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Generalized phase space version of Langevin equations and associated Fokker-Planck equations

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Abstract. Generic Langevin equations are almost always given as first-order stochastic ordinary differential equations for the phase space variables of a system, with noise and damping terms in the equation of motion of every variable. In contrast, Langevin equations for mechanical systems with canonical position and momentum variables usually include the noise and damping forces only in the equations for the momentum variables. In this paper we derive Langevin equations and associated Fokker-Planck equations for mechanical systems that include noise and damping terms in the equations of motion for all of the canonical variables. The derivation is done by comparing a distinctive derivation of a phase space Fokker-Planck equation, given by Langer, to the usual derivation relating Langevin equations to their associated Fokker-Planck equations. The resulting equations have simple reductions to overdamped and underdamped limits. They should prove useful for numerical simulation of systems in contact with a heat bath, since they provide one additional parameter that can be used, for example, to control the rate of approach to thermal equilibrium. The paper concludes with a brief description of the modification of Kramers' result for the escape rate from a metastable well, using the new form of the Fokker-Planck equation obtained here.

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1 Introduction

A familiar form of the Langevin equations of motion (EOMs) for a system of particles with N degrees of freedom is

$$M\ddot{x}_i = F_i(\{x\}) - M\gamma^{(2)}\dot{x}_i + \nu_i^{(2)}(t), \quad i = 1, \cdots, N. \quad (1)$$

Here $x_i(t)$ is a Cartesian component of the position at time t of a particle which has mass M, and $F_i(\{x\})$ is a component of the deterministic force acting on the particle; it is a function of the position of the other particles. $\gamma^{(2)}$ is a damping constant [with dimensions of (time)$^{-1}$], and $\nu_i^{(2)}(t)$ is a component of a random force acting on the particle; only statistical information is known about this function. (The superscripts are included for later convenience.)

The form of the above EOM might constrain one to think solely within the configuration space of the system, labeled by the variables $\{x\} = (x_1, x_2, \cdots, x_N)$. Here we want to expand our perspective to phase space, so we rewrite these EOMs in terms of both momentum and displacement

$$\dot{x}_i = \frac{p_i}{M},$$
$$\dot{p}_i = F_i(\{x\}) - \gamma^{(2)}p_i + \nu_i^{(2)}(t). \quad (2)$$

Now we recall that at least part of the motivation both for introducing (generalized) momentum variables and for combining them with the position variables to construct phase space is to be able to consider the positions and momenta on an identical footing. Then a much larger class of variable transformations (canonical transformations) becomes available for use in solving the EOMs. If the deterministic force in equations (2) is obtained from a potential energy Φ, as $F_i = -\partial\Phi/\partial x_i$, then the deterministic pieces of equations (2) are just Hamilton's equations, which do treat the positions and momenta in an equivalent way. However, the stochastic differential equations in equations (2) do not treat the position and momentum variables equivalently, because the damping and noise forces act to change only the momentum in the second equation. We want to retain a symmetric treatment of the two kinds of variables, by adding damping and noise terms to the right-hand side of the first of equations (2). Such

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terms would mean, for example, that the velocity is not exactly proportional to the momentum. However, it is not clear *a priori* what terms to add, so one purpose of this paper is to answer that question. In addition we will also obtain the corresponding Fokker-Planck equation (FPE).

A recent paper [1] treats the related question of how to obtain a form for Langevin EOMs and the associated FPE that is manifestly canonically invariant. Our approach does not have that same global viewpoint, but we are pursuing the idea that a phase space treatment should treat the two sets of variables in the same way.

Our approach starts from a distinctive derivation by Langer [2] of a Fokker-Planck equation. His method is very general in one way, in that it treats an arbitrary set of phase space variables; they could be local concentrations, or magnetic moments, or canonical coordinates and momenta, as we will consider them to be. But his method is restrictive in another way, in that it treats a system in contact with a heat bath in thermal equilibrium; as a consequence the solutions of the obtained FPE always have asymptotic approach to thermal equilibrium. For our purposes this derivation is ideal because it treats all of the phase space variables in the same way. When we compare this FPE to the one obtained by the typical derivation from a Langevin equation, we are able to identify the damping and random noise terms to add to the first of equations (2).

2 Langer's derivation of the Fokker-Planck equation

This derivation is of course best explained in the original paper (Ref. [2]), but we repeat some of it here to establish notation and to emphasize features that are important for our purposes. The derivation begins from consideration of a general system described by a set of discrete phase space variables $\{\eta\} = (\eta_1, \eta_2, \cdots)$, whose precise physical nature is not so important initially. In the application we will make, these variables will be canonical displacement and momentum variables. Therefore the index i runs from $1, \ldots, 2N$, where N is the number of degrees of freedom of the system.

