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A Mean-Field Equation of Motion for the Dynamic Ising Model

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A mean-field type of approximation is used to derive two differential equations, one approximately representing the average behavior of the Ising model with Glauber (spin-flip) stochastic dynamics, and the other doing the same for Kawasaki (spin-exchange) dynamics. The proposed new equations are compared with the Cahn–Allen and Cahn–Hilliard equations representing the same systems and with information about the exact behavior of the microscopic models.

KEY WORDS: Dynamic Ising model; mean-field theories; kinetics of phase transitions; approximate kinetic equations.

1. INTRODUCTION

Partial differential equation models such as the Cahn–Allen[1] and Cahn–Hilliard[2] equations have been used with great success as representations of the broad characteristics of kinetic phase-transition phenomena, such as spinodal decomposition. The Cahn–Hilliard equation also gives[4] quantitative predictions of the scaling functions which have been found to encapsulate the time dependence of the structure function and the pair distribution in the late stages of spinodal decomposition.

There are, however, some theoretical difficulties associated with these equations [which are exhibited below as Eqs. (27) and (28)]. One is that the equations contain a function, normally interpreted as the thermodynamic free energy density, which is a nonconvex function of the magnetization or the density, in violation of the general theorem [(3.4.4)

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of ref. 10], that the free energy function must be convex. Moreover, as we shall see in Section 5, this interpretation is incompatible with the exact microscopic dynamics of the kinetic Ising model. Another difficulty, if the equations are to be used for quantitative predictions, is that they contain a rate parameter for which there is no obvious microscopic theory.

The purpose of this paper is to propose a different type of equation, which avoids some of these difficulties and which can be derived from a microscopic model, namely the kinetic Ising model, by the use of a well-defined approximation. This approximation is closely related to the mean-field theory of the equilibrium properties of this Ising model.

2. DERIVATION OF THE EQUATIONS

Consider an Ising model on a lattice Λ, and denote the spin at site $a \in \Lambda$ by s_a (so that $s_a = \pm 1$ for all $a \in \Lambda$). We assume nearest-neighbor interactions so that the energy of a configuration $s = \{s_a, a \in \Lambda\}$ is

$$W(s) = -\frac{1}{2} \sum_a \sum_b J_{ab} s_a s_b \tag{1}$$

where J_{ab} is the Ising interaction between sites a and b. For simplicity we shall assume throughout that $J_{ab} \geqslant 0$, although much of the discussion applies to other cases as well.

We shall consider two different kinds of stochastic dynamics: the spin-flip dynamics of Glauber,[5] in which each spin has a probability per unit time $w_a(s)$ of reversing its sign, and the spin-exchange dynamics of Kawasaki,[6] in which, for each nearest-neighbor pair ab of sites, there is a probability $w_{ab}(s)$ per unit time that the spins at the two sites will change places. If a, b are not nearest neighbors, we take $w_{ab} = 0$.

We denote expectations by the symbol $\mathbf{E}$. For Glauber dynamics the expectation of s_a obeys[5] the time evolution law

$$\frac{d}{dt} \mathbf{E}(s_a) = -2\mathbf{E}(s_a w_a) \tag{2}$$

For Kawasaki dynamics the corresponding law is

$$\frac{d}{dt} \mathbf{E}(s_a) = \sum_{b \in N(a)} \mathbf{E}[(s_b - s_a) w_{ab}] \tag{3}$$

where $N(a)$ means the set of sites that are nearest neighbors of site a.

The choice of the transition rates w_a and w_{ab} is to some extent arbitrary, but on general principles they should satisfy the detailed balance conditions

$$w_a(s)\, e^{-\beta W(s)} = w_a(s^a)\, e^{-\beta W(s^a)} \tag{4}$$

$$w_{ab}(s)\, e^{-\beta W(s^{ab})} = w_{ab}(s^{ab})\, e^{-\beta W(s^{ab})} \tag{5}$$

where β is the inverse temperature, s^a is the configuration obtained from s by reversing s_a [so that $(s^a)_b = s_b$ if $a \neq b$, but $= -s_b$ if $a = b$], and s^{ab} is the configuration obtained from s by interchanging s_a and s_b [so that $(s^{ab})_c = s_c$ if $c \neq a$, b, but $= s_b$ if $c = a$, and $= s_a$ if $c = b$].

