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Continuum Description for Nonequilibrium Competing Dynamic Models

P. L. Garrido and M. A. Muñoz

Instituto Carlos I de Física Teórica y Computacional, Facultad de Ciencias, Universidad de Granada, 18071-Granada, Spain
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In contrast to what happens in systems at thermodynamic equilibrium, microscopic dynamics plays an essential role in the macroscopic behavior of nonequilibrium systems. Usually, continuum descriptions of nonequilibrium systems do not model accurately enough this microscopic dependence. For a broad class of nonequilibrium lattice models, defined through a master equation, we construct a continuous representation, i.e., a Fokker-Planck equation. It is constructed in such a way that its deterministic stationary states and the fluctuations in a neighborhood of them are exactly represented. Therefore any future analysis based on this new Fokker-Planck equation will lead to more confident results.

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The description of systems at thermodynamic equilibrium by means of continuum dynamical equations has been proved to be very useful [1]. One of the reasons for the success of this approach is that, as the renormalization group establishes, the static and dynamic properties of the system near a critical point are independent of many of their microscopic details. In fact, the systems at equilibrium can be classified into universality classes depending only on macroscopic properties, such as symmetries, dimensionality, conserved quantities, etc. [1,2]. These classes are very robust with respect to changes in other microscopic details. Let us consider a given system at equilibrium. When an external agent is applied to it, say, for instance, a temperature gradient or a driving field, the system behavior changes essentially: Its stationary state cannot be represented by a Gibbsian probability measure. In order to describe this kind of nonequilibrium situation by means of continuum dynamical equations, the standard procedure consists of adding some extra term representing the action of the external agent to the corresponding equilibrium dynamical equation (see, for example, [3]). In this way, the original equilibrium description is recovered when the agent is turned off. However, this scheme assumes that the influence of the microscopic dynamical details on the macroscopic properties is irrelevant. This assumption is at least dangerous when applied without further examination. In fact, as has been broadly reported

[4–8], the microscopic dynamic plays an essential role in the nonequilibrium systems' behavior; their phase diagrams and even their critical properties can be dramatically modified by small changes in the microscopic dynamical rules. Therefore, in order to establish the real influence of the microscopic details on the macroscopic behavior of nonequilibrium systems, it is necessary to study carefully the connection between their microscopic and continuum representations. To achieve this goal, we derive in this paper a systematic and rigorous way to construct continuous, Fokker-Planck equations to characterize a particular family of nonequilibrium models. These models are defined by a Markovian master equation in which the transition probabilities (or rates) are given by the stochastic superposition of different microscopic mechanisms. Each of the individual microscopic dynamics drives the system to a different equilibrium state. The simultaneous presence of more than one of them induces a *dynamical frustration*, and the associated stationary state becomes a nonequilibrium one.

The Fokker-Planck equation (FPE) that we propose is constructed very carefully in order to treat properly the microscopic information. In particular, the stationary states and phase diagrams associated with the FPE are exact in the sense that will be specified below.

Specifically, from a microscopic Markovian master equation that defines these models, we get a continuum FPE with the following properties.

(i) In general, its associated stationary nonequilibrium distribution is locally exact around the extremals of the true one.

(ii) When only one microscopic mechanism acts, its stationary distribution is the corresponding equilibrium Gibbsian one (independent of the microscopic rates used).

(iii) The FPE depends explicitly on the microscopic rates.

(iv) The deterministic limits of both the master and Fokker-Planck equations coincide.

None of the FPE's commonly used in the literature (say, for instance, Hohenberg and Halperin's model A [1] or the Kramers-Moyal FPE's [9]) fulfills at the same time the last four requirements. However, some other interesting attempts have been made in order to build better FPE descriptions [10].

The last four properties guarantee that any future analysis based on this new Fokker-Planck equation (for instance, the study of critical properties by means of the path integral formalism) will lead to confident results.

Now we introduce the family of nonequilibrium models we are going to deal with. Our system consists of a d -dimensional lattice, where at each site there is a spinlike variable. We define at each point $\underline{r} \in R^d$ a field variable $\Phi(\underline{r}) \in R$, which is the averaged value of the spins on a region of volume Ω around \underline{r} . When Ω is large enough, Φ is assumed to be a continuous function of \underline{r} . The probability of finding a field configuration $\underline{\Phi} = \{\Phi(\underline{r}); \underline{r} \in R^d\}$ at time t , say, $P_t^\Omega(\underline{\Phi})$, evolves according to a Markovian master equation:

