Heuristic derivation of continuum kinetic equations from microscopic dynamics

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We present an approximate and heuristic scheme for the derivation of continuum kinetic equations from microscopic dynamics for stochastic, interacting systems. The method consists of a mean-field-type, decoupled approximation of the master equation followed by the ''naive'' continuum limit. The Ising model and driven diffusive systems are used as illustrations. The equations derived are in agreement with other approaches, and consequences of the microscopic dependences of coarse-grained parameters compare favorably with exact or high-temperature expansions. The method is valuable when more systematic and rigorous approaches fail, and when microscopic inputs in the continuum theory are desirable.

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I. INTRODUCTION

Ever since its introduction in a classic treatment of the Brownian motion [1], the Langevin equation has been playing an important role in modern statistical physics. It provides a mathematical framework and a physical basis for studying stochastic processes in statistical, mechanical systems. Applications are wide-ranging [2], including chemical reactions, laser physics, diffusive processes, and modern theories of dynamical critical phenomena [3]. Recent topics such as surface growth [4] and pattern formation [5] also rely heavily on the Langevin equation.

It is fair to say, however, that despite its popularity, the Langevin equation for a specific problem is seldom derived from the corresponding microscopics. It is often postulated on the grounds of symmetry and physical reasoning. Only rarely in simple circumstances is it derived with reasonable mathematical rigor from the more fundamental master equation. To this end, the Ω expansion introduced by van Kampen [6] is a well-established technique. It consists of a decomposition of the slow variable into a macroscopic part and a fluctuating part, followed by a systematic expansion of the master equation in inverse powers of the volume Ω of the coarse-graining block. While the leading order in the expansion gives the deterministic equation of motion for the slow variable, the next order yields a Fokker-Planck equation for the fluctuating part, from which the noise term of the associated Langevin equation can be identified. An independent method, based on a Fock space representation of classical objects using creation and annihilation operators, was introduced by Doi [7] and reformulated by Rose [8] and Grassberger and Scheunert [9]. Although not directly cast in the Langevin language, it also addresses the dynamics of classical many-particle systems. The method is noted for its application in birth-death processes such as chemical reactions. Later, Peliti [10] recast it in a path-integral form and treated random walks and aggregation problems.

In this paper, we shall present an approximate scheme somewhat in between a mere postulation and rigorous formulations, for deriving the Langevin equation from the microscopic specification of the dynamics. Our goal is not to propose a new formal derivation, but rather to give a quick, simple, and heuristic means that can be applied generally to stochastic systems, several of which shall be discussed below.

Expositions of the historical, philosophical, and technical aspects of the Langevin equation are beyond the scope of this paper. Interested readers are thus referred to the relevant literature [2]. This paper is organized as follows. An elementary recapitulation of the master equation and Langevin equation is presented in Sec. II. Section III contains several examples as illustrations of the method, as well as assessment of the quality of the approximation involved. Conclusions are given in Sec. IV. A discussion of the noise correlation is given in the Appendix.

II. MASTER EQUATION AND TIME-DEPENDENT GINZBURG-LANDAU EQUATION

In statistical physics, one of the most important applications of the Langevin equation is in the theories of dynamical critical phenomena [3]. Therefore, our discussion shall be cast in that language, although it should be obvious that the method itself is not limited to systems exhibiting those phenomena. For concreteness, consider the kinetic Ising model that obeys Glauber (i.e., spin-flip) dynamics [11]. At the classical, microscopic level of description, the system consists of N spins σ_i interacting via the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j , \tag{1}$$

where J is the coupling constant and $\langle i,j \rangle$ denotes a sum over nearest-neighbor pairs. The time evolution of the system is governed by a master equation

$$P(\vec{\sigma};t+1) - P(\vec{\sigma};t) = \sum_{\vec{\sigma}'} [w(\vec{\sigma}' \to \vec{\sigma}) P(\vec{\sigma}';t) - w(\vec{\sigma} \to \vec{\sigma}') P(\vec{\sigma};t)], \tag{2}$$

where $P(\vec{\sigma};t)$ is the joint probability of finding the system in the spin configuration $\vec{\sigma} \equiv \{\sigma_1, \sigma_2, \ldots, \sigma_N\}$ at time t, and