A convenient choice of transition rates satisfying detailed balance is Glauber's[5] hyperbolic tangent rule

$$w(s) = \tfrac{1}{2}\{1 - \tanh[\tfrac{1}{2}\beta \delta W(s)]\} \tag{6}$$

where $\delta W(s)$ is the increase in energy brought about by the transition and the unit of time is chosen so that $w(s) \to 1$ as $\delta W(s) \to -\infty$. More specifically, for Glauber dynamics the w on the left of (6) means w_a and δW is given by

$$\begin{aligned} \delta W(s) &= W(s^a) - W(s) \\ &= 2 s_a \sum_{b \neq a} J_{ab} s_b \qquad \text{by (1)} \end{aligned} \tag{7}$$

For Kawasaki dynamics, the w means w_{ab} and δW is given by

$$\begin{aligned} \delta W(s) &= w(s^{ab}) - w(s) \\ &= (s_a - s_b) \sum_{c \neq a, b} (J_{ac} - J_{bc})\, s_c \qquad \text{by (1)} \end{aligned} \tag{8}$$

However, in this case the formula (6) for w applies only if a and b are nearest neighbors; if they are not, we take $w_{ab} = 0$.

The general solution of the detailed balance condition is a formula like (6) with the right-hand side multiplied by an arbitrary even function of $\delta W(s)$ which approaches 1 as $\delta W(s) \to -\infty$. For example, the Metropolis probability rule[7] can be obtained by multiplying the right-hand side of (6) by $1 + \exp(-\beta\, |\delta W(s)|)$. In the present paper, however, only the hyperbolic tangent rule (6) will be used.

Substitution of (6) into the time evolution law for Glauber dynamics, Eq. (2), gives

$$\begin{aligned} \frac{d}{dt}\mathbf{E}(s_a) &= -\mathbf{E}(s_a) + \mathbf{E}\left[s_a \tanh\left(\beta s_a \sum_{b \neq a} J_{ab} s_b \right) \right] \\ &= -\mathbf{E}(s_a) + \mathbf{E}(\tanh r_a) \qquad \text{since} \quad s_a^2 = 1 \end{aligned} \tag{9}$$

where we have defined

$$r_a = \sum_{b \neq a} \beta J_{ab} s_b \tag{10}$$

For Kawasaki dynamics the corresponding result, from (6) and (3), is

$$\frac{d}{dt} \mathbf{E}(s_a) = \sum_{b \in N(a)} I_{ba} \tag{11}$$

where

$$\begin{aligned} I_{ba} &= \tfrac{1}{2}\mathbf{E}\left\{(s_b - s_a)\left[1 - \tanh \tfrac{1}{2}\beta(s_a - s_b) \sum_{c \neq a,b} (J_{ac} - J_{bc})\, s_c\right]\right\} \\ &= \tfrac{1}{2}\mathbf{E}(s_b - s_a) + \tfrac{1}{4}\mathbf{E}\left\{(s_a - s_b)^2 \tanh\left[\sum_{c \neq a,b} \beta(J_{ac} - J_{bc})\, s_c\right]\right\} \\ &\qquad [\text{since } s_a - s_b = \pm 2 \text{ or } 0] \\ &= \tfrac{1}{2}\mathbf{E}(s_b - s_a) + \tfrac{1}{2}\mathbf{E}\{(1 - s_a s_b) \tanh[r_a - r_b + \beta J_{ab}(s_a - s_b)]\} \end{aligned} \tag{12}$$

with r defined as in (10).

In order to turn (9) or (12) into a closed equation for $\mathbf{E}(s_a)$ we need an approximation for the expectation involving a hyperbolic tangent. The approximation we shall use is motivated by consideration of the limiting case where the interaction is very weak and of very long range; in this limit, equilibrium mean-field theory becomes exact.[8] For this case, the quantity r_a defined in (10) is the sum of a large number of contributions from many different parts of the system. Assuming that the fluctuations of these contributions about their mean values are independent, so that a law of large numbers applies, then the fluctuations of r_a about its mean value will be small, so that in the limit $\mathbf{E}(\tanh r_a) = \tanh \mathbf{E}(r_a)$. Our approximation, which may be expected to be the more accurate the more nonvanishing terms there are in the sum (10) for r_a, is thus to replace $\mathbf{E}(\tanh r_a)$ by $\tanh \mathbf{E}(r_a)$ in (9). This gives the following approximate kinetic equation, for Glauber dynamics with the hyperbolic tangent rule:

$$\frac{d}{dt} \mathbf{E}(s_a) = -\mathbf{E}(s_a) + \tanh \mathbf{E}(r_a) \tag{13}$$

This equation may be written

$$\frac{du_a}{dt} = -u_a + \tanh v_a \tag{14}$$

where u_a means $\mathbf{E}(s_a)$ and v_a is defined by

$$v_a = \mathbf{E}(r_a) = \sum_{b \neq a} \beta J_{ab} u_b \tag{15}$$

In the special case where u_a is independent of a, Eq. (14) reduces to the mean-field equation of Suzuki and Kubo.[11]

For Kawasaki dynamics the corresponding approximation is to replace the argument of the tangent in (12) by its expectation; however, the resulting approximate kinetic equation still involves $\mathbf{E}(s_a s_b)$, and so a further closure approximation is necessary. The simplest such approximation is

$$\mathbf{E}(s_a s_b) \simeq \mathbf{E}(s_a)\,\mathbf{E}(s_b) \tag{16}$$

and it leads to the approximate kinetic equation

$$\frac{du_a}{dt} = \frac{1}{2} \sum_{b \in N(a)} \{(u_b - u_a) + (1 - u_b u_a) \tanh[v_a - v_b + \beta J_{ab}(u_a - u_b)]\} \tag{17}$$

with u_a and v_a defined as before.

The two approximate kinetic equations (14) and (17) are the core of this paper.

3. THE LYAPUNOV PROPERTY

One of the attractive features of the Cahn–Allen and Cahn–Hilliard equations is that for each of them the free energy functional is a Lyapunov functional, that is, it decreases monotonically with time. This corresponds to what we expect on physical grounds, and is also useful for deducing mathematical properties of the solutions of the equation, such as their approach to equilibrium as $t \to \infty$.

The approximate kinetic equations derived in Section 2 also have a Lyapunov function, which may also be interpreted as a free energy. In the case of Glauber dynamics, the Lyapunov function is the following expression, which can be interpreted as a mean-field approximation to the free energy:

$$F_G\{u\} = \beta^{-1} \sum_a g(u_a) - \frac{1}{2} \sum_a \sum_b J_{ab} u_a u_b \tag{18}$$

where g is defined by

$$g(u) = \tfrac{1}{2}(1+u)\log(1+u) + \tfrac{1}{2}(1-u)\log(1-u) \tag{19}$$

From these definitions it follows that the derivative of g is

$$g'(u) = \operatorname{arc\,tanh} u \tag{20}$$

and that

$$\beta \frac{\partial F_G}{\partial u_a} = \operatorname{arc\,tanh} u_a - v_a \tag{21}$$

with v_a defined as in (15).

To prove the Lyapunov property of our approximate kinetic equation (14) for Glauber dynamics, we calculate the time derivative of F_G, using (14) and (21). We obtain

$$\begin{aligned} \beta \frac{dF_G}{dt} &= \beta \sum_a \frac{\partial F}{\partial u_a} \frac{du_a}{dt} \\ &= -\sum_a (\operatorname{arc\,tanh} u_a - v_a)(u_a - \tanh v_a) \\ &\leqslant 0 \end{aligned} \tag{22}$$

since $\operatorname{arc\,tanh} u - v$ and $u - \tanh v$ necessarily have the same sign.

In the Kawasaki case a Lyapunov function exists provided that J_{ab} takes the same value, call it J_{nn}, for all nearest-neighbor pairs J_{ab}. This Lyapunov function is

$$F_K = F_G - \frac{1}{2} J_{nn} \sum_a u_a^2 \tag{23}$$

The time derivative of this function can be written, using (11),

$$\begin{aligned} \frac{dF_K}{dt} &= \sum_a \frac{\partial F_K}{\partial u_a} \sum_{b \in N(a)} I_{ba} = \sum_b \frac{\partial F_K}{\partial u_b} \sum_{a \in N(b)} I_{ab} \\ &= -\frac{1}{2} \sum_a \sum_{b \in N(a)} \left(\frac{\partial F_K}{\partial u_a} - \frac{\partial F_K}{\partial u_b} \right) I_{ab} \qquad \text{since } I_{ba} = -I_{ab} \end{aligned} \tag{24}$$

The approximation used in (17) for I_{ab} now gives, if we define $w_a = v_a + \beta J_{nn} u_a$,

$$\begin{aligned} \beta \frac{dF_K}{dt} &= -\frac{1}{4} \sum_a \sum_{b \in N(a)} [g'(u_a) - w_a - g'(u_b) + w_b] \\ &\quad \times [u_a - u_b - (1 - u_a u_b) \tanh(w_a - w_b)] \\ &= -\frac{1}{4} \sum_a \sum_{b \in N(a)} (1 - u_a u_b)[g'(u_a) - g'(u_b) - w_a + w_b] \\ &\quad \times \{\tanh[g'(u_a) - g'(u_b)] - \tanh(w_a - w_b)\} \\ &\leqslant 0 \end{aligned} \tag{25}$$

by (20), since $x-y$ and $\tanh x-\tanh y$ always have the same sign. In the penultimate line we have used the addition formula for hyperbolic tangents.

4. THE DISCRETE CAHN–ALLEN AND CAHN–HILLIARD EQUATIONS

For comparison purposes, it is useful to have discrete analogues of the Cahn–Allen and Cahn–Hilliard equations. These equations are normally obtained from the continuous-space free energy functional

$$F=\int \{f(u(\mathbf{x}))+\tfrac{1}{2}\varepsilon[\nabla u(\mathbf{x})]^2\}\, d^3\mathbf{x} \tag{26}$$

where f is the free energy per unit volume and ε is a constant. The Cahn–Allen equation is

$$\frac{\partial u}{\partial t}=-M\frac{\delta F}{\delta u(\mathbf{x})}=-M\{f'(u)-\varepsilon\nabla^2 u\} \tag{27}$$

where M is a rate constant and $\delta F/\delta u(\mathbf{x})$ denotes a functional derivative. The Cahn–Hilliard equation is

$$\frac{\partial u}{\partial t}=M\nabla^2\frac{\delta F}{\delta u}=M\nabla^2\{f'(u)-\varepsilon\nabla^2 u\} \tag{28}$$

The free energy formula (26) has a discrete analogue

$$\begin{aligned} F &\simeq \sum_a f(u_a)+\tfrac{1}{4}\varepsilon\sum_a\sum_{b\in N(a)}(u_a-u_b)^2 \\ &=\sum_a[f(u_a)+\tfrac{1}{2}z\varepsilon u_a^2]-\tfrac{1}{2}\varepsilon\sum_a\sum_{b\in N(a)}u_a u_b \end{aligned} \tag{29}$$

where z is the coordination number of the lattice. By applying the discrete analogue of the recipe used in (27) to this free energy function, we obtain a discrete analogue of the Cahn–Allen equation:

$$\frac{du_a}{dt}=-M\frac{\partial F}{\partial u_a}=-M\left[f'(u_a)-\sum_{b\in N(a)}\varepsilon(u_b-u_a)\right] \tag{30}$$

Likewise, by applying the discrete analogue of the recipe used in (28) we obtain a discrete analogue of the Cahn–Hilliard equation

$$\begin{aligned} \frac{du_a}{dt} &= M\sum_{b\in N(a)}\left(\frac{\partial F}{\partial u_b}-\frac{\partial F}{\partial u_a}\right) \\ &= M\sum_{b\in N(a)}\left[f'(u_b)-f'(u_a)-\sum_{c\in N(b)}\varepsilon(u_c-u_b)+\sum_{c\in N(a)}\varepsilon(u_c-u_a)\right] \end{aligned} \tag{31}$$

The correspondence between Eqs. (30) and (31) on the one hand and our approximate kinetic equations (14) and (17) on the other becomes particularly close if we arrange for the corresponding Lyapunov functions, (29) on the one hand and (18) and (23) on the other, to be the same. To do this we choose nearest-neighbor interactions with $J_{nn} = \varepsilon$ and take the free energy per site to be

$$f(u) = \beta^{-1} g(u) - \tfrac{1}{2} z \varepsilon u^2 \qquad \text{(Glauber dynamics)} \tag{32}$$

$$f(u) = \beta^{-1} g(u) - \tfrac{1}{2}(z+1)\, \varepsilon u^2 \qquad \text{(Kawasaki dynamics)} \tag{33}$$

With the use of the free energy formula (32), the discrete Cahn–Allen equation (30) now becomes

$$\frac{du_a}{dt} = -M \frac{\partial F_G}{\partial u_a} = -\beta^{-1} M (\operatorname{arc\,tanh} u_a - v_a) \tag{34}$$

By way of comparison, if we were to set $M = \beta$ and replace each of the two terms on the right side of (34) by their hyperbolic tangents, we would get the approximate kinetic equation (14).

Likewise, using (33) in the discrete Cahn–Hilliard equation (31), we get

$$\frac{du_a}{dt} = \beta^{-1} M \sum_{b \in N(a)} [g'(u_b) - g'(u_a) - w_b + w_a] \tag{35}$$

where $w_a = v_a + J_{nn} u_a$ as before. If we were to set $M = \beta/2$, insert a factor $(1 - u_a u_b)$, and replace $g'(u_b) - g'(u_a)$ and $-w_b + w_a$ by their hyperbolic tangents, we would get (17).

5. SOME COMPARISONS

As the approximate kinetic equations (14) and (17) are being put forward here as possible improvements on the Cahn–Allen and Cahn–Hilliard equations, we would like to compare the accuracy of the two types of equation as representations of the true behavior of the kinetic Ising model. In order to compare like with like, we shall compare with the discrete Cahn–Allen and Cahn–Hilliard equations (30) and (31) rather than the original partial differential equations.

Consider first of all the equilibrium solutions. These can be obtained by minimizing the Lyapunov functions (18) and (23); therefore, provided we use the appropriate correspondence from (32) and (33) when choosing $f(u)$, the equations compared will have the same Lyapunov functions and therefore the same equilibrium solutions, whatever boundary conditions

are imposed. In the case of Glauber dynamics this makes good sense, because the free energy expression (32) we use in the approximate Cahn–Allen equation is precisely the free energy expression given by mean-field equilibrium theory. For the Kawasaki case, however, the situation is a little different: this time, to make the equilibrium solutions agree we must use the free energy expression (33), which is *not* the same as the mean-field approximation to the true free energy density. Although even the correct mean-field approximation is not particularly accurate, especially at low dimension numbers, the appearance of a free energy density which does not follow from any recognized approximate equilibrium theory is a defect. This defect presumably arises from the simplifying approximation (16), which at low temperatures is not a good one.

Consider now the simplest nonequilibrium case, namely infinite temperature ($\beta = 0$). In this case the exact kinetic equations are, by (9) and (11), (12),

$$\frac{du_a}{dt} = -u_a \qquad \text{(Glauber dynamics)} \tag{36}$$

$$\frac{du_a}{dt} = \frac{1}{2} \sum_{b \in N(a)} (u_b - u_a) \qquad \text{(Kawasaki dynamics)} \tag{37}$$

Our approximate kinetic equations (14) and (17) agree precisely with these exact equations when $\beta = 0$. The discrete Cahn–Allen and Cahn–Hilliard equations (30) and (31), on the other hand, give in the high-temperature limit

$$\frac{du_a}{dt} = -M_0 \operatorname{arc\,tanh} u_a \qquad \text{(Glauber)} \tag{38}$$

$$\frac{du_a}{dt} = M_0 \sum_{b \in N(a)} (\operatorname{arc\,tanh} u_b - \operatorname{arc\,tanh} u_a) \qquad \text{(Kawasaki)} \tag{39}$$

where $M_0 = \lim_{\beta \to 0} \beta^{-1} M$, since the asymptotic form of $f(u)$ at high temperatures is the ideal lattice-gas form $f(u) = \beta^{-1} g(u)$ with $g(u)$ as in (19).

The discrete Cahn–Allen and Cahn–Hilliard equations can of course be saved in this case by relaxing the condition that f be the free energy per site and choosing instead $f(u) = u^2/2M$. Indeed, it is a common practice among users of these equations to take f to be a polynomial (see, for example, refs. 3 and 9), but for a lattice system this form for $f(u)$, with u capable of all real values instead of being restricted to the interval $[-1, 1]$, seems more appropriate to a continuous-spin model than to the Ising model.

For finite temperatures it is not possible (apart from one special case, which we consider below) to solve the exact kinetic equation (9) or (11), (12), but we can obtain an inequality which leads to similar conclusions about the comparison we are considering here. For Glauber dynamics, the exact equation (9) implies

$$\left|\frac{du_a}{dt}+u_a\right| = \left|\mathbf{E}\left[s_a \tanh\left(\beta s_a \sum_{b\neq a} J_{ab}s_b\right)\right]\right|$$
$$\leqslant \tanh\beta \sum_{b\neq a} J_{ab}$$
$$\leqslant 1 \tag{40}$$

Our approximate kinetic equation (14) is consistent with (40), whereas the discrete Cahn–Allen equation is consistent with it only if

$$|f'(u)| \leqslant 2/M + 2\beta z\varepsilon \tag{41}$$

[a condition derived by substituting for du_a/dt from (30) into (40) and using the fact that u_a and u_b are $\leqslant 1$]. Once again we have an inconsistency with the interpretation of $f(u)$ as the free energy per site, since under that interpretation $f'(u)$ is the chemical potential and tends to $\pm\infty$ as u tends to ± 1.

A similar argument applies in the case of Kawasaki dynamics, for which the exact kinetic equation (11), (12) implies

$$\left|\frac{du_a}{dt}+\sum_{b\in N(a)}\frac{1}{2}(u_a-u_b)\right| \leqslant z \tag{42}$$

where z is the coordination number of the lattice. This inequality is consistent with (17), but taken together with the discrete Cahn–Hilliard equation (31), it implies (for nearest-neighbor interaction strength $J_{nn}=\varepsilon$)

$$\left|\sum_{b\in N(a)}[f'(u_a)-f'(u_b)]\right| \leqslant 2z(1/M+2z\varepsilon) \tag{43}$$

To see that this last inequality is inconsistent with the interpretation of $f(u)$ as free energy per site, consider any lattice—such as the simple cubic—whose sites can be colored, as on a chessboard, in such a way that every nearest-neighbor pair consists of one site of each color, and take u_a to be $+u$ if a is a "black" site and $-u$ if b is "white" site, where u is a number to be chosen. Then (43) becomes

$$|2zf'(u)| \leqslant 2z(1/M+2z\varepsilon) \tag{44}$$

which like (41) is inconsistent with the requirement $\lim_{u\to\pm 1} f'(u) = \pm\infty$.

There is one further test to which these kinetic equations can be subjected, and neither comes out of it well. The test is to apply them to Glauber's[5] exactly soluble model, the one-dimensional Ising chain with nearest-neighbor interactions. For this model, since r_a can now take only the values $\pm 2\beta J_{nn}$ and 0, Eq. (9) reduces exactly to

$$\frac{du_a}{dt} = -u_a + \frac{\tanh(2\beta J_{nn})}{2\beta J_{nn}} v_a \tag{45}$$

Our approximate kinetic equation (14) agrees with this only in the high-temperature limit, and the discrete Cahn–Allen equation agrees with it only if we make $f(u)$ proportional to u^2, which, for the reasons already explained, is inconsistent with the thermodynamic interpretation of $f(u)$.

A practical disadvantage afflicting our kinetic equations (14) and (17) and the discrete Cahn–Hilliard and Cahn–Allen equations equally, but not the original continuous-space Cahn–Hilliard and Cahn–Allen equations (27) and (28), is that if the lattice being considered has a very large number of sites, then the number of differential equations to be solved is very large. A possible way to overcome this would be to use instead the partial differential equation to which it is the discrete approximation, obtained (in the case of nearest-neighbor interactions on a square or simple cubic lattice with unit spacing) by replacing the definition (15) of v_a by

$$v_a = \beta J_{nn}(z u_a + \nabla^2 u_a) \tag{46}$$

The resulting nonlinear partial differential equation, containing a hyperbolic tangent of a space derivative, is of a very unusual type.

To conclude, the approximate kinetic equations proposed here differ from the Cahn–Hilliard and Cahn–Allen equations in that they can be derived directly from a macroscopic model, contain no adjustable parameters or functions, and avoid the difficulties of interpreting the function $f(u)$ which are associated with the latter equations. They seem well worth further investigation.

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NOTE ADDED IN PROOF

Another way of converting our kinetic equations into a partial differential equation is to look for solutions in which u_a varies only very

slowly from one lattice site to the next. For example, in the case of Kawasaki dynamics we may look for solutions of Eq. (17) in the form $u_a(t) = U(\mathbf{r}_a/L, t/L^2)$ where $\mathbf{r}_a$ is the position vector of lattice site a and L is a parameter representing the length scale for variations of u_a. Then, writing $\mathbf{R}$ for $\mathbf{r}_a/L$ and T for t/L^2, and taking the limit where L becomes very large we obtain as the limiting form of (17) (assuming for simplicity a simple cubic lattice, with lattice constant 1)

$$\frac{\partial}{\partial T} U(\mathbf{R}, T) = \frac{1}{2} \operatorname{div}[D(U)\ \mathbf{grad}\ U]$$

where $D(U) = 1 - (1 - U^2)\,\beta(J_{nn} + \sum_{b \neq a} J_{ab})$ and the vector differentiations are taken with respect to $\mathbf{R}$. A limiting equation of precisely this form has been derived rigorously by Lebowitz, Orlandi and Presutti [12] in a case where the interaction is very weak and of very long range, there is only one space dimension and the initial values of U (that is, of u) lie in the range where $D(U)$ is positive.

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