# Kawasaki-type dynamics: Diffusion in the kinetic Gaussian model

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In this Brief Report, we retain the basic idea and at the same time generalize Kawasaki's dynamics, the spin-pair exchange mechanism, to a spin-pair redistribution mechanism, and present a normalized redistribution probability. This serves to unite various order-parameter-conserved processes into a universal framework in microscopics and provides the basis for further treatment. As an example of the applications, we treated the kinetic Gaussian model and obtained the exact diffusion equation. We observed critical slowing down near the critical point and found that the critical dynamic exponent $z=1/v=2$ is independent of space dimensionality and the assumed mechanism, whether Glauber type or Kawasaki type.

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Irreversible dynamic systems exhibit complicated but interesting nonequilibrium phenomena near the critical point. In spite of their complexity, the interesting dynamic critical behaviors have attracted a lot of researchers for many decades. Within the vast body of literature, pioneering work completed by Glauber [1] and Kawasaki [2] has been regarded as a milestone. Great progress has been achieved with the application of Glauber's single-spin-flip mechanism and Kawasaki's spin-pair exchange mechanism, which have proved to catch the inherent essential process.

Kawasaki's dynamics deals with a system consisting of an array of $N$ coupled spins. The coupling between the spins is represented by a set of probabilities of spin exchange. Initially, the focus was on the Ising model. The spins may exchange with their nearest neighbors, and in this way the system evolves while the total spin remains conserved. In later studies the idea of exchange has proved very successful as it catches the essential nature of the process. As the basic mechanism in order-parameter-conserved processes, it has important applications in Ising [3] and Ising-like models such as the lattice gas model [4], the Blume-Emery-Griffiths model [5], and others [6].

However, its initial embodiment was closely tied up with the simplicity of the Ising model, in which the spins can only take two values, $\pm 1$, and there exist only nearest-neighbor interactions. It turned to be limited when applied to other more complicated systems. The same situation exists in Glauber's dynamics. Recently Zhu and Yang successfully generalized Glauber's single-spin-flip mechanism to a single-spin transition mechanism and gave a normalized version of the transition probability [7]. Applications yielded encouraging results [7,8]. In this article, along the same line, we retain the basic idea and at the same time generalize Kawasaki's dynamics, the spin-pair exchange mechanism, to a spin-pair redistribution mechanism, also with a normalized redistribution probability.

The limit is to be removed and the spins may take various discrete values (discrete-spin model) or continuous values (continuous-spin model). Because in the Ising model spins can only be $+1$ or $-1$, simple direct exchange may be enough to describe the way the system evolves. In other different models, such as the Gaussian model, Potts model, or $XY$ model, this simple picture may not be as capable. On the other hand, as mentioned above, the conservation of the order parameter has been regarded as the most important feature of this class of processes (and a necessary result of the exchange mechanism). Based on these considerations, in a generalized mechanism, two neighboring spins $\sigma_k$ and $\sigma_{k+1}$ no longer merely exchange with each other. Instead, they may take any values $\hat{\sigma}_k$ and $\hat{\sigma}_{k+1}$ as long as their sum remains conserved; their sum is redistributed, and we call this spin-pair redistribution.

The probability distribution function $P(\sigma_1, \ldots, \sigma_N; t)$, or simply $P(\{\sigma\};t)$, denotes the probability of the $N$-spin system being in the state $(\sigma_1, \ldots, \sigma_N)$, or simply $\{\sigma\}$, at time $t$. $W_{jl}(\sigma_j\sigma_l \rightarrow \hat{\sigma}_j\hat{\sigma}_l)$ is the probability per unit time that two neighboring spins $\sigma_j$ and $\sigma_l$ are redistributed while the others remain unchanged. Then, on the supposition of neighboring spin-pair redistributions, we have

$$\frac{d}{dt}P(\{\sigma\};t)=\sum_{\langle jl\rangle}\sum_{\hat{\sigma}_j,\hat{\sigma}_l}\{-W_{jl}(\sigma_j\sigma_l\rightarrow\hat{\sigma}_j\hat{\sigma}_l)P(\{\sigma\};t) + W_{jl}(\hat{\sigma}_j\hat{\sigma}_l\rightarrow\sigma_j\sigma_l)P(\{\sigma_{i\neq j,l}\},\hat{\sigma}_j,\hat{\sigma}_l;t)\}. \tag{1}$$

This is a probability equation, in which the first term on the right-hand side denotes the decrease of the probability distribution function $P(\{\sigma\};t)$ per unit time, due to the redistribution of the spin pair from initially $\sigma_j\sigma_l$ to various values $\hat{\sigma}_j\hat{\sigma}_l$; and the second term denotes the contrary situation. (Clearly, in Ising and Ising-like systems, it does become Kawasaki's picture.) We shall refer to Eq. (1) as the master equation since its solution would contain the most complete description of the system.