$$\begin{aligned} \partial_t P_t^\Omega(\underline{\Phi}) &= \int_{R^d} d\underline{r} \int_R d\eta f(\eta) \\ &\times [w^\Omega(\underline{\Phi}^{\eta,\underline{r}} \rightarrow \underline{\Phi}) P_t^\Omega(\underline{\Phi}^{\eta,\underline{r}}) \\ &- w^\Omega(\underline{\Phi} \rightarrow \underline{\Phi}^{\eta,\underline{r}}) P_t^\Omega(\underline{\Phi})], \end{aligned} \quad (1)$$

where $f(\eta)$, an even and analytical real function around the origin, stands for the field increment distribution, $\underline{\Phi}^{\eta,\underline{r}} = \{\Phi(\underline{r}') + (\eta/\Omega)\delta_{\underline{r},\underline{r}'}; \underline{r}' \in R^d\}$, and $w^\Omega(\underline{\Phi} \rightarrow \underline{\Phi}')$ represents the transition probabilities per unit time. These are defined as follows:

$$w^\Omega(\underline{\Phi} \rightarrow \underline{\Phi}') = \int_{R^d} d\underline{K} p(\underline{K}) w^\Omega(\underline{\Phi} \rightarrow \underline{\Phi}'; \underline{K}), \quad (2)$$

where $w^\Omega(\underline{\Phi} \rightarrow \underline{\Phi}'; \underline{K}) = D[H^\Omega(\underline{\Phi}'; \underline{K}) - H^\Omega(\underline{\Phi}; \underline{K})]$, the function D has the property $D[\lambda] = e^{-\lambda} D[-\lambda] \geq 0$, $H^\Omega(\underline{\Phi}; \underline{K}) = \Omega \int_{R^d} d\underline{r} h[\underline{\Phi}(\underline{r}); \underline{K}]$ is a continuum interaction Hamiltonian which depends on the parameters $\underline{K} = \{K_i, i = 1, \dots, n\}$, and $p(\underline{K})$ is any probability distribution for the parameters. In particular, for $p(\underline{K}) = \delta(\underline{K} - \underline{K}_0)$ the stationary solution of the master equation (1) is the Gibbsian distribution $P_{eq}^\Omega(\underline{\Phi}; \underline{K}_0) \propto \exp[-H^\Omega(\underline{\Phi}; \underline{K}_0)]$. That is, we are superposing several equilibrium dynamics with different \underline{K} parameters. In this way, each rate tries to lead the system to a different equilibrium state, and the system is *dynamically frustrated*. The system stationary state is expected (*a priori*) to be non-Gibbsian in this kind of situation (i.e., there is no effective Hamiltonian describing the stationary state). When we rescale the time variable $\tau = \Omega^{-1}t$ and we take the limit $\Omega \rightarrow \infty$, the solution of the master equation (1) is $P_\tau(\underline{\Phi}) = \delta(\underline{\Phi} - \underline{v}_\tau)$, where \underline{v}_τ is the solution of the so-called *deterministic equation*

$$\begin{aligned} \partial_\tau \underline{v}_\tau(\underline{r}) &= \Xi_0^{\text{exact}}(\underline{v}_\tau(\underline{r})) \\ &= \int_R d\eta f(\eta) \eta \langle\langle D(U_\eta(\underline{v}_\tau(\underline{r}); \underline{K})) \rangle\rangle, \end{aligned} \quad (3)$$

where $U_\eta(\underline{\Phi}(\underline{r}); \underline{K}) = \eta \delta \hat{H}(\underline{\Phi}; \underline{K}) / \delta \Phi(\underline{r})$ and $\langle\langle A \rangle\rangle = \int_{R^n} d\underline{K} p(\underline{K}) A(\underline{K})$. In general, for large enough Ω , the stationary probability distribution solution of the master equation (1) can be written as $P_{st}^\Omega(\underline{\Phi}) \propto \exp[-V_{st}^\Omega(\underline{\Phi})]$, where $V_{st}^\Omega(\underline{\Phi}) = \Omega V_{0,st}(\underline{\Phi}) + V_{1,st}(\underline{\Phi}) + O(\Omega^{-1})$. The nonequilibrium potential $V_{st}^\Omega(\underline{\Phi})$ is expected to be continuous but not differentiable in some small regions in the phase space (see, for instance, [11]), and it can be shown that it is a Lyapunov function for the underlying deterministic dynamical system [12]. Anyway, we are going to work where the potential is assumed to be locally differentiable, that is, near its local minima.

