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Canonically invariant formulation of Langevin and Fokker-Planck equations

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Abstract. We present a canonically invariant form for the generalized Langevin and Fokker-Planck equations. We discuss the role of constants of motion and the construction of conservative stochastic processes.

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The Langevin equation represents the dynamics of a Hamiltonian system coupled to a heat bath in a very specific way: every degree of freedom can be considered to have its own, independent and infinitely large heat bath.

Even within this assumption, the way in which such a dynamics is formulated implies some further restrictions. Consider the usual Langevin equation:

$$m\ddot{q}_i = -\frac{\partial V}{\partial q_i} - \dot{q}_i + \xi_i(t) \tag{1}$$

with $\xi_i(t)$ Gaussian white noise $\langle \xi_i(t)\xi_j(t')\rangle = 2T \times\delta_{ij}\delta(t-t')$, and T the temperature of the thermal bath. Rewriting this as a set of phase-space equations:

$$\begin{cases} \dot{q}_i = & \dfrac{p_i}{m} \\ \dot{p}_i = -\dfrac{\partial V}{\partial q_i} - \dfrac{p_i}{m} + \xi_i(t) \end{cases} \tag{2}$$

we notice two things. Firstly, the form of the first equation is restricted to a Hamiltonian H of the form $H = \sum_i p_i^2/m + V(q)$. Secondly, the interaction with the bath has introduced an asymmetry in the treatment of coordinates and momenta by assuming that the thermal noise couples only to the coordinates and not to the velocities. This latter fact is usually taken as obvious, although one can envisage a scenario in which this is not the case.

Here we wish to reformulate the Langevin and Fokker-Planck processes in such a way as to treat all phase-space variables on an equal footing. Our aim is not so much to study systems whose kinetic energy is not quadratic or having more general couplings with the heat bath, but to be able to regain the canonical phase-space structure that is lost in the usual formulation. The hope is that, as in ordinary classical mechanics, a canonical formulation can be helpful in clarifying the properties of the dynamics, and may provide tools for the solutions of certain problems.

In general, Langevin equations can be motivated [1,2] by considering the system with Hamiltonian H, coupled to an infinite set of harmonic oscillators with random phases at some initial time and energies given by equipartition at temperature T. Upon solving for the oscillators, and reinjecting their dependence on the equation of motion, one gets a Langevin equation which can be made Markovian by a suitable choice of distribution of the oscillators' frequencies.

Actually, equations (1, 2) are associated with a particular coupling of the form:

$$H_{\rm coup} = \sum_i q_i \left[\sum_{a=1}^{N} A_a^i y_a^i\right] \tag{3}$$

where y_a^i are the coordinates of the oscillators of frequencies ω_a^i.

In order to obtain a canonically invariant generalization, one can repeat the exercise with a coupling with the "bath" of oscillators of a more general form:

$$H_{\rm coup} = \sum_i \sum_{a=1}^{N} \left[A_a^i G_i^1(\mathbf{q},\mathbf{p}) y_a^i + B_a^i G_i^2(\mathbf{q},\mathbf{p})\dot{y}_a^i\right]. \tag{4}$$

Such a very general form of the couplings may seem unphysical, but one should bare in mind that in the present formulation we may wish to re-express the problem in new generalized variables that mix the original coordinates and momenta, and terms like that will be generated by the transformation.

In order to obtain a Langevin equation starting from (4), it is convenient to consider the limit of small coupling between system and bath, thus avoiding the introduction

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of additional "counterterms" necessary to compensate for the interaction energy (see Ref. [1]). The procedure is standard [1], here we outline the steps:

- One solves the linear equations for the variables y_a^i with initial amplitudes and velocities $y_a^i(t=0)$, $\dot{y}_a^i(t=0)$. The solution is expressed in terms of the $G_i^1(\mathbf{q},\mathbf{p})(t)$, $G_i^2(\mathbf{q},\mathbf{p})(t)$ which act as external fields for the oscillators.
- One can write the equations of motion for the $\mathbf{q},\mathbf{p}$ substituting the $y_a^i(t)$, $\dot{y}_a^i(t)$ obtained in the previous step. One thus obtains an equation of motion that is non-local in time but involves only $\mathbf{q},\mathbf{p}$ and the initial conditions for the oscillators.
- The initial energies of the oscillators are set to $k_\mathrm{b}T$, thus defining the temperature of the bath. The initial phases of the bath's oscillators are taken as random variables: *this is where stochasticity enters.* Averages over the heat bath will in fact be averages over the initial phases.
- One thus obtains a "generalized Langevin equation" [3] with correlated noise and a friction term that is non-local in time. One can make the equation local in time by choosing a suitable distribution of frequencies of the oscillators.