The statistical evolution of the phase space variables is described by a phase space probability distribution function (PDF) $\rho(\{\eta\}, t)$. Langer supposes that the time evolution of the PDF develops both from internal dynamics of the system and from fluctuations created by interactions with a heat bath. The total time rate of change is the sum of these two effects,

$$\left(\frac{\partial \rho}{\partial t}\right) = \left(\frac{\partial \rho}{\partial t}\right)_{\text{dyn}} + \left(\frac{\partial \rho}{\partial t}\right)_{\text{fluct}}. \tag{3}$$

The η variables are assumed to be canonical, so the internal dynamics is described by Hamilton's equations obtained from an energy function $H(\eta)$. These are conveniently summarized by

$$\dot{\eta}_i = \sum_{j=1}^{2N} A_{ij} \frac{\partial H}{\partial \eta_j}, \tag{4}$$

where A_{ij} is the symplectic matrix [3]

$$A_{ij} = \begin{cases} \delta_{i+N,j} & i \le N, \\ -\delta_{i,j+N} & j \le N, \\ 0, & \text{otherwise,} \end{cases} \qquad i, j = 1, \cdots, 2N. \tag{5}$$

The dynamical rate of change of the PDF is obtained in the usual way from Liouville's equation to be

$$\left(\frac{\partial \rho}{\partial t}\right)_{\text{dyn}} = -\sum_{i=1}^{2N} \frac{\partial \rho}{\partial \eta_i} \dot{\eta}_i = -\sum_{i,j=1}^{2N} \frac{\partial \rho}{\partial \eta_i} A_{ij} \frac{\partial H}{\partial \eta_j}. \tag{6}$$

We perform some transformations here to get this expression into a convenient form. Because of the antisymmetry of A_{ij} and the symmetry of $\partial^2 H / \partial \eta_i \partial \eta_j$, the quantity $\rho \sum_{ij} A_{ij} \partial^2 H / \partial \eta_i \partial \eta_j$ is zero and can be added to the right-hand side of equation (6). Then the dynamical rate of change of the PDF can be written

$$\left(\frac{\partial \rho}{\partial t}\right)_{\text{dyn}} = -\sum_{i=1}^{2N} \frac{\partial}{\partial \eta_i} \left[\sum_{j=1}^{2N} A_{ij} \frac{\partial H}{\partial \eta_j} \rho \right]. \tag{7}$$

The evolution of the fluctuations induced by the heat bath is described by a master equation

$$\left(\frac{\partial \rho}{\partial t}\right)_{\text{fluct}} = \int \left[\prod_{i=1}^{2N} \mathrm{d}\eta_i' \right] \left[P\left(\{\eta\} \leftarrow \{\eta'\}\right) \rho(\{\eta'\}, t) - P\left(\{\eta'\} \leftarrow \{\eta\}\right) \rho(\{\eta\}, t) \right]. \tag{8}$$

Here $P(\{\eta\} \leftarrow \{\eta'\})$ is the rate at which transitions are induced by the bath from configuration $\{\eta'\}$ to $\{\eta\}$. The details of the transition process are described by this rate function. First, the bath is assumed to interact independently with each phase space variable, so that

$$P\left(\{\eta\} \leftarrow \{\eta'\}\right) = \sum_{i=1}^{2N} \prod_{j=1, j\neq i}^{2N} \delta\left(\eta_j - \eta_j'\right) R_i\left(\{\eta\} \leftarrow \{\eta'\}\right). \tag{9}$$

The function R_i embodies the important restriction that the heat bath is in thermal equilibrium before each interaction with the system; therefore

$$R_i\left(\{\eta\} \leftarrow \{\eta'\}\right) = \int \mathrm{d}s \int \mathrm{d}s' \frac{1}{Z_R} \exp\left[-\epsilon(s')/k_{\text{B}}T\right] T_i\left((s, \eta_i) \leftarrow (s', \eta_i')\right) \times \delta\left(\epsilon(s) + H(\{\eta\}) - \epsilon(s') - H(\{\eta'\})\right). \tag{10}$$

