf{0}$ in our quenching simulations. Only five quenchings with different initial configurations were carried out for each temperature because of the difficulty in simulating a system with continuous variables. Fortunately, for a system with continuous symmetry, the results from each individual quench are very close, probably due to the large degree of randomness in the initial configuration of the system [6]. Since there is no domain in the usual sense in the system, the ordering was monitored by calculating the time-dependent structure factor $S(q,t)$ which is the Fourier transform of the correlation function $C(r,t)$ in Eq. (1). By assuming translational invariance, the spherically averaged structure factor in three dimensions $L^3$ can be obtained as

$$S(q,t) = \frac{\displaystyle\sum_{q_n \le |\mathbf{q}| < q_{n+1}} \left\langle L^{-3} \left| \sum_{\mathbf{r}_i} \mathbf{S}_{\mathbf{r}_i} e^{i\mathbf{q}\cdot\mathbf{r}_i} \right|^2 \right\rangle}{\displaystyle\sum_{q_n \le |\mathbf{q}| < q_{n+1}} 1}, \tag{3}$$

where $\mathbf{q} = \frac{2\pi}{L}(l\hat{\mathbf{i}} + m\hat{\mathbf{j}} + n\hat{\mathbf{k}})$, $q_n = \frac{2\pi n}{L}$, and $q = |\mathbf{q}|$, with $l, m, n = 0, 1, 2, \ldots$. As measures of the linear domain size, the length scales were derived from the moments of $S(q,t)$ as follows:

$$k_m(t) = \left( \frac{\sum_q{}' q^m S(q,t)}{\sum_q{}' S(q,t)} \right)^{-1/m}, \tag{4}$$

and

$$K(t) = \frac{\sum_q{}' q^{-2} S(q,t)}{\sum_q{}' q^{-1} S(q,t)}, \tag{5}$$

where the primed sums in Eqs. (4) and (5) are restricted by an ultraviolet cutoff.

Figure 1 shows the evolution of the internal energy, $E(t)$, in time, measured in the Monte Carlo steps per lattice site (MCS/S), as obtained from the quench from the isotropic, disordered phase to two different temperatures in the ordered, ferromagnetic phase of the Heisenberg spin system. Results for both GKD and KD are shown for each temperature. They are not distinguishable at the higher temperature. However, at the lower temperature, it is clearly shown that the system reaches thermodynamic equilibrium faster by GKD than by KD. To see the evolution of energy in more detail, we have investigated the distribution in the angle between nearest-neighbor spin pairs at different moments after quenching. The angle $\delta_{ij}$ between nearest-neighbor spin pairs $\mathbf{S}_i$ and $\mathbf{S}_j$ is defined by $\cos\delta_{ij} = \mathbf{S}_i \cdot \mathbf{S}_j$. The distribution of $\delta_{ij}$, $n(\delta)$, over all nearest-neighbor spin pairs within the intervals of $\delta_{ij}$ is then calculated. In Fig. 2 are shown the distributions for both GKD and KD at several selected times in the period from $10^2$ to $10^4$ MCS/S at the lower temperature. The peak of the distribution gets sharper and shifts to the small angle side when the ordering of the system develops with time. The initial distribution, for a configuration of spins that distribute uniformly in the orientational space, is very close to what one expects for the

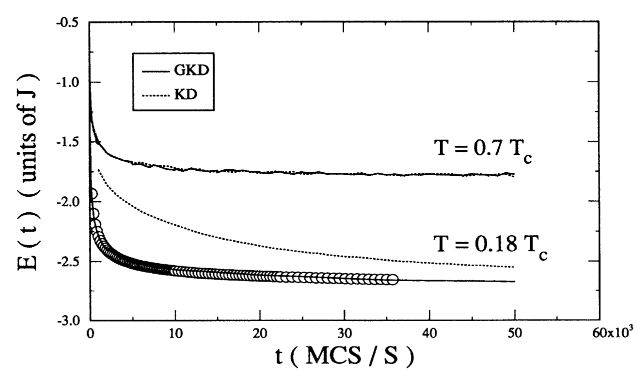


FIG. 1. The internal energy per spin $E(t)$ in units of $J$, as a function of time $t$, in MCS/S, obtained in quenches of the Heisenberg spin system from the isotropic, disordered phase to the two temperatures, $T = 0.7T_c$ and $0.18T_c$, in the ordered, ferromagnetic phase. All the data were obtained from a system of $28^3$ spins except those for GKD, shown as [$\circ$], which were obtained from a system of $64^3$ spins.