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w's are the transition rates between two configurations that differ only by one spin flip. There is a great deal of freedom in the choice of w, as long as the following detailed balance condition is satisfied to ensure the same equilibrium distribution $P_{\rm eq}(\vec{\sigma}) \sim e^{-\beta H(\vec{\sigma})}$,

$$\frac{w(\vec{\sigma}' \to \vec{\sigma})}{w(\vec{\sigma} \to \vec{\sigma}')} = \frac{P_{\rm eq}(\vec{\sigma})}{P_{\rm eq}(\vec{\sigma}')} = e^{-\beta[H(\vec{\sigma}) - H(\vec{\sigma}')]}, \tag{3}$$

with $\beta = 1/k_B T$. In practice, the choice is largely dictated by mathematical convenience. The most common choices of w are the Metropolis rate in Monte Carlo simulations for its ease of implementation, and the heat-bath rate (also known as the Kawasaki rate [12]) in analytic calculations for its analyticity. In this paper, we confine our attention to the latter choice. It is given by

$$w(\vec{\sigma} \to \vec{\sigma}') = \frac{1}{1 + e^{-\beta[H(\vec{\sigma}) - H(\vec{\sigma}')]}}. \tag{4}$$

Since the master equation is not very convenient for analytic purposes such as a renormalization-group analysis, one often turns to a mesoscopic, continuum representation. For an Ising system with Glauber dynamics, the relevant continuum field is the local magnetization density $\phi(\vec{r},t)$, which obeys a kinetic equation

$$\frac{\partial \phi}{\partial t} = -\Gamma \frac{\delta \mathcal{H}}{\delta \phi} + \zeta, \tag{5}$$

$$\mathcal{H} = \int d^d r \left\{ \frac{1}{2} (\nabla \phi)^2 + V(\phi) \right\}, \tag{6}$$

$$V(\phi) = \frac{u}{2} \phi^2 + \frac{g}{4!} \phi^4 + \cdots. \tag{7}$$

This is an example of the time-dependent Ginzburg-Landau (TDGL) kinetic equation. In Eq. (6), d is the dimensionality of the system, and $\mathcal{H}$ is a coarse-grained Hamiltonian. For Eq. (5) to describe a stochastic process, the noise term $\zeta(\vec{r},t)$ is needed, which accounts for the effect of thermal fluctuations and prevents the system from trapping in metastable states. For mathematical convenience, it is often taken to be Gaussian with zero mean:

$$\langle \zeta(\vec{r},t) \rangle = 0, \tag{8}$$

$$\langle \zeta(\vec{r},t) \zeta(\vec{r}',t') \rangle = 2D \delta(\vec{r} - \vec{r}') \delta(t - t'). \tag{9}$$

For equilibrium systems, the correlation D in Eq. (9) has to be chosen to ensure that the stationary solution of Eq. (5) is consistent with the Boltzmann weight $\mathcal{P}_{\rm eq} \sim e^{-\mathcal{H}}$ (cf. the Appendix). For a system as simple as the Ising model, the *static* continuum Hamiltonian $\mathcal{H}$ can actually be derived from the microscopic H via the partition function by means of the Hubbard-Stratonovich transformation [13], which is a trick based on the Gaussian integral. For the dynamics, the TDGL equation has been derived by coarse graining the master equation [14], which in principle yields expressions of the coarse-grained parameters Γ, u, and g in Eqs. (5)–(7) as functions of microscopic ones in Eq. (2).

However, for more complicated H, the Hubbard-Stratonovich transformation fails and the coarse graining cannot be done explicitly. Moreover, these methods rely on the existence of a Hamiltonian H and the associated equilibrium Boltzmann weight $e^{-\beta H}$, which is not valid in generic nonequilibrium situations defined only by the dynamics [15]. For those cases, alternative to the established techniques [6–10], it is highly desirable to have a straightforward method to extract a continuum description directly from the dynamics [16]. In the next section, we shall present such a method.

III. FACTORIZATION AND NAIVE CONTINUUM EXPANSION

Our method is very simple. It consists of two steps: a mean-field-type factorization of joint probabilities into singlet ones in the master equation, followed by a ''naive'' continuum expansion. The result is a continuum kinetic equation with full knowledge of the microscopic dependence of the coarse-grained parameters [17]. Since the input is the master equation, whether the system is an equilibrium one or not [15] is irrelevant. To illustrate, we now discuss several examples in increasing order of sophistication.