In this equation T is the temperature and k_{B} is Boltzmann's constant, s denotes the state of the bath, $\epsilon(s)$ is

the energy of that state, and Z_R is the bath partition function. T_i is the transition rate between the states listed in its arguments and is a symmetric function of those arguments. There is an assumption of weak coupling between the system and the bath built into equation (10), because there is no interaction energy term between them included in the argument of the energy-conserving delta function. By using the conservation of total energy condition for the system plus bath, we can manipulate the Boltzmann factor in equation (10) into

$$R_i = \exp\left(\frac{H\left(\{\eta'\}\right) - H\left(\{\eta\}\right)}{2k_{\mathrm{B}}T}\right)\bar{T}_i\left(\{\eta\} \leftarrow \{\eta'\}\right), \quad (11)$$

where the function $\bar{T}_i$ is a symmetric function of its arguments. Langer's final assumption is that this transition function can be modeled by a Gaussian,

$$\bar{T}_i(\{\eta\} \leftarrow \{\eta'\}) = 2\Gamma_i \frac{1}{\Delta\sqrt{2\pi\Delta}} \exp\left[-\frac{(\eta_i - \eta_i')^2}{2\Delta}\right]. \quad (12)$$

The quantity Δ is the mean-square jump size of the variable η_i due to interaction with the bath. We assume that Δ is small so that an expansion can be performed in equation (8) up to second order in Δ. Then the integrals in equation (8) can be done, and the constant Δ disappears (the details are in Ref. [2]). Only Γ_i, which describes the rate of variation of η_i, remains to describe the details of the jump process. The question of whether the Γ_i are strictly constant or perhaps are temperature dependent is left open at this point (see Sect. 5.2). The final result for the bath-induced rate of change of the PDF is

$$\left(\frac{\partial\rho}{\partial t}\right)_{\mathrm{fluct}} = \sum_{i=1}^{2N} \Gamma_i \frac{\partial}{\partial\eta_i}\left(\frac{1}{k_{\mathrm{B}}T}\frac{\partial H}{\partial\eta_i}\rho + \frac{\partial\rho}{\partial\eta_i}\right). \quad (13)$$

To complete the derivation we combine equations (3, 6, 13) and find the total rate of change of ρ can be written as a continuity equation in phase space,

$$\frac{\partial\rho}{\partial t} = -\sum_{i=1}^{2N}\frac{\partial J_i}{\partial\eta_i}. \quad (14)$$

The components of the probability current density are

$$J_i = \left(\sum_{j=1}^{2N} A_{ij}\frac{\partial H}{\partial\eta_j}\right)\rho - \frac{\Gamma_i}{k_{\mathrm{B}}T}\left(\frac{\partial H}{\partial\eta_i}\rho + k_{\mathrm{B}}T\frac{\partial\rho}{\partial\eta_i}\right), \quad i = 1, \cdots, 2N. \quad (15)$$

The final step here is for convenience rather than for fundamental reasons. The thermal equilibrium PDF $\rho \propto \exp(-H/k_{\mathrm{B}}T)$ should be a steady-state solution of equation (14), and it is. But if we substitute this solution into equation (15), from the first term we obtain a nonzero but divergenceless current. By adding a second nonzero, divergenceless term in equation (15), Langer makes the current zero in equilibrium. The final expression for the current components, to be used in subsequent analysis, is

$$J_i = \left[\sum_{j=1}^{2N} A_{ij}\left(\frac{\partial H}{\partial\eta_j}\rho + k_{\mathrm{B}}T\frac{\partial\rho}{\partial\eta_j}\right)\right] - \frac{\Gamma_i}{k_{\mathrm{B}}T}\left(\frac{\partial H}{\partial\eta_i}\rho + k_{\mathrm{B}}T\frac{\partial\rho}{\partial\eta_i}\right), \quad i = 1, \cdots, 2N. \quad (16)$$

Equations (14, 16) are (one form of) Langer's FPE. It treats all of the phase space variables on an equal footing, because it assumes that the deterministic evolution of the phase space variables is governed by Hamilton's equations and because the interaction with the heat bath is introduced in the same way for all variables. Because of the assumption made in its derivation, that the heat bath is in equilibrium at every interaction with the system, the time-dependent solutions of this equation approach the thermal equilibrium PDF as $t \to \infty$.

3 Generic derivation of the Fokker-Planck equation from Langevin equations

Another approach to derive the FPE starts from stochastic differential EOMs or Langevin equations. This derivation is given in many places [4,5]. We have found the monograph by Zinn-Justin [6] to be particularly useful.