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The key to the master equation is the redistribution (or exchange, flip, transition, etc.) probability. Usually it cannot be uniquely determined by the detailed balance condition, and thus in Kawasaki's and Glauber's pioneering work some arbitrariness remained. We hope to make our choice of the spin-pair redistribution probability able to contain the original form in the specific Ising model, and applicable to other various spin systems, while at the same time clearer and more definite. Now we consider it in both mathematical and physical respects. In mathematics, generally speaking, the probability must be positive and normalized; in physics, we often require that a system in thermodynamic equilibrium satisfy the detailed balance condition; the probability should also be ergodic as long as the total spin remains conserved. Based on these considerations, for arbitrary neighboring $j$th and $l$th spins, the redistribution probability $W_{jl}$ should satisfy the following conditions.

(a) Ergodicity, positivity, and conservation of spin:

$$W_{jl}(\sigma_j\sigma_l\rightarrow\hat{\sigma}_j\hat{\sigma}_l)\begin{cases} >0, & \forall \quad \hat{\sigma}_j+\hat{\sigma}_l=\sigma_j+\sigma_l \\ =0, & \forall \quad \hat{\sigma}_j+\hat{\sigma}_l\neq\sigma_j+\sigma_l . \end{cases}$$

(b) Normalization:

$$\sum_{\hat{\sigma}_j,\hat{\sigma}_l} W_{jl}(\sigma_j\sigma_l\rightarrow\hat{\sigma}_j\hat{\sigma}_l)=1.$$

(c) Detailed balance:

$$\frac{W_{jl}(\sigma_j\sigma_l\rightarrow\hat{\sigma}_j\hat{\sigma}_l)}{W_{jl}(\hat{\sigma}_j\hat{\sigma}_l\rightarrow\sigma_j\sigma_l)}=\frac{P_{eq}(\sigma_1,\ldots,\hat{\sigma}_j,\hat{\sigma}_l,\ldots,\sigma_N)}{P_{eq}(\sigma_1,\ldots,\sigma_j,\sigma_l,\ldots,\sigma_N)},$$

where $P_{eq}$ is the equilibrium distribution function.

Although the redistribution probabilities are still not determined uniquely by the above restrictions, there is less room left. The consideration that we use is similar to that in the generalization of Glauber's dynamics [7], that the redistribution of a neighboring pair depends merely on the momentary values of the surrounding spins and the influence of the heat bath. Based on this, we can similarly assume that the redistribution probability $W_{jl}$ depends only on the heat Boltzmann factor of the system,

$$W_{jl}(\sigma_j\sigma_l\rightarrow\hat{\sigma}_j\hat{\sigma}_l)=\frac{1}{Q_{jl}}\delta_{\sigma_j+\sigma_l,\hat{\sigma}_j+\hat{\sigma}_l} \times\exp[-\beta\mathcal{H}_{jl}(\hat{\sigma}_j,\hat{\sigma}_l,\{\sigma_m\}_{m\neq j,l})], \tag{2}$$

where the factor $Q_{jl}$ can be determined by the normalization condition. Compared with Kawasaki's expression, Eq. (2) is a normalized version. In his expression of the exchange probability, there is an $\alpha$ assumed to be a constant. In the Ising model, redistribution is in fact exchange and actually our expression is only a definite selection for constant $\alpha$ by extra considerations.

Usually, we are interested in local magnetization. It is defined as

$$q_k(t)=\langle\sigma_k(t)\rangle=\sum_{\{\sigma\}}\sigma_k P(\{\sigma\};t). \tag{3}$$

According to the definition (3) and the master equation (1), and using the normalization condition (b), the time-evolving equation of $q_k(t)$ can be derived as

$$\frac{d}{dt}q_k(t)=-2dq_k(t)+\sum_{\{\sigma\}}\sum_w\left[\sum_{\hat{\sigma}_k,\hat{\sigma}_{k+w}}\hat{\sigma}_k \times W_{k,k+w}(\sigma_k\sigma_{k+w}\rightarrow\hat{\sigma}_k\hat{\sigma}_{k+w})\right]P(\{\sigma\};t), \tag{4}$$

where $d$ is the system dimensionality, and $\Sigma_w$ means summation taken over the nearest neighbors (clearly it is related to the dimensionality, too).