A. 1D Ising model

Focusing on a spin at position x in a one-dimensional (1D) Ising model, it is easy to find by integrating out all other spins in Eq. (2) that

$$\begin{aligned} P_+(x;t+1) - P_+(x;t) = {} & P_{---} w_{---} + P_{--+} w_{--+} \\ & + P_{+-+} w_{+-+} + P_{+--} w_{+--} \\ & - P_{-+-} w_{-+-} - P_{-++} w_{-++} \\ & - P_{++-} w_{++-} - P_{+++} w_{+++}, \end{aligned} \tag{10}$$

where $P_+(x;t)$ denotes the singlet probability of finding the spin up at site x at time t, and $P_{+++}(x;t)$ denotes the joint probability of finding three spins up at site $x-1$, x, $x+1$, respectively, and so on. From Eq. (4), the heat-bath transition rates are given by $w_{---} = w_{+++} = W_4$, $w_{--+} = w_{+--} = w_{-++} = w_{++-} = W_0$, and $w_{+-+} = w_{-+-} = W_{-4}$, where

$$W_n \equiv \frac{1}{1 + e^{n\beta J}}. \tag{11}$$

Adopting a mean-field approximation, the joint probabilities are replaced by their factorizations, e.g., $P_{++-}(x;t) \to P_+(x-1;t) P_+(x;t) P_-(x+1;t)$. Since $\Sigma_\sigma \sigma P_\sigma(x;t) = P_+(x;t) - P_-(x;t) = \langle \sigma \rangle$ and $\Sigma_\sigma P_\sigma(x;t) = P_+(x;t) + P_-(x;t) = 1$, in the spirit of coarse graining we proceed to make the identification

$$P_{\pm}(x;t) \leftrightarrow \frac{1 \pm \phi(x;t)}{2}, \tag{12}$$

where ϕ is the local magnetization density. By using ϕ instead of spin number densities, we take advantage of symmetries anticipated in the final kinetic equation. Since a spin flip depends on a total of $z+1$ spins in Eq. (2), where $z=2d$ for hypercubic lattices, the factorization effectively produces a power-series expansion in ϕ up to ϕ^{z+1}. After replacing P's by ϕ's, we make the transition to the continuum by ''naively'' expanding about x, such as

$$\phi(x \pm 1;t) \rightarrow \phi(x;t) \pm \frac{\partial \phi(x;t)}{\partial x} + \frac{1}{2} \frac{\partial^2 \phi(x;t)}{\partial x^2} + \cdots. \tag{13}$$

For most applications, we are only interested in the long-distance behavior, hence it suffices to stop at the lowest derivatives as shown. This procedure results in a deterministic kinetic equation for ϕ in precisely the form of Eqs. (5)–(7), barring the noise term ζ:

$$\frac{\partial \phi}{\partial t} = -\Gamma\left(-\frac{\partial^2 \phi}{\partial x^2} + r\phi + \frac{g}{6}\phi^3 \right),$$

where the coefficients are given by

$$\Gamma = \frac{1}{2}(W_{-4} - W_4),$$

$$r = \frac{1}{2\Gamma}(3W_4 - W_{-4} + 2W_0),$$

$$g = \frac{3}{\Gamma}(W_4 + W_{-4} - 2W_0). \tag{14}$$

Several remarks are in order.

(i) Symmetries in the resulting continuum equation (with respect to ϕ, x, and t) are as expected, because the approximations respect those symmetries and leave them intact.

(ii) There are explicit temperature dependences in the coefficients that cannot be deduced by symmetry or physical reasoning. Such dependences are specific to the choice of jump rates that are manifest through the approximations used.

(iii) Noting that $W_{-n} = 1 - W_n$ for any n, we find $\Gamma = \frac{1}{2} - W_4 > 0$ and $g = 0$ at any T [18], and $r = 2W_4/\Gamma$ has one zero, at $T = 0$. This is consistent with the absence of phase transition in the 1D Ising model at any finite temperature, an improvement over the usual mean-field result $T_c^{\mathrm{MF}} = 2J/k_B$. There is no stability problem arising from $g = 0$ because the quadratic coefficient is positive for $T > 0$.

(iv) In the presence of an external magnetic field h, the degeneracies in jump rates are lifted [e.g., $W_{+\pm-} = (1 + e^{\pm 2\beta h})^{-1}$]. To $O(h)$, the kinetic equation acquires a new term $\Gamma\mu h$ on the right-hand side, where

$$\mu = \frac{2\beta}{\Gamma}(W_0^2 + W_4 W_{-4}). \tag{15}$$

Linear response then determines that the susceptibility is $\chi = \mu/r = \beta(1-\gamma^2/2)/(1-\gamma)$, where $\gamma \equiv \tanh 2\beta J$. In the Appendix, we show that μ is needed to fix the noise correlation.