Let us write a general FPE with arbitrary coefficients up to first order in Ω^{-1} :

$$\partial_t P_t^\Omega(\underline{\Phi}) = \frac{1}{\Omega} \int_{R^d} d\underline{r} \frac{\delta}{\delta \Phi(\underline{r})} \left[\Xi_0(\underline{\Phi}(\underline{r})) + \frac{1}{\Omega} \Xi_1(\underline{\Phi}(\underline{r})) + \frac{1}{\Omega} \Xi_2(\underline{\Phi}(\underline{r})) \frac{\delta}{\delta \Phi(\underline{r})} \right] P_t^\Omega(\underline{\Phi}). \quad (4)$$

We would like to fit the functionals Ξ_0 , Ξ_1 , and Ξ_2 in such a way that the above four properties hold. That is, we expect to reproduce, at least, the two first leading terms in a Ω perturbation scheme of the true nonequilibrium stationary distribution. Because our parameter Ω

is large, the latter will be a good approximation of the real system behavior. In particular, we have been able to prove the following theorems.

Theorem 1.—Let $H(\underline{\Phi}; \underline{K}_0) = \Omega \hat{H}(\underline{\Phi}; \underline{K}_0)$ be the interaction Hamiltonian that characterizes the system

equilibrium stationary state, i.e., $p(\underline{K}) = \delta(\underline{K} - \underline{K}_0)$. Then the FPE (4) with coefficients

$$\begin{aligned}\Xi_0(\underline{\Phi}(\underline{r})) &= \Xi_0^{\text{exact}}(\underline{\Phi}(\underline{r})), \\ \Xi_1(\underline{\Phi}(\underline{r})) &= 0, \\ \Xi_2(\underline{\Phi}(\underline{r})) &= \frac{\Xi_0^{\text{exact}}(\underline{\Phi}(\underline{r}))}{\delta\hat{H}(\underline{\Phi})/\delta\Phi(\underline{r})},\end{aligned}\quad (5)$$

has the following properties:

(i) it reproduces the exact deterministic dynamics given by Eq. (3); (ii) its stationary solution is the exact Gibbsian one: $P_{\text{st}}(\Phi) \propto \exp(-H(\Phi; \underline{K}_0))$.

Theorem 2.—Let any FPE (4) be such that its coefficients have the properties

$$\begin{aligned}\Xi_0(\underline{\Phi}(\underline{r})) &= \Xi_0^{\text{exact}}(\underline{\Phi}(\underline{r})), \\ \Xi_2(\underline{v}^*(\underline{r})) &= \frac{1}{2} \int_R d\eta f(\eta) \langle\langle D(U_\eta(v^*(\underline{r}); \underline{K})) \rangle\rangle \eta^2,\end{aligned}\quad (6)$$

where \underline{v}^* is any dynamically stable solution of the stationary deterministic equation (3), i.e., $\partial_\tau \underline{v}^*(\underline{r}) = 0$. Then (i) it reproduces the exact deterministic dynamics given by Eq. (3); (ii) the $V_{0,\text{st}}$ part of its stationary solution almost coincides with the exact one in a suitable neighborhood of \underline{v}^* .

Theorem 3.—Let any FPE (4) such that its coefficients have the form

$$\begin{aligned}\Xi_0(\underline{\Phi}(\underline{r})) &= \frac{1}{2} [D_-(\underline{\Phi}(\underline{r})) - D_+(\underline{\Phi}(\underline{r}))], \\ \Xi_1(\underline{\Phi}(\underline{r})) &= 0, \\ \Xi_2(\underline{\Phi}(\underline{r})) &= \frac{D_-(\underline{\Phi}(\underline{r})) - D_+(\underline{\Phi}(\underline{r}))}{2 \ln[D_-(\underline{\Phi}(\underline{r}))/D_+(\underline{\Phi}(\underline{r}))]},\end{aligned}\quad (7)$$

where $D_\eta(\underline{\Phi}(\underline{r})) = \langle\langle D(U_\eta(\underline{\Phi}(\underline{r}); \underline{K})) \rangle\rangle$. When $f(\eta) = \frac{1}{2}[\delta(\eta - 1) + \delta(\eta + 1)]$, then (i) it reproduces the exact deterministic dynamics given by Eq. (3); and (ii) the $V_{0,\text{st}}$ and $V_{1,\text{st}}$ parts of its stationary solution almost coincide with the exact one in a suitable neighborhood of all spatially homogeneous deterministic solutions \underline{v}^* .

Corollary: The FPE defined in Theorem 3 is the same as the one in Theorem 1 when $p(\underline{K}) = \delta(\underline{K} - \underline{K}_0)$ and $f(\eta) = \frac{1}{2}[\delta(\eta - 1) + \delta(\eta + 1)]$.

Let us mention here that the functional form of $f(\eta)$ in Theorem 3 and its Corollary is the most common one used in the literature.