Kawasaki's exchange mechanism was initially designed for study of the diffusion constant, and he himself obtained an approximate result for the Ising model by first deriving an expression for the spin flux [2]. As an application of the redistribution mechanism, we will now study the same phenomenon in the kinetic Gaussian model, while our method is a direct one.

The Gaussian model, proposed by Berlin and Kac initially in order to make the Ising model more tractable, is a continuous-spin model. It has the same Hamiltonian form as the Ising model (three dimensional),

$$-\beta\mathcal{H}=K\sum_{i,j,k=1}^{N}\sum_w\sigma_{ijk}(\sigma_{i+w,jk}+\sigma_{ij+w,k}+\sigma_{ij,k+w}). \tag{5}$$

Compared with the Ising model, it has two extensions. First, the spins $\sigma_{ijk}$ can take any real value between $(-\infty,+\infty)$. Second, to prevent the spins from tending to infinity, the probability of finding a given spin between $\sigma_{ijk}$ and $\sigma_{ijk}+d\sigma_{ijk}$ is assumed to be the Gaussian-type distribution

$$f(\sigma_{ijk})d\sigma_{ijk}=\sqrt{\frac{b}{2\pi}}\exp\left(-\frac{b}{2}\sigma_{ijk}^2\right)d\sigma_{ijk},$$

where $b$ is a distribution constant independent of temperature. Although it is an extension of the Ising model, the Gaussian model is quite different. In the equilibrium case, on translationally invariant lattices the Gaussian model is exactly solvable, and later as a starting point to study the unsolvable models it has also been investigated with mean field theory and the momentum-space renormalization-group method.

In the three-dimensional (3D) kinetic Gaussian model, there are six combined terms in the 3D *type* time-evolving equation of the local magnetization, Eq. (4). Because the spins take continuous values, the summation for the spin value turns into the integration

$$\sum_{\sigma} \rightarrow \int_{-\infty}^{\infty} f(\sigma)d\sigma.$$

Because of its length, here we give only the results:

$$\sum_{\hat{\sigma}_{ijk},\hat{\sigma}_{i\pm1,j,k}} \hat{\sigma}_{ijk} W_{i,j,k;i\pm1,j,k}(\sigma_{ijk}\sigma_{i\pm1,j,k} \rightarrow \hat{\sigma}_{ijk}\hat{\sigma}_{i\pm1,j,k}) = \frac{1}{2(b+K)}[K(\sigma_{i,j+1,k}+\sigma_{i\mp1,j,k}+\sigma_{i,j-1,k}+\sigma_{i,j,k-1}+\sigma_{i,j,k+1}+\sigma_{ijk}$$
$$+\sigma_{i\pm1,j,k}-\sigma_{i\pm1,j+1,k}-\sigma_{i\pm2,j,k}-\sigma_{i\pm1,j-1,k}-\sigma_{i\pm1,j,k+1}$$
$$-\sigma_{i\pm1,j,k-1})+b(\sigma_{ijk}+\sigma_{i\pm1,j,k})],$$

$$\sum_{\hat{\sigma}_{ijk},\hat{\sigma}_{i,j\pm1,k}} \hat{\sigma}_{ijk} W_{i,j,k;i,j\pm1,k}(\sigma_{ijk}\sigma_{i,j\pm1,k} \rightarrow \hat{\sigma}_{ijk}\hat{\sigma}_{i,j\pm1,k}) = \frac{1}{2(b+K)}[K(\sigma_{i,j,k+1}+\sigma_{i,j\mp1,k}+\sigma_{i,j,k-1}+\sigma_{i-1,j,k}+\sigma_{i+1,j,k}+\sigma_{ijk}$$
$$+\sigma_{i,j\pm1,k}-\sigma_{i,j\pm1,k+1}-\sigma_{i,j\pm2,k}-\sigma_{i,j\pm1,k-1}-\sigma_{i+1,j\pm1,k}$$
$$-\sigma_{i-1,j\pm1,k})+b(\sigma_{ijk}+\sigma_{i,j\pm1,k})],$$