(v) Besides capturing the correct symmetries, our results compare quite well with exact results. From Eq. (5), the relaxation time can be read off easily as $\tau = 1/\Gamma r = 1/(1-\gamma)$. This turns out to be exact [11]. For the susceptibility, deviation from the exact result $\beta e^{2\beta J}$ [11] shows up only at $O((\beta J)^5)$ when expanded in βJ. Hence, our method has the advantage that it embodies a refined mean-field theory, as already applied to studies of stochastic resonance in Ising systems [19].

(vi) Finally, due to the factorizations, only the deterministic terms in Eq. (5) can be derived. The noise term has to be deduced separately (see the Appendix). The result for the noise correlation D in Eq. (9) is $D = k_B T \mu \Gamma$.

Having gone through the details of our method, we now turn to a few less trivial examples.

B. 2D Ising model

The same procedure can be applied to the 2D Ising model with Glauber dynamics. Again we obtain Eq. (5), with the parameters given by

$$\Gamma = \frac{1}{8}(-2W_4 + 2W_{-4} - W_8 + W_{-8}), \tag{16}$$

$$r = \frac{1}{8\Gamma}(6W_0 + 12W_4 - 4W_{-4} + 5W_8 - 3W_{-8}), \tag{17}$$

$$g = \frac{3}{2\Gamma}(-6W_0 - 4W_4 + 4W_{-4} + 5W_8 + W_{-8}), \tag{18}$$

$$\mu = \frac{\beta}{2\Gamma}(3W_0^2 + 4W_4 W_{-4} + W_8 W_{-8}). \tag{19}$$

It is worth noting that Γ, g, and μ are positive definite for all $T > 0$, whereas r has one zero at $T_c^{\mathrm{GL}} \approx 3.0898 J/k_B \approx 1.3616 T_c$, again an improvement over the mean-field prediction $T_c^{\mathrm{MF}} = 4J/k_B$, where $T_c = -2J/k_B \ln(\sqrt{2}-1) \approx 2.2692 J/k_B$ is the exact critical temperature. As expected, there is no ϕ^5 and higher-order term [18].

The results of τ and χ for the Gaussian case ($g = 0$) are quite satisfactory. They differ from high-temperature series expansions [20] at order $O((\beta J)^5)$ and $O((\beta J)^4)$, respectively, whereas the usual mean-field results are worse, at $O((\beta J)^3)$ and $O((\beta J)^2)$.

C. 3D Ising model

Despite being more tedious (128 terms on the right-hand side of the master equation), we also derive the kinetic equation for the 3D Ising model with Glauber dynamics. The results are

$$\Gamma = \frac{1}{32}(W_{-12} + 4W_{-8} + 5W_{-4} - 5W_4 - 4W_8 - W_{12}), \tag{20}$$

$$r=\frac{1}{32\Gamma}(-5W_{-12}-18W_{-8}-15W_{-4}+20W_0+45W_4 +30W_8+7W_{12}), \tag{21}$$

$$g=\frac{15}{16\Gamma}(-W_{-12}+6W_{-8}+9W_{-4}-12W_0-15W_4+6W_8 +7W_{12}), \tag{22}$$

$$\mu=\frac{\beta}{8\Gamma}(10W_0^2+15W_{-4}W_4+6W_{-8}W_8+W_{-12}W_{12}). \tag{23}$$

As for the 2D Ising model, Γ, g, and μ are positive definite for all $T>0$, and r has one zero at $T_c^{\mathrm{GL}}\approx 5.0733J/k_B$, 12% higher than the best estimate [21], compared to $T_c^{\mathrm{MF}}=6J/k_B$.

D. 1D driven lattice gas

In many generic nonequilibrium systems [15], the free energy does not exist and one has to start from the dynamics, such as described by the master equation. A notable example is the driven diffusive system [22], which is regarded as a paradigm of spatially extensive interacting systems that exhibit cooperative phenomena in steady-state nonequilibrium situations. In its standard form, it models an Ising-like lattice gas of particles whose motion along a certain direction is biased by an external drive denoted by E. For $E=0$, the model reduces to the ordinary kinetic Ising model with Kawasaki, or spin-exchange, dynamics (model B in [3]).