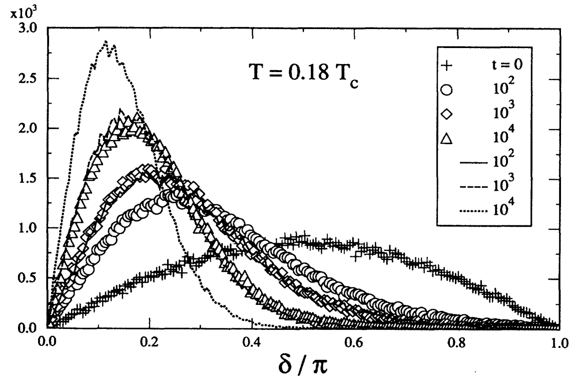


FIG. 2. The distribution in the angle between nearest-neighbor spins pairs, $n(\delta)$, at $T = 0.18T_c$ and at $t = 10^2$, $10^3$, and $10^4$ MCS/S for both GKD (lines) and KD (open symbols). The initial distribution, shown as [+], was generated by a configuration of spins which distribute uniformly in the orientational space. All the data were obtained from a system of $32^3$ spins.

spin system at very high temperatures, i.e., $n(\delta) \sim \sin\delta$. As shown in Fig. 2, the distributions for GKD at $t = 10^2$ and $10^3$ nearly overlap those for KD at $t = 10^3$ and $10^4$, respectively. It is consistent with the results presented in Fig. 1 that the ordering develops about 10 times faster for GKD than for KD at the lower temperature. However, the distributions for GKD and KD at the higher temperature are always very similar at any time. Three domain length scales derived from the moments of the structure factor for GKD are illustrated in Fig. 3. At the late stage the data for $k_1(t)$, $k_2(t)$, and $K(t)$, obtained according to Eqs. (4) and (5), conform clearly to a power law. In fact, $k_{m=1,2}(t) \sim t^{-0.26\pm0.01}$ and $K(t) \sim t^{-0.25\pm0.01}$, where the exponents were obtained from the best fits to the data at the late stage. They are consistent with each other within the statistical errors, although the result from the data of $K(t)$ is generally expected to be more accurate [15]. The same length scales were also calculated for the system at higher temperature and almost the same power law was observed. It indicates that the domain size $R(t)$, characterized by the length scales, grows as $R(t) \sim t^n$ with $n \approx \frac{1}{4}$ at the late stage, and the growth exponent is, within statistical errors, independent of temperature in contrast to the observations made in the Monte Carlo study in the case of the nonconserved order parameter [6]. This result is consistent with those obtained from studies on the Langevin dynamics [1,3]. The domain growth of KD is similar to that of GKD at the higher temperature, but the former is much slower than the latter at the lower temperature and even has not reached the scaling regime before finite size effects show up. The difference between GKD and KD in a quenching experiment can also be observed in the orientational distribution of the spins. In Fig. 4 is shown the orientational distribution of the spins before and after a quenching to $T = 0.18T_c$. The difference between GKD and KD in the orientational distribution is very obvious. In a quench the orientational distribution of the spins for KD does not change since only exchanges of the spatial positions of spins are involved. However, the orientational distribution of the spins for GKD changes in such a way that the vector order parameter $\mathbf{M}$ can keep the initial value, namely, $\mathbf{M} \approx \mathbf{0}$, in the quench. A certain order appears in the distribution for GKD in correspondence with establishing spin waves, the equilibrium state of the Heisenberg model. The spin wave with wavelength $\phi \approx \pi$ instead of $\phi \approx 2\pi$, as shown in Fig. 4, seems to be always observed in different runs although the understanding of the observation is still lacking.