$$\sum_{\hat{\sigma}_{ijk},\hat{\sigma}_{i,j,k\pm1}} \hat{\sigma}_{ijk} W_{i,j,k;i,j,k\pm1}(\sigma_{ijk}\sigma_{i,j,k\pm1} \rightarrow \hat{\sigma}_{ijk}\hat{\sigma}_{i,j,k\pm1}) = \frac{1}{2(b+K)}[K(\sigma_{i+1,j,k}+\sigma_{i,j,k\mp1}+\sigma_{i-1,j,k}+\sigma_{i,j-1,k}+\sigma_{i,j+1,k}+\sigma_{ijk}$$
$$+\sigma_{i,j,k\pm1}-\sigma_{i+1,j,k\pm1}-\sigma_{i,j,k\pm2}-\sigma_{i-1,j,k\pm1}-\sigma_{i,j+1,k\pm1}$$
$$-\sigma_{i,j-1,k\pm1})+b(\sigma_{ijk}+\sigma_{i,j,k\pm1})],$$

Substituting them into the time-evolving equation of the local magnetization (4), we get

$$\frac{d}{dt}q_{ijk}(t) = \frac{1}{2(b+K)}b\{[(q_{i+1,j,k}-q_{ijk})-(q_{ijk}-q_{i-1,j,k})]+[(q_{i,j+1,k}-q_{ijk})-(q_{ijk}-q_{i,j-1,k})]+[(q_{i,j,k+1}-q_{ijk})-(q_{ijk}$$
$$-q_{i,j,k-1})]\}+\frac{K}{2(b+K)}[2(2q_{i-1,j,k}-q_{i-1,j+1,k}-q_{i-1,j-1,k})+(2q_{i-1,j,k}-q_{ijk}-q_{i-2,j,k})+2(2q_{i+1,j,k}$$
$$-q_{i+1,j+1,k}-q_{i+1,j-1,k})+(2q_{i+1,j,k}-q_{ijk}-q_{i+2,j,k})+2(2q_{i,j-1,k}-q_{i,j-1,k+1}-q_{i,j-1,k-1})+(2q_{i,j-1,k}-q_{ijk}$$
$$-q_{i,j-2,k})+2(2q_{i,j+1,k}-q_{i,j+1,k+1}-q_{i,j+1,k-1})+(2q_{i,j+1,k}-q_{ijk}-q_{i,j+2,k})+2(2q_{i,j,k-1}-q_{i+1,j,k-1}$$
$$-q_{i-1,j,k-1})+(2q_{i,j,k-1}-q_{ijk}-q_{i,j,k-2})+2(2q_{i,j,k+1}-q_{i+1,j,k+1}-q_{i-1,j,k+1})+(2q_{i,j,k+1}-q_{ijk}-q_{i,j,k+2})]. \tag{6}$$

With lattice constant $a$ we can transform the above equation to

$$\frac{d}{dt}q(t) = \frac{a^2}{2(b+K)}b(\nabla_x^2+\nabla_y^2+\nabla_z^2)q(t)-\frac{a^2}{2(b+K)}K[2(2\nabla_y^2+\nabla_x^2)+2(2\nabla_z^2+\nabla_y^2)+2(2\nabla_x^2+\nabla_z^2)]q(t)$$
$$=\frac{3a^2}{b+K}\left(\frac{b}{6}-K\right)\nabla^2 q(t). \tag{7}$$

It is of the form of a diffusion equation:

$$\frac{dq(t)}{dt} = D\nabla^2 q(t), \quad D=\frac{3a^2}{b+K}\left(\frac{b}{6}-K\right)a^2.$$

The one- and two-dimensional Gaussian models can be treated in the same way. Here we give only the results,

$$\frac{d}{dt}q(t) = \frac{da^2}{b+K}\left(\frac{b}{2d}-K\right)\nabla^2 q, \tag{8}$$

where $d$ is the system dimensionality. This diffusion equation reveals that the diffusion will get much slower when it is near its critical point, which is already known to be $K_c = J/k_B T_c = b/2d$. The linear equations we obtained for a single spin can be directly solved, but the solution of the diffusion equations may already give us satisfying information. For example, in the 1D case, we have

$$q(x,t) = \frac{1}{2\sqrt{D\pi t}}\int_{-\infty}^{\infty} q(\xi,0)e^{-(x-\xi)^2/4Dt}d\xi.$$