The system is again assumed to be described by some set of phase space variables η_i, $i = 1, \cdots, 2N$. (There is no actual requirement for the number of variables to be even; we choose $2N$ here for comparison with the formulas of the preceding section.) These variables are assumed to evolve according to Langevin equations of the form

$$\dot{\eta}_i = f_i(\{\eta(t)\}) + \nu_i(t), \quad i = 1, \cdots, 2N. \quad (17)$$

The $f_i(\{\eta(t)\})$ are prescribed functions. The $\nu_i(t)$ are random noise sources whose PDF $\rho_\nu(\{\nu\})$ is assumed to be a multivariate Gaussian,

$$\rho_\nu(\{\nu\}) \propto \exp\left[-\sum_{i=1}^{2N}\frac{1}{2D_i}\int_{-\infty}^{\infty}\mathrm{d}t\,\nu_i^2(t)\right]. \quad (18)$$

The factorized nature of this PDF implies that the noise at each point and time are independent random variables; this property corresponds to the independence of the interactions of the bath with each of the phase space variables expressed in equation (9). From equation (18) it is straightforward to show that the average value and correlation functions of the noise sources are given by the familiar formulas,

$$\langle\nu_i(t)\rangle_\nu = 0, \qquad \langle\nu_i(t)\nu_{i'}(t')\rangle_\nu = D_i\delta_{ii'}\delta(t-t'). \quad (19)$$

(The subscript on the average is to indicate that these averages are to be calculated with the PDF for the noise.)

With this PDF one can also obtain the Novikov theorem [7]: for any functional of the noise source $F(\{\nu\})$

$$\langle F(\{\nu\})\nu_j(t')\rangle_\nu = D_j \left\langle \frac{\delta F(\{\nu\})}{\delta \nu_j(t')} \right\rangle_\nu . \tag{20}$$

The PDF for the dynamical variables is

$$\rho(\{\eta\},t) = \left\langle \prod_{i=1}^{2N} \delta\left(\eta_i(t) - \eta_i\right) \right\rangle_\nu , \tag{21}$$

where the variables $\{\eta\}$ are the coordinates of an arbitrary point in phase space, and the functions $\eta_i(t)$ are the solution of the Langevin equations for a specific realization of the noise. The derivation of the EOM for the phase space PDF begins by differentiating equation (21) with respect to t, and then substituting from the Langevin equation for the $\dot{\eta}_i$'s that appear. One then has an expression to which the Novikov theorem can be applied. After some further steps, which can be found in reference [6], we arrive at the following FPE for the phase space PDF:

$$\frac{\partial \rho(\{\eta\},t)}{\partial t} = - \sum_{j=1}^{2N} \frac{\partial}{\partial \eta_j} \left[f_j\left(\{\eta\}\right) \rho(\{\eta\},t) - \frac{1}{2} D_j \frac{\partial}{\partial \eta_j} \rho(\{\eta\},t) \right]. \tag{22}$$

We note that without additional assumptions of certain relations between the functions f_j and the constants D_j, the time evolution of solutions of this equation is not constrained to approach thermal equilibrium.

4 Specialization to coordinate-momentum variables

At this point we specialize to the system of our interest. It is a system of particles with N degrees of freedom, and the phase space variables divide into the sets of positions x_i and conjugate momenta p_i:

$$\eta_i = \begin{cases} x_i, & i = 1, \cdots, N, \\ p_{i-N}, & i = N+1, \cdots 2N. \end{cases} \tag{23}$$

We now have to specialize the two forms of FPEs obtained in the preceding two section to this choice of variables.

4.1 Langer's form

Corresponding to the categorization of the phase space variables in equation (23), the probability current components of equation (16) divide into two categories; the first half are displacement components J_{x_i} and the second half are momentum components J_{p_i}. Equation (14) becomes

$$\frac{\partial \rho}{\partial t} = - \sum_{i=1}^{N} \left(\frac{\partial J_{x_i}}{\partial x_i} + \frac{\partial J_{p_i}}{\partial p_i} \right). \tag{24}$$

In the expressions for the current components the rate constants Γ_i could in principle be different for each of the phase space variables. For our purposes it is sufficient to have just two constants, one for the positions, $\Gamma^{(1)}$, and one for the momenta, $\Gamma^{(2)}$. It is also necessary to have two different constants, because they have different dimensions: $[\Gamma^{(1)}] = (\text{length})^2/(\text{time})^2$ and $[\Gamma^{(2)}] = (\text{mass})^2(\text{length})^2/(\text{time})^3$. Taking into account the definition of A_{ij} in equation (5), we obtain the following formulas for the probability current components for this system:

$$\begin{aligned} J_{x_i} &= \left(\frac{\partial H}{\partial p_i} - \frac{\Gamma^{(1)}}{k_\mathrm{B}T} \frac{\partial H}{\partial x_i} \right) \rho - \Gamma^{(1)} \frac{\partial \rho}{\partial x_i} + k_\mathrm{B}T \frac{\partial \rho}{\partial p_i}, \\ J_{p_i} &= \left(-\frac{\partial H}{\partial x_i} - \frac{\Gamma^{(2)}}{k_\mathrm{B}T} \frac{\partial H}{\partial p_i} \right) \rho - \Gamma^{(2)} \frac{\partial \rho}{\partial p_i} - k_\mathrm{B}T \frac{\partial \rho}{\partial x_i} . \end{aligned} \tag{25}$$