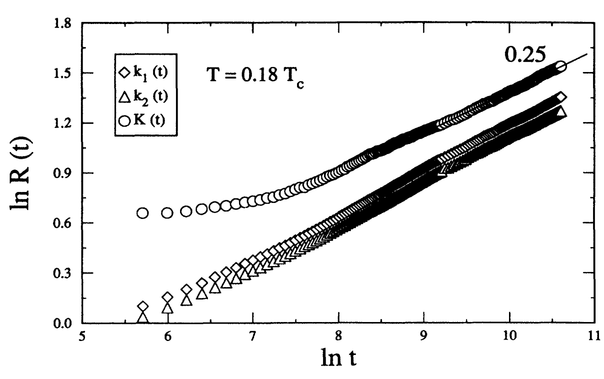


FIG. 3. Log-log plot of the length scales, $k_1(t)$, $k_2(t)$, and $K(t)$, in Eq. (4) and Eq. (5) vs time $t$ (in units of MCS/S) for quenches from the disordered phase to the temperature, $T = 0.18T_c$, in the ordered phase. The data were obtained from a system of $64^3$ spins for GKD. The solid straight line, the best fitting to the data of $K(t)$ at the late stage, has the slope as indicated.

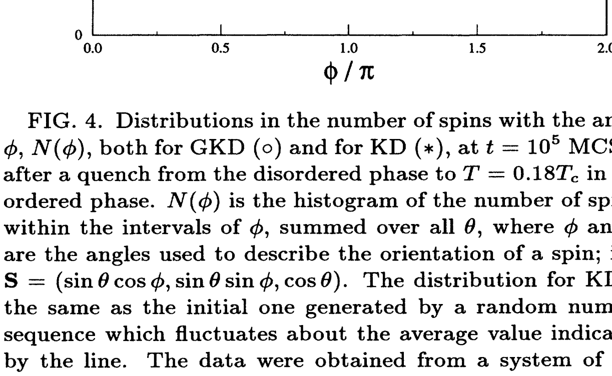


FIG. 4. Distributions in the number of spins with the angle $\phi$, $N(\phi)$, both for GKD (○) and for KD (∗), at $t = 10^5$ MCS/S after a quench from the disordered phase to $T = 0.18T_c$ in the ordered phase. $N(\phi)$ is the histogram of the number of spins, within the intervals of $\phi$, summed over all $\theta$, where $\phi$ and $\theta$ are the angles used to describe the orientation of a spin; i.e., $\mathbf{S} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. The distribution for KD is the same as the initial one generated by a random number sequence which fluctuates about the average value indicated by the line. The data were obtained from a system of $32^3$ spins.

The theoretical analysis made by Bray [1], in which the growth with $n = \frac{1}{4}$ is related to the existence of spin waves in a system with continuous symmetry, can be used to interpret our simulation results. In fact, our Monte Carlo simulation data for GKD and KD seem to indicate some links between domain growth and spin waves. Both the growth exponent $n \approx \frac{1}{4}$ and the evidence for building up spin waves were observed in the simulations for GKD at low temperature, but not in the simulations for KD in the same situation. The dynamics proposed in this paper (GKD) can effectively establish spin waves so that the same growth law predicated by Bray [1] can be observed at low temperatures. Therefore, from this point of view, GKD may be more favorable than KD in real situations. At higher temperatures, the spin waves are less-well defined because of large thermal fluctuations, so there is not much difference between GKD and KD. We have also done the simulations for GKD for several different systems up to $64^3$ spins. No obvious finite size effect was found for the growth exponent of $n \approx \frac{1}{4}$.

In summary, we present dynamics for the Heisenberg model with a conserved vector order parameter. The Monte Carlo simulation study on the microscopic model with continuous symmetry shows that the dynamics enables the system to reach thermodynamic equilibrium faster than the Kawasaki dynamics does. Domain growth with the exponent, $n = \frac{1}{4}$, was observed in our Monte Carlo simulations, consistent with previous studies on the Langevin equations. Evidence for spin waves was found in the orientational distribution of the spins for the dynamics in our Monte Carlo quenching simulations.

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