A question subject to recent debate concerns the form of nonlinearities associated with E [23,24]. That is an important issue because the nonlinearities decide to which universality class of critical behavior the system belongs. It is interesting to see what the present method says about that. First, we consider a one-dimensional, simplified version in which the particles are not interacting except being hard core, but their hoppings to nearest neighbors are biased by having different jump rates, p and q, to the right and left, respectively. Hence, the master equation reads

$$P_+(x;t+1)-P_+(x;t)=pP_{+-}(x-1;t)+qP_{-+}(x;t) -pP_{+-}(x;t)-qP_{-+}(x-1;t), \tag{24}$$

where as usual an up (down) spin corresponds to the occupation of a particle (hole), and joint probabilities such as $P_{+-}(x-1;t)$ mean the probability of finding a particle-hole pair at site $x-1$ and x. After factorizations and applications of Eq. (12) and (13), we readily find

$$\frac{\partial\phi}{\partial t}=\mathcal{D}\frac{\partial^2\phi}{\partial x^2}+\frac{\mathcal{E}}{2}\frac{\partial\phi^2}{\partial x}, \tag{25}$$

where the diffusion coefficient is $\mathcal{D}=(p+q)/2$, as expected, and the coefficient of driving is $\mathcal{E}=(p-q)$. The nonlinear term is the same as in the ''standard'' field theoretic model [25], which was proposed on the grounds of symmetries. As side remarks, note that we obtain the diffusion equation for $p=q$, and that $\mathcal{E}$ is smooth in the ''infinite'' drive limit ($p=1,q=0$), which is used in most Monte Carlo simulations of driven diffusive systems.

E. 2D driven lattice gas

Generalization of the previous result to the 2D interacting driven lattice gas is immediate, despite the unpleasant fact that there are altogether 512 terms in the master equation. In the presence of a drive E along the $+y$ direction and attractive [$J>0$ in Eq. (1)] interaction between particles, the heat-bath rates for hoppings of particles along and against the drive take the form

$$W_{n,\pm E}\equiv\frac{1}{1+e^{n\beta J\mp E\beta J}}, \tag{26}$$

where the dimensionless E ($0\leqslant E<\infty$) represents the ''work done'' on the particle by the field. Obviously, the rates for hoppings perpendicular to E are $W_{n,0}=W_n$.

Going through the same procedure as above, we eventually obtain a kinetic equation that is in complete agreement with the standard field theory of the driven diffusive system [25]:

$$\frac{\partial\phi}{\partial t}=-\left(\alpha_x\frac{\partial^4}{\partial x^4}+2\alpha_{xy}\frac{\partial^4}{\partial x^2\partial y^2}+\alpha_y\frac{\partial^4}{\partial y^4}\right)\phi +\left(r_x\frac{\partial^2}{\partial x^2}+r_y\frac{\partial^2}{\partial y^2}\right)\phi+\frac{1}{6}\left(g_x\frac{\partial^2}{\partial x^2}+g_y\frac{\partial^2}{\partial y^2}\right)\phi^3 +\frac{\mathcal{E}}{2}\frac{\partial\phi^2}{\partial y}. \tag{27}$$

The anisotropies are generated by the drive. Excluding the last term, this is the anisotropic generalization of the deterministic TDGL equation with conserved magnetization, i.e., model B [3]:

$$\frac{\partial\phi}{\partial t}=\nabla^2\left(-\alpha\nabla^2\phi+r\phi+\frac{g}{6}\phi^3\right). \tag{28}$$

All coefficients are determined as follows:

$$\alpha_x=\frac{1}{384}(69-85W_4-68W_8-17W_{12}), \tag{29}$$

$$\alpha_{xy}=\frac{1}{256}(20-20W_4-16W_8-4W_{12}+W_{-12,-E}+W_{-12,E} +4W_{-8,-E}+4W_{-8,E}+5W_{-4,-E}+5W_{-4,E}-5W_{4,-E} -5W_{4,E}-4W_{8,-E}-4W_{8,E}-W_{12,-E}-W_{12,E}), \tag{30}$$

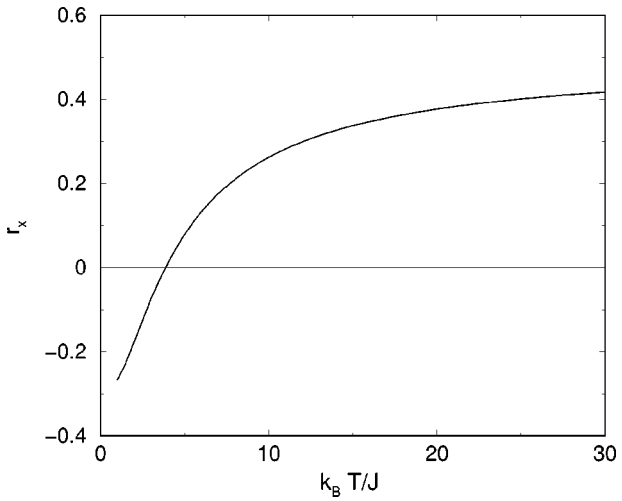


FIG. 1. Quadratic coefficient in the transverse direction r_x plotted vs temperature. Its zero locates the critical temperature T_c^{GL}.