Finally we make one more restriction on the nature of the system, that the Hamiltonian has the form

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2M} + \Phi(\{x\}). \tag{26}$$

Then

$$\frac{\partial H}{\partial p_i} = \frac{p_i}{M}, \quad \text{and} \quad - \frac{\partial H}{\partial x_i} = - \frac{\partial \Phi}{\partial x_i} = F_i, \tag{27}$$

the i-th component of the deterministic force. With these results, the probability current components are

$$\begin{aligned} J_{x_i} &= \left[\frac{p_i}{M} + \frac{\Gamma^{(1)}}{k_\mathrm{B}T} F_i \right] \rho - \Gamma^{(1)} \frac{\partial \rho}{\partial x_i} + k_\mathrm{B}T \frac{\partial \rho}{\partial p_i}, \\ J_{p_i} &= \left[F_i - \frac{\Gamma^{(2)}}{k_\mathrm{B}T} \frac{p_i}{M} \right] \rho - \Gamma^{(2)} \frac{\partial \rho}{\partial p_i} - k_\mathrm{B}T \frac{\partial \rho}{\partial x_i}, \\ & i = 1, \cdots, N. \end{aligned} \tag{28}$$

4.2 Generic form

The Langevin equations in equation (17), when specialized to position and momentum variables, as we did at equation (23), become

$$\begin{aligned} \dot{x}_i &= f_{x_i}(\{x,p\}) + \tilde{\nu}_i^{(1)}(t), \\ \dot{p}_i &= f_{p_i}(\{x,p\}) + \nu_i^{(2)}(t), \\ & i = 1, \cdots, N. \end{aligned} \tag{29}$$

Here $\tilde{\nu}_i^{(1)}$ is the same function as ν_i of Section 3 for $i = 1, \cdots, N$; it is a a random noise source, with dimensions of length/time. $\nu_i^{(2)}$ is the same as ν_{i+N} of Section 3 for $i = 1, \cdots, N$; it is a random force. Similarly, the generic FPE in equation (22) becomes the same form as in equation (24), with the following formulas for the currents,

$$\begin{aligned} J_{x_i} &= f_{x_i}(\{x,p\})\rho - \frac{1}{2} D^{(1)} \frac{\partial \rho}{\partial x_i}, \\ J_{p_i} &= f_{p_i}(\{x,p\})\rho - \frac{1}{2} D^{(2)} \frac{\partial \rho}{\partial p_i}, \\ & i = 1, \cdots, N. \end{aligned} \tag{30}$$

Here we have restricted the constants D_i (see Eq. (18)) to two different values, one describing the coordinate noise source and the other the momentum noise force.

4.3 Comparison

The comparison between the two different expressions for the probability current densities in equations (28, 30), we can identify the following terms:

$$\begin{aligned} f_{x_i}(\{x,p\}) &= \frac{p_i}{M} + \frac{\Gamma^{(1)}}{k_\mathrm{B}T}F_i, \\ f_{p_i}(\{x,p\}) &= F_i - \frac{\Gamma^{(2)}}{Mk_\mathrm{B}T}p_i, \\ \frac{1}{2}D^{(1)} &= \Gamma^{(1)}, \\ \frac{1}{2}D^{(2)} &= \Gamma^{(2)}. \end{aligned} \tag{31}$$

We substitute the second of equations (31) into the second of equations (29) and obtain

$$\dot{p}_i = F_i - \frac{\Gamma^{(2)}}{Mk_\mathrm{B}T}p_i + \nu_i^{(2)}(t). \tag{32}$$

Then we compare this with the second of equations (2) and obtain the relation between the damping constant in the usual Langevin equation and the constants appearing in Langer's derivation of the FPE,

$$\gamma^{(2)} = \frac{\Gamma^{(2)}}{Mk_\mathrm{B}T}\,. \tag{33}$$

Now we define a new constant, with dimensions of $(\mathrm{time})^{-1}$, from the constants appearing in the first of equations (31),

$$\gamma^{(1)} = \frac{k_\mathrm{B}T}{M\Gamma^{(1)}}\,. \tag{34}$$

From equation (12) in Langer's derivation of the FPE, we see that for there to be no stochastic element in the evolution of the x_i variables, it is necessary that $\Gamma^{(1)} \to 0$. From equation (34) this obviously translates to $\gamma^{(1)} \to \infty$.