Performing these steps, one arrives at the following Langevin equation, valid for any phase-space variable $A(\mathbf{q},\mathbf{p})$, in particular the coordinates and momenta q_i, p_i:

$$\dot{A} = \kappa\{A,H\} + \sum_j \{A,G_j\}(\xi_j(t) + \{G_j,H\}). \quad (5)$$

Here $\{A,B\} = \sum_i \left(\frac{\partial A}{\partial q_i}\frac{\partial A}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i}\right)$ are the Poisson brackets.

We have denoted $G_i(\mathbf{p},\mathbf{q})$ $(i = 1,...,R)$ the set $G_i^1(\mathbf{q},\mathbf{p})$, $G_i^2(\mathbf{q},\mathbf{p})$ consisting of R arbitrary phase-space functions. The noise is white and Gaussian. The inverse time-constant κ will be useful below, it has been added by rescaling the time.

In fact, one does not have to worry about the details of the derivation, because it will be shown in what follows that this equation is a Langevin equation having all the good properties, in particular that it leads to the canonical distribution at temperature T. The definition of equation (5) is completed by specifying that it should be understood *in the Stratonovitch sense:* in a discretized form all phase-space functions in the right hand side have to be evaluated as an average of their values in the previous and the incremented time.

Indeed, one can adopt *Itô's convention* in which the r.h.s. is evaluated in the previous time, and the equation now reads:

$$\dot{A} = \kappa\{A,H\} + \sum_j \{A,G_j\}(\xi_j(t) + \{G_j,H\}) + T\{G_j,\{G_j,A\}\}. \quad (6)$$

Two particular cases are $G_i = -q_i\ \forall i;\ \kappa = 1$, which yields to equations (1,2), and $G_i = p_i\ \forall i;\ \kappa = 0$ which yields the *massless* version of (1). Note that in general the Poisson brackets between the G_i need not vanish, in which case the equations (5) cannot be taken through a canonical transformation to the form (1).

Let us now turn to the (Fokker-Planck) equation satisfied by the probability distribution $P(\mathbf{q},\mathbf{p},t)$. Denoting collectively $\{x_i\}$ the set $\{\mathbf{q},\mathbf{p}\}$ equations (5) can be written as:

$$\dot{x}_i = \{x_i,H\} + \{x_i,G_j\}(\xi_j(t) + \{G_j,H\}) \quad (7)$$

in the Stratonovitch convention. This leads (see Chap. 3 of Ref. [3])to the following Fokker-Planck equation:

$$\frac{\partial P}{\partial t} = \hat{L}_\mathrm{FP} P \quad \text{with} \quad \hat{L}_\mathrm{FP} = -\frac{\partial}{\partial x_i} D_i + \frac{\partial^2}{\partial x_i \partial x_k} D_{ik}. \quad (8)$$

With the specific form of (7) the coefficients read:

$$D_i(\{x_p\}) = \{x_i,H\} + \{x_i,G_j\}\{G_j,H\} + T\{x_l,G_j\}\frac{\partial}{\partial x_l}\{x_i,G_j\}$$
$$D_{ik}(\{x_p\}) = \{x_i,G_j\}\{x_k,G_j\}. \quad (9)$$

It is now a simple exercise to re-express (8) in terms of Poisson brackets. The result is:

$$\frac{\partial P}{\partial t} + \kappa\{P,H\} = \sum_j \{G_j\{G_j,H\}P + \{G_j,P\}\}. \quad (10)$$

It is now clear that $P = \exp(-H/T)$ is a stationary solution of (10). Again, with the choice $G_i = -q_i\ \forall i;\ \kappa = 1$ we obtain the Kramer's equation. If instead we make $G_i = p_i\ \forall i;\ \kappa = 0$ we obtain the usual Fokker-Planck equation for diffusion without inertia.

By writing $\langle A\rangle(t) = \int \mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p} A(\mathbf{q},\mathbf{p})P(\mathbf{q},\mathbf{p},t)$ we obtain for the evolution of the average of an observable $A(\mathbf{q},\mathbf{p})$:

$$\frac{\mathrm{d}\langle A\rangle(t)}{\mathrm{d}t} = \langle\{A,H\}\rangle - \sum_i \langle\{G_i,A\}\{G_i,H\}\rangle - T\sum_i \langle\{G_i,\{A,G_i\}\}\rangle. \quad (11)$$

All three equations (5, 10 and 11) are canonically invariant in form: a canonical transformation of variables is obtained directly by transforming H and the G_i. Furthermore, the pure Hamiltonian term and the bath-coupling terms are explicitly separated.

Equilibration

In order to study the equilibration properties, let us define an $\mathcal{H}$-function as [5,6]:

$$\mathcal{H}(t) = \int \mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p} P(\mathbf{q},\mathbf{p},t)(T\ln P(\mathbf{q},\mathbf{p},t) + H(\mathbf{q},\mathbf{p})) \quad (12)$$

which cannot increase, since:

$$\dot{\mathcal{H}} = -\sum_i \int \mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p} \frac{(\{G_i, H\}P + T\{G_i, P\})^2}{P} \leq 0. \quad (13)$$

Note that only the bath-terms contribute.
If the equilibrium measure exists, $\mathcal{H}$ is bounded from below, and we have that

$$\{G_i, H\}P + T\{G_i, P\} \to 0 \ \forall i. \quad (14)$$

If we parameterize $P(\mathbf{q}, \mathbf{p}, t)$ as:

$$P(\mathbf{q}, \mathbf{p}, t) = Q(\mathbf{q}, \mathbf{p}, t) \exp(-H/T) \quad (15)$$

the limit (14) implies that, once stationarity is achieved:

$$\{G_i, Q\} = 0 \ \forall i. \quad (16)$$

Using this equation, we have that $\dot{Q} = \{H, Q\}$. Since at stationarity (16) has to be valid at all times, we obtain the necessary conditions:

$$\{Q_i, Q\} = 0; \quad \{G_i\{H, Q\}\} = 0;$$
$$\{G_i\{H, \{H, Q\}\}\} = 0; \ ... \quad (17)$$

In the usual Langevin case (1,2), $G_i = x_i$, $H = \sum_i p_i^2/2m + V(x)$ and the first two sets of equations suffice to prove that $Q =$ constant is the only stationary solution.

Constants of motion

Suppose the Hamiltonian has some constants of motion $\{H, K_a\} = 0$. Depending on the choice of G_i, these constants will be preserved or not by the coupling with the bath. Indeed, equation (5) implies:

$$\frac{\mathrm{d}K_a}{\mathrm{d}t} = \sum_j \{K_a, G_j\}(\xi_j(t) + \{G_j, H\}). \quad (18)$$

The evolution of K_a is then purely dictated by the heat-bath, and will be "slow" in the limit of small coupling to the bath $G_i \sim 0$.

If we wish to construct a K_a-preserving noisy dynamics, we have to choose the G_i such that $\{K_a, G_i\} = 0 \ \forall i$ [7].

If, on the other hand, we couple the system to the bath through some constants of motion, that is $G_i = K_i$, the Langevin dynamics for any $A(\mathbf{q}, \mathbf{p})$ becomes:

$$\dot{A} = \kappa\{A, H\} + \sum_j \{A, K_j\}\xi_j(t) \quad (19)$$

which expresses the fact that the system receives random kicks in the direction generated by the K_j.

An extreme and rather amusing form of this is the case in which we put a single $G = H$ and $\kappa = 0$. We then have

$$\dot{A} = \{A, H\}\xi(t) \quad (20)$$

and the associated Fokker-Planck equation:

$$\frac{\partial P}{\partial t} = T\{H, \{H, P\}\}. \quad (21)$$

The system diffuses back an forth along its classical trajectories. The probability distribution tends for long times to the smallest invariant structure compatible with the original distribution, and the entropy $\int \mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p} P(\mathbf{q}, \mathbf{p}, t) \times \ln P(\mathbf{q}, \mathbf{p}, t)$ becomes stationary.

Motion within a group

Another simple application is the construction of a heat-bath dynamics on a group. Suppose the Hamiltonian is constructed in terms of the generators L_i of a group, satisfying $\{L_i, L_j\} = C_{ijl} L_l$. Then,

$$\dot{L}_i = \{L_i, H\} + C_{ijl} L_l(\xi_j(t) + \{L_j, H\})$$
$$= C_{ijl}(\omega_j + \xi_j)L_l + C_{ijl} C_{j\mathrm{sr}} \omega_\mathrm{s} L_\mathrm{r} L_l \quad (22)$$

where the "angular velocities" are