$$\alpha_y=\frac{1}{768}(8W_{-12,-E}+8W_{-12,E}+31W_{-8,-E}+31W_{-8,E}+35W_{-4,-E}+35W_{-4,E}-10W_{0,-E}-10W_{0,E}-50W_{4,-E}-50W_{4,E}-37W_{8,-E}-37W_{8,E}-9W_{12,-E}-9W_{12,E}), \tag{31}$$

$$r_x=\frac{1}{32}(-9+25W_4+20W_8+5W_{12}), \tag{32}$$

$$r_y=\frac{1}{64}(-2W_{-12,-E}-2W_{-12,E}-7W_{-8,-E}-7W_{-8,E}-5W_{-4,-E}-5W_{-4,E}+10W_{0,-E}+10W_{0,E}+20W_{4,-E}+20W_{4,E}+13W_{8,-E}+13W_{8,E}+3W_{12,-E}+3W_{12,E}), \tag{33}$$

$$g_x=\frac{5}{16}(3+W_4-4W_8-3W_{12}), \tag{34}$$

$$g_y=\frac{1}{32}(6W_{-12,-E}+6W_{-12,E}+7W_{-8,-E}+7W_{-8,E}-W_{-4,-E}-W_{-4,E}+6W_{0,-E}+6W_{0,E}+4W_{4,-E}+4W_{4,E}-13W_{8,-E}-13W_{8,E}-9W_{12,-E}-9W_{12,E}), \tag{35}$$

$$\mathcal{E}=\frac{1}{16}(-W_{-12,-E}+W_{-12,E}-3W_{-8,-E}+3W_{-8,E}-3W_{-4,-E}+3W_{-4,E}-2W_{0,-E}+2W_{0,E}-3W_{4,-E}+3W_{4,E}-3W_{8,-E}+3W_{8,E}-W_{12,-E}+W_{12,E}). \tag{36}$$

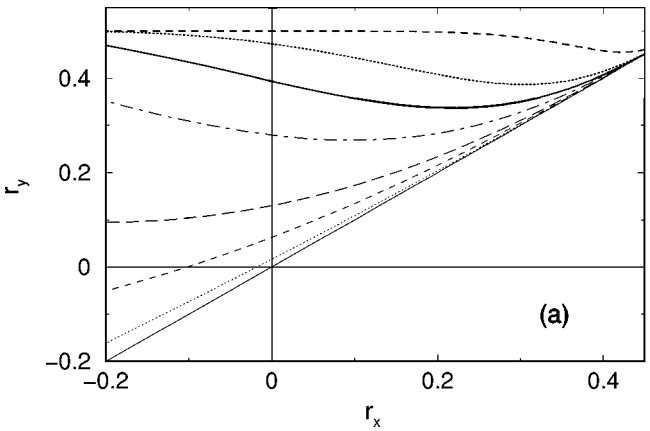
They have the following important properties.

(i) All but $\mathcal{E}$ are even in E, consistent with the invariance of the dynamics under $\{E\to -E, y\to -y\}$.

(ii) The quadratic coefficient r_x is independent of E. It has one zero at $T_c^{\mathrm{GL}}=3.861\,43J/k_B$, as shown in Fig. 1. In contrast, r_y depends on E. Figure 2 displays the behavior of $r_y(T,E)$ versus $r_x(T)$ as T is lowered from above T_c^{GL} at fixed E, as well as $r_y(T=T_c^{\mathrm{GL}},E)$ versus E. It shows that for any $E>0$, r_x always vanishes before r_y does when T is decreased. For small E, $r_y\approx r_x+cE^2$, where $c>0$. Consequently, at the critical temperature, the dominant derivatives come from the r_y and α_x terms, leading to the identification of an intrinsically anisotropic critical theory with scaling of momenta $k_y\sim k_x^2$. This agrees with a previous perturbative argument [25].

(iii) The coefficient $\mathcal{E}$ of the leading nonlinearity induced by the drive vanishes linearly in E at small E, and saturates to a constant at $E=\infty$. This dependence, exhibited in Fig. 3, is already anticipated above from the 1D model and argued previously [24], but at odds with the claims in [23].