With the definition in equation (34) and the first of equations (31), the first of equations (29) becomes

$$\dot{x}_i = \frac{p_i}{M} + \frac{1}{M\gamma^{(1)}}F_i + \tilde{\nu}_i^{(1)}(t). \tag{35}$$

Next we multiply this equation through by $M\gamma^{(1)}$ and find that it is natural to define a second random force function by

$$\nu_i^{(1)} = M\gamma^{(1)}\tilde{\nu}_i^{(1)}. \tag{36}$$

The resulting equation here, along with the combination of equations (32, 33), give the phase space Langevin equations with coordinates and momenta treated equivalently:

$$\begin{aligned} M\gamma^{(1)}\dot{x}_i &= \gamma^{(1)}p_i + F_i + \nu_i^{(1)}(t), \\ \dot{p}_i &= F_i - \gamma^{(2)}p_i + \nu_i^{(2)}(t), \\ i &= 1,\ldots,N. \end{aligned} \tag{37}$$

Equations (37) are the equations we are seeking, as described in the Introduction.

Equation (19) gives the correlation function of the noise sources in the generic form of the Langevin equation. When the constants are specialized to the values obtained in this section, using equations (19, 31, 33, 34, 36), these correlation functions become

$$\begin{aligned} \left\langle \nu_i^{(r)}(t)\nu_{i'}^{(s)}(t') \right\rangle_\nu &= 2M\gamma^{(r)}k_\mathrm{B}T\delta_{rs}\delta_{ii'}\delta(t-t'), \\ i,i' &= 1,\ldots,N;\ \ r,s = 1,2. \end{aligned} \tag{38}$$

One implication of equation (38) is that for large values of the damping constants, $\gamma^{(r)} \to \infty$, the magnitudes of the noise forces $\nu^{(r)}$ increase proportionally to $[\gamma^{(r)}]^{1/2}$.

The final form of the FPE, obtained from equations (14, 28) and the identification of the constants in this section, is

$$\begin{aligned} \frac{\partial\rho}{\partial t} = \\ -\sum_{i=1}^{N}\left\{ \frac{\partial}{\partial x_i}\left[\left(\frac{p_i}{M} + \frac{1}{M\gamma^{(1)}}F_i\right)\rho - \frac{k_\mathrm{B}T}{M\gamma^{(1)}}\frac{\partial\rho}{\partial x_i} + k_\mathrm{B}T\frac{\partial\rho}{\partial p_i}\right]\right. \\ \left. + \frac{\partial}{\partial p_i}\left[\left(F_i - \gamma^{(2)}p_i\right)\rho - Mk_\mathrm{B}T\gamma^{(2)}\frac{\partial\rho}{\partial p_i} - k_\mathrm{B}T\frac{\partial\rho}{\partial x_i}\right]\right\}. \end{aligned} \tag{39}$$

In this equation, the force F_i is obtained from the potential energy using the second of equations (27).

5 Consequences

5.1 Limiting cases

The "phase space" form of the Langevin equations in equation (37) are novel because there are damping and random force terms in both equations and because the deterministic force F_i appears in both equations. However, in appropriate limits equations (37) reduce to two forms of Langevin equations that are familiar.

The form where we started in equation (1) is obtained by taking the limit $\gamma^{(1)} \to \infty$. We noted after equation (34) that this limit removes the random forces which act directly on the x_i variables. The first of equations (37) simplifies to $\dot{x}_i = p_i/M$ (before taking the limit, divide by $M\gamma^{(1)}$ and recall that $\nu^{(1)}$ increases proportionally to $[\gamma^{(1)}]^{1/2}$), and the desired result is obtained on substitution into the second of equations (37). The appropriate form of the FPE for this limit is

$$\begin{aligned} \frac{\partial\rho}{\partial t} = -\sum_{i=1}^{N}\left\{ \frac{\partial}{\partial x_i}\left[\frac{p_i}{M}\rho + k_\mathrm{B}T\frac{\partial\rho}{\partial p_i}\right]\right. \\ \left. + \frac{\partial}{\partial p_i}\left[\left(F_i - \gamma^{(2)}p_i\right)\rho - Mk_\mathrm{B}T\gamma^{(2)}\frac{\partial\rho}{\partial p_i} - k_\mathrm{B}T\frac{\partial\rho}{\partial x_i}\right]\right\}. \end{aligned} \tag{40}$$

Another important limit is obtained by letting $\gamma^{(2)} \to \infty$. In the second of equations (37) the dominance of the damping term forces p_i to zero very rapidly. Then, setting $p_i = 0$ in the first of equations (37) reduces it to the overdamped form of the Langevin equation,

$$M\gamma^{(1)}\dot{x}_i = F_i + \nu_i^{(1)}(t). \tag{41}$$

To obtain the FPE appropriate for this limit, we divide equation (39) by $\gamma^{(2)}$; the terms that remain when we take $\gamma^{(2)} \to \infty$ are

$$\sum_i \frac{\partial}{\partial p_i}\left[p_i\rho + Mk_{\mathrm{B}}T\frac{\partial\rho}{\partial p_i}\right] = 0. \tag{42}$$

The normalizable solution of this equation is the Maxwell-Boltzmann distribution for each momentum component. Thus in this limit the phase space PDF is a product of separate momentum and configuration factors with the form

$$\begin{aligned}\rho(\{x,p\},t) &= N_{\mathrm{MB}}\exp\left(-\sum_{i=1}^{N}\frac{p_i^2}{2Mk_{\mathrm{B}}T}\right)\rho_{\mathrm{c}}(\{x\},t)\\ &\equiv \rho_{\mathrm{MB}}(\{p\})\rho_{\mathrm{c}}(\{x\},t),\end{aligned} \tag{43}$$

where N_{MB} is a normalization constant. We substitute this form into equation (39) and obtain

$$\begin{aligned}\rho_{\mathrm{MB}}\frac{\partial\rho_{\mathrm{c}}}{\partial t} = -\sum_{i=1}^{N}\Bigg\{&\frac{p_i}{M}\rho_{\mathrm{MB}}(\{p\})\frac{\partial\rho_{\mathrm{c}}(\{u\})}{\partial x_i}\\ &+\frac{1}{M\gamma^{(1)}}\rho_{\mathrm{MB}}\frac{\partial}{\partial x_i}(F_i\rho_{\mathrm{c}}) - \frac{k_{\mathrm{B}}T}{M\gamma^{(1)}}\rho_{\mathrm{MB}}\frac{\partial^2\rho_{\mathrm{c}}}{\partial x_i^2} - \frac{p_i}{M}\rho_{\mathrm{MB}}\rho_{\mathrm{c}}\\ &+\frac{\partial}{\partial p_i}\left[F_i\rho_{\mathrm{MB}}\rho_{\mathrm{c}} - k_{\mathrm{B}}T\rho_{\mathrm{MB}}\frac{\partial\rho_{\mathrm{c}}}{\partial x_i}\right]\Bigg\}.\end{aligned} \tag{44}$$

Next we integrate equation (44) over all of momentum space. The terms proportional to $p_i\rho_{\mathrm{MB}}(\{p\})$ integrate to zero. The term with the derivative with respect to p_i can be integrated, and the result vanishes because ρ_{MB} vanishes at infinity. We obtain the following overdamped FPE or Smoluchowski [8] equation:

$$\frac{\partial\rho_{\mathrm{c}}(\{x\},t)}{\partial t} = -\sum_{i=1}^{N}\frac{\partial}{\partial x_i}\left[\frac{1}{M\gamma^{(1)}}F_i\rho_{\mathrm{c}} - \frac{k_{\mathrm{B}}T}{M\gamma^{(1)}}\frac{\partial\rho_{\mathrm{c}}}{\partial x_i}\right]. \tag{45}$$

This reduction of the Fokker-Planck equation in phase space to the Smoluchowski equation in configuration space is shorter than the one usually given [9].

5.2 Temperature dependence

In equations (33, 34) we obtained relations between the damping constants $\gamma^{(i)}$ that appear in the usual Langevin equations and Langer's constants $\Gamma^{(i)}$ that give the rate of variation of the phase space variables induced by interaction with the heat bath. Here we want to point out that it is not consistent to assume that both of these sets of constants are temperature-independent. In many computer simulations that have been carried out using Langevin equations, it is common to assume that the $\gamma^{(i)}$ (only one of them has been present in previous work) are independent of temperature. In that case the $\Gamma^{(i)}$ must be proportional to temperature. It seems natural that the rate of variation induced by the heat bath should increase with the temperature of the bath.