In a specific example of the diffusion of a Gaussian type packet $q(\xi,0)=e^{-\xi^2}$, one will obtain

$$q(x,t)=\sqrt{\frac{1}{1+t/\tau}}\exp\left[-\frac{x^2}{1+t/\tau}\right],$$
$$\tau=\frac{1}{4D}=\left[\frac{4a^2}{b+K}\left(\frac{b}{2}-K\right)\right]^{-1}. \tag{9}$$

When $K\to K_c=b/2$, $D\to 0$ and the relaxation time $\tau\to\infty$, and this is a typical critical slowing down phenomenon. With the correlation length critical exponent $\nu=1/2$ and the dynamical scaling hypotheses $\tau\sim\xi^z$, $\xi\sim|T-T_c|^{-\nu}$, one can obtain the dynamic critical exponent $z=2$. The same result can be obtained for 2D and 3D models. In earlier studies [7,8] the same result $z=1/\upsilon=2$ for any dimensionality was obtained with a Glauber-type mechanism. Thus we find that, in the kinetic Gaussian model, *the critical dynamic exponent is independent of space dimensionality and the dynamic mechanism*.

To summarize, in this Brief Report, we presented a systematic formulation of the Kawasaki-type dynamics: spin-pair redistribution. As a natural generalization of the exchange mechanism, it gives the system more freedom while keeping the order parameter conserved. The master equation has been given, with a normalized redistribution probability determined by the heat Boltzmann factor. The presentation of this probability, which is the key of the whole formulation, makes the mechanism mathematically well organized and physically meaningful. In much of the earlier work there are already ideas of ''redistribution'' and these efforts often turned out to be rather fruitful. This Brief Report serves to provide a general foundation upon which the generalized Kawasaki dynamics becomes universal and can be *directly* applied to microscopic systems. Without any extra requirements, it has an advantage compared with some earlier approaches covering the same ground, such as numerical Ginzburg-Landau approaches.

The formulation is compact in mathematics, while on the other hand it is also quite open. People are able to introduce other elements into it. For example, one can easily give the mathematical form of the competing dynamics, Glauber type and Kawasaki type, both with a probability, to study self-organization phenomena in a wide range of systems. One can also modify the mechanism by some means and directly study the small-world network effect in nonequilibrium statistical dynamics. We have already obtained some interesting results, which will be reported in a later paper as a further application.

Up to this point we have successfully generalized Glauber's single-spin-flipping mechanism to a single-spin transition mechanism, and Kawasaki's spin-pair exchange mechanism to a spin-pair redistribution mechanism. These two generalizations are of similar mathematical form and may become counterparts of each other in nonconserved and conserved dynamics, respectively.

The formulation of the mechanism is the chief purpose of this Brief Report. As an example of its applications we studied the diffusion process in a kinetic Gaussian model, which people were previously unable to treat. The temperature-dependent diffusion coefficient, which becomes zero at the critical point, reveals critical slowing down in the diffusion process. In this specific case, interestingly, the critical dynamic exponent is independent of space dimensionality and the dynamic mechanism. The redistribution mechanism (and transition) can also be directly applied to the Potts model, $XY$ model, Heisenberg model, and many other types (in principle arbitrary). Although an exact treatment may be difficult, other methods can be used later based on this foundation. There have been many such efforts. For example, in a Monte Carlo simulation of the three-dimensional ferromagnetic Heisenberg model [9], Zhang has suggested that two neighboring spins $\sigma_i$ and $\sigma_j$ may rotate with their conserved sum being the axis. He found that this scheme enabled the system to evolve to thermodynamic equilibrium faster, and commented that it might be more favorable in reality. This is just a successful exploration of the spin-pair redistribution mechanism, and there are many other such examples, though assuming different forms. At the same time the redistribution mechanism can be almost directly applied to conserved processes other than those in spin-lattice models; for example, the relaxation of granular material under shaking (mass conserved), or the activities of particles in space (particle number conserved). One may first present an analogous lattice model and define the parameter. Then one can write the master equation, modified if necessary, and the evolving equation of the parameter one is interested in. This serves to unite the various conserved processes into a universal framework in microscopics, and provides the basis for further treatment, either exact, approximate, or Monte Carlo. The same is true for the single-spin transition mechanism. This in turn brings more significance back to the original mechanisms.

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