(iv) The $E=0$ limit. Setting $E=0$, we readily recover the isotropic model B with $\alpha_x=\alpha_y$, $r_x=r_y$, and $g_x=g_y$, making use of the identity $W_{-n,0}=1-W_{n,0}$. We also find $\alpha_{xy}\neq\alpha_x$ — the continuum model derived is not rotationally invariant. While this is not surprising since the symmetry is absent in the original lattice model, it turns out that $\alpha_{xy}=\alpha_x$ at T_c^{GL}. At present, we are not sure whether this ac-



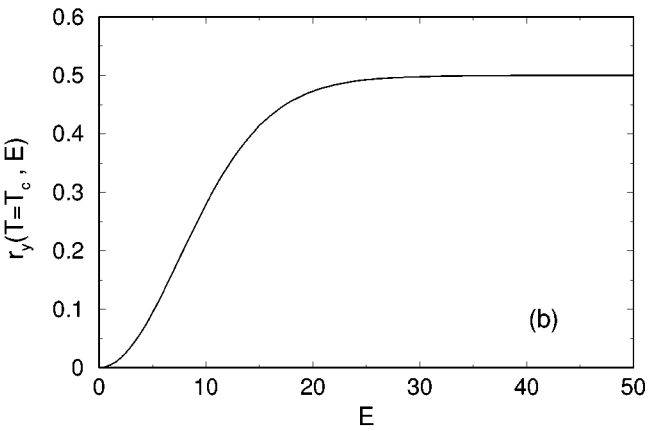


FIG. 2. (a) Trends of r_y vs r_x as T is varied across T_c^{GL} at fixed E. From bottom to top: $E=0$, 2, 4, 6, 10, 14, 20, and 50. (b) Intercept $r_y(r_x=0)$ in (a) plotted vs E.

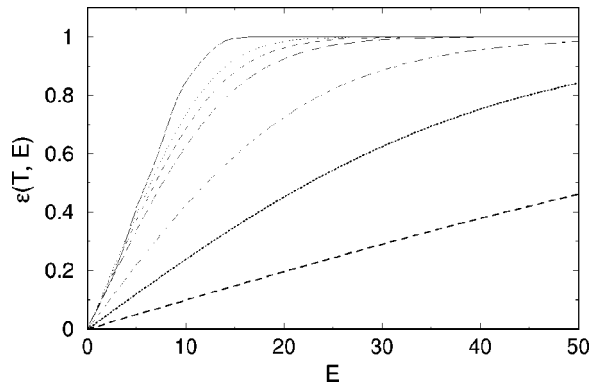


FIG. 3. The coefficient of the leading nonlinearity, $\mathcal{E}$, vs the microscopic drive, E, at different temperatures. From top to bottom: $k_BT/J=1$, 3, 3.861 43 $(=T_c^{\mathrm{GL}})$, 5, 10, 20, and 50.

quirement of higher symmetry at the critical point is general for the underlying lattice model or specific to the method.

F. Two-species driven lattice gas

In all the above examples, each site has only two local states (spin up or down). In the two-species driven lattice-gas model [26], motivated in part by multi-ionic conductors and traffic flow problems, there are three possibilities: as a hole or either of two types of particles. The two types of particles are driven in opposite directions as if they were oppositely charged and driven by an electric field, with local particle densities denoted by ρ_+ and ρ_-. Due to the extra local state, it is not easy to write down the correct set of equations by symmetry and intuition alone. One way to proceed [26] is to express the entropy in terms of ρ_+ and ρ_-, and obtain the diffusion terms by functional differentiations. The driving terms can then be added to the kinetic equations by generalizing that for the one-species model. Another way is to use the Ω expansion [6,27]. The current method has also been applied [28]. The equations derived are the same as in [26,27], with the advantage of tractable microscopic origins in each coefficient. Hence, this model further testifies the usefulness of the present approach when symmetry and intuition are not very helpful.

We end this section with a final remark. Since the method begins with a factorization of joint probabilities, the ensuing equation is deterministic. All information about correlations seems to have been lost. The situation can be remedied, however, by introducing a noise term to restore a probabilistic description. Correlations can then be computed by averaging over the noise by means of standard field-theoretic techniques [29]. For equilibrium systems, the noise can be fixed by requirements such as the fluctuation-dissipation theorem (Appendix A). For nonequilibrium systems, there is no general rule. One usually has to resort to extrapolation from equilibrium or to the Ω expansion [6,27].