5.3 Example: The Kramers' problem

One of the touchstone problems which has been analyzed by use of the Fokker-Planck equation is the calculation of escape rates from metastable states. The most quoted early paper on the subject is probably by Kramers [10], although it is evidently not the first [11]. In the interval since Kramers' paper an enormous literature on the subject has been created. There are recent reviews on the subject to which we refer for detailed summaries [12,13]. In its simplest form, the problem concerns a single Brownian particle moving in a one-dimensional potential energy with a well (minimum) and a barrier (maximum). The minimum is located at $x = x_{\mathrm{A}}$, and the maximum at $x = x_{\mathrm{B}}$. Near these two locations, the potential energy is approximated by quadratic forms

$$\begin{aligned}U(x) &= \frac{1}{2}M\omega_{\mathrm{A}}^2(x-x_{\mathrm{A}})^2 + \cdots, \quad x \approx x_{\mathrm{A}},\\ U(x) &= E_{\mathrm{b}} - \frac{1}{2}M\omega_{\mathrm{B}}^2(x-x_{\mathrm{B}})^2 + \cdots, \quad x \approx x_{\mathrm{B}};\end{aligned} \tag{46}$$

E_{b} is the barrier height, and ω_{A} and ω_{B} are positive. The problem is to calculate the rate of escape from the well over the barrier under the influence of the noise and damping forces.

The solution is obtained from the (one degree of freedom form of the) FPE in equation (40). Here we want to give the solution as obtained from our FPE with two damping constants (Eq. (39)). The solution is obtained in exactly the same way as for the simpler FPE in equation (40), and those details are described, for example, in references [10,12]. Therefore we give just the answer for the rate constant, which is

$$\begin{aligned}k(\gamma^{(1)},\gamma^{(2)}) = \frac{1}{2\pi}\frac{\omega_{\mathrm{A}}}{\omega_{\mathrm{B}}}\Bigg\{&\sqrt{\left[\frac{1}{2}\left(\frac{\omega_{\mathrm{B}}^2}{\gamma^{(1)}}+\gamma^{(2)}\right)\right]^2+\omega_{\mathrm{B}}^2}\\ &+\frac{1}{2}\left(\frac{\omega_{\mathrm{B}}^2}{\gamma^{(1)}}-\gamma^{(2)}\right)\Bigg\}\mathrm{e}^{-E_{\mathrm{b}}/k_{\mathrm{B}}T}.\end{aligned} \tag{47}$$

As discussed in references [10,12], the method of solution of the FPE used to obtain equation (47) is valid only for moderate and large damping. Familiar results are obtained by taking limits on equation (47), similarly to the discussion in Section 5.1. If we take $\gamma^{(1)} \to \infty$, then

equation (47) reduces to Kramers' result for moderate damping,

$$k(\infty,\gamma^{(2)}) = \frac{1}{2\pi}\frac{\omega_{\rm A}}{\omega_{\rm B}}\left\{\sqrt{\left[\frac{1}{2}\gamma^{(2)}\right]^2+\omega_{\rm B}^2}-\frac{1}{2}\gamma^{(2)}\right\} \times {\rm e}^{-E_{\rm b}/k_{\rm B}T}. \quad (48)$$

And if we let $\gamma^{(2)} \to \infty$ in equation (47), then to first order in $1/\gamma^{(2)}$ and for arbitrary values of $1/\gamma^{(1)}$ we get,

$$\lim_{\gamma^{(2)}\to\infty} k(\gamma^{(1)},\gamma^{(2)}) = \frac{1}{2\pi}\omega_{\rm A}\omega_{\rm B}\left(\frac{1}{\gamma^{(1)}}+\frac{1}{\gamma^{(2)}}\right){\rm e}^{-E_{\rm b}/k_{\rm B}T}. \quad (49)$$

Either term here is Kramers' result for large damping. With these two damping constants, the rate is essentially determined by the larger term. Finally, the limit

$$\lim_{\gamma^{(2)}\to 0} k(\infty,\gamma^{(2)}) = \frac{1}{2\pi}\omega_{\rm A}{\rm e}^{-E_{\rm b}/k_{\rm B}T} \quad (50)$$

is the result of transition state theory [14].

6 Summary

By comparing two different derivations of the Fokker-Planck equation, we have obtained Langevin equations of motion for a mechanical system that have consistent damping and noise forces in the equations for all the phase space variables. These equations reduce in appropriate limits to previously used forms of the Langevin equations. The equations could be useful for performing dynamical computer simulations of systems in contact with a heat bath, because of the additional flexibility allowed by the existence of two damping constants. For example in simulations of lightly damped systems, the computer time required to bring the simulation system to thermal equilibrium can be excessive. With these equations, one could set a value for $\gamma^{(1)}$ that would rapidly thermalize the system, and then remove that damping source ($\gamma^{(1)} \to \infty$) and continue the simulation with the desired small value of $\gamma^{(2)}$. We plan to demonstrate the usefulness of equations (37) in a forthcoming publication.

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