It is not possible to give here the details of the proofs, but let us expose the general ideas we have followed. The main question to answer is how can we guarantee that our FPE reproduces the exact stationary distribution without explicitly solving the equation? When we substitute the expansion in Ω of the stationary distribution into the ME (1), we get a set of nontrivial Hamiltonian-Jacobi (HJ)

type of differential equations, where the unknowns are the components of the stationary potential $V_{i,\text{st}}$. For example, at order Ω^0 we get a closed equation for $V_{0,\text{st}}$ at order Ω^{-1} one equation for $V_{1,\text{st}}$ which depends also on the previous $V_{0,\text{st}}$ and so on. We are unable to solve any of those equations which, in general, are nonintegrable. Nevertheless, locally around the solutions of the stationary deterministic equation (3), we can apply the method of the characteristics to those HJ equations. That is, we can define a generating Hamiltonian in which the first derivative of the potential in the HJ equation is converted into conjugate moments $\pi(\underline{r})$ of the fields $\Phi(\underline{r})$. Then the solution of the HJ equation at point $\underline{\Phi}$ is given by the integral of π along the trajectory connecting the point $(\pi_0, \underline{\Phi})$ with $M = (\underline{\pi}^*, \underline{v}^*)$, where π_0 is fixed by choosing the trajectory that reaches M when $t \rightarrow -\infty$, and M is the fixed point for the generating Hamiltonian dynamics. Therefore we have reduced the problem of finding the nonequilibrium potential to the knowledge of a Hamiltonian from which we can generate it. In fact, we can apply the same scheme to the FPE (4). That is, we again substitute the expansion in Ω of the stationary potential into the FPE, and again we get a set of nontrivial HJ equations for each component of the potential. Therefore to show that we are going to get the same solution in both cases we only need to show that the corresponding generating Hamiltonians are equal *locally*, that is, they have equal fixed points and their expansions around them are equal. With this requirement, the coefficients of the FPE (4) can be fixed order by order in Ω .

Finally, it is worth comparing the results coming from our FPE and from other FPE commonly used in the literature (say, for instance, the FPE coming from a truncated Kramers-Moyal expansion). To achieve this goal, we have considered a simple nonequilibrium model. This model was introduced to study the dynamical frustration originated by the competition of two dynamics based in ferromagnetic and antiferromagnetic equilibrium Hamiltonians. A state is completely characterized by two variables, v_F and v_A , which represent the ferromagnetic and antiferromagnetic order parameters in a lattice, respectively (see Ref. [7] for more details). In Fig. 1 we represent an arbitrary section of the three stationary potentials, $V_{0,\text{st}}$, $V_{0,\text{st}}^{\text{KM}}$, and $V_{0,\text{st}}^{\text{N}}$, which are the solutions of the master equation, the Kramers-Moyal FPE, and our FPE, respectively. All those potentials have been computed by using standard methods explained in Refs. [7,11,12]. It is clearly shown in the figure that $V_{0,\text{st}}^{\text{N}}$ is a very good approximation to the exact solution $V_{0,\text{st}}$. In fact, this behavior can be shown to be generic all over the phase space. However, $V_{0,\text{st}}^{\text{KM}}$ presents large and systematic deviations with respect to the exact potential in almost all phase space. Therefore the properties which depend on the global potential shape, for instance, the first passage

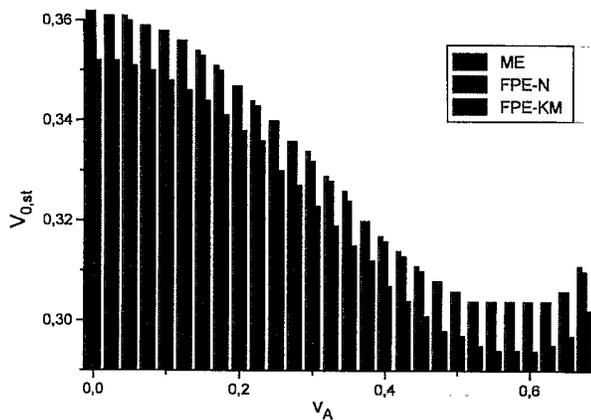


FIG. 1. The section $v_F = 0.2$ of three different nonequilibrium potential solutions of the exact master equation (ME), the FPE coming from the truncation of the Kramers-Moyal expansion (FPE-KM), and the FPE built by Theorem 3 in the text (FPE-N).

time, escape rates, etc., will only be accurately reproduced by our FPE.

In conclusion, we have constructed a new FPE that characterizes a broad class of nonequilibrium models. It is shown in this Letter that this new modeling reproduces the exact nonequilibrium stationary distribution at least in the neighborhood of the potential extremals. As far as we know, this is the first time that it has been possible to obtain a FPE for nonequilibrium systems with such a property. Any future analysis based on this FPE will lead to more confident conclusions.

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