IV. CONCLUSION

We have presented in detail a very simple and straightforward method to derive the deterministic kinetic equations from known microscopic dynamics for stochastic, interacting systems. The method has a mean-field flavor. It preserves the underlying symmetries of the dynamics and is in line with the spirit of coarse graining. The resulting equations are in good agreement with other either more or less rigorous approaches, as demonstrated explicitly via several examples. Hence, despite the approximate and heuristic nature of our approach, it proves to be a useful and convenient means to obtain a correct continuum theory, especially (i) when other more rigorous approaches do not apply or are too involved; (ii) when symmetries of the system are not intuitively obvious; and (iii) when microscopic dependences of the continuum parameters are wanted.

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APPENDIX A: NOISE CORRELATION

Since the present method only gives the deterministic part of the kinetic equation, the noise term has to be considered separately. Here we follow the common practice of assuming that the noise ζ is Gaussian distributed and correlated over negligible ranges. Then the only question is to determine its correlation D in Eq. (9).

There are two ways to do it. The first makes use of the correspondence between the Langevin equation,

$$\frac{\partial\phi}{\partial t}=-\Gamma\frac{\delta\mathcal{H}}{\delta\phi}+\zeta, \tag{A1}$$

$$\langle\zeta(\vec{r},t)\zeta(\vec{r}',t')\rangle=2D\,\delta(\vec{r}-\vec{r}')\,\delta(t-t'), \tag{A2}$$

and the Fokker-Planck equation,

$$\frac{\partial\mathcal{P}}{\partial t}=-\int d^dx\frac{\delta}{\delta\phi}\left(-\Gamma\frac{\delta\mathcal{H}}{\delta\phi}\,\mathcal{P}-D\frac{\delta\mathcal{P}}{\delta\phi}\right), \tag{A3}$$

which is a continuity equation. A stationary solution of the Fokker-Planck equation is obtained by setting the probability current to zero, i.e., $(\cdots)=0$, which gives $\mathcal{P}\propto e^{-\Gamma\mathcal{H}/D}$. Since the free energy $\mathcal{F}[h]$ in the presence of an external field h is of the form $\mathcal{F}[h]=\mathcal{F}[0]-h\phi$, it differs from $\mathcal{H}$ by a factor of μ. Hence, by matching $e^{-\mathcal{F}[h]/k_BT}$ and $e^{-\Gamma\mathcal{H}[h]/D}$, we deduce that

$$D=k_BT\mu\Gamma. \tag{A4}$$

In passing, it is worth noting that the kinetic coefficient defined in

$$\frac{\partial\phi}{\partial t}=-\lambda\frac{\delta\mathcal{F}}{\delta\phi}+\zeta \tag{A5}$$

is $\lambda=D/k_BT$, which is the Einstein relation.

An alternative way to determine D is to use the fluctuation-dissipation theorem, which in momentum-frequency space takes the form

$$\frac{2k_BT}{\omega}\mathrm{Im}\chi(k,\omega)=G(k,\omega). \tag{A6}$$

Although neither the susceptibility χ nor the two-point correlation function G can be calculated in closed form for general $\mathcal{H}$, Eq. (A6) holds order by order so that we only need to consider the Gaussian model in the case of $g=0$. Thus, by Fourier transforms, we obtain $\chi(k,\omega)=\Gamma\mu/[-i\omega+\Gamma(k^2+r)]$ and $G(k,\omega)=2D/[\omega^2+\Gamma^2(k^2+r)^2]$, which by virtue of Eq. (A6) also gives Eq. (A4).

Since the above deductions require the knowledge of the equilibrium distribution, they do not apply to nonequilibrium situations [15]. In those cases, there are no similar shortcuts. Extrapolation from equilibrium analogy or application of the Ω expansion [6,27] seems to be all one can do.

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[15] By ''generic'' we refer to systems that have nonzero probability current in configuration space [the terms enclosed by large parentheses in Eq. (A3)] even in stationary states. In the master equation, this corresponds to the breakdown of detailed balance, i.e., the right-hand side of Eq. (2) does not vanish term-by-term in stationary states but only after summation. Usually this is also accompanied by a breakdown of the fluctuation-dissipation theorem, and the lack of a well-defined free energy.

[16] For critical properties, this is not a serious problem because the relevant physics is in the long-wavelength, long-time limits, where by virtue of universality, a kinetic equation postulated solely by symmetry considerations is sufficient. However, this often requires physical intuition and insight, whereas the present method does not.

[17] Similar approaches exist in other contexts, such as in the surface growth problem, where the equation of motion for the surface profile may be derived by approximating the transtion rate by a power series in the slow variable (the height difference), followed by taking the continuum limit. See Z. Racz, M. Siegert, D. Liu, and M. Plischke, Phys. Rev. A **43**, 5275 (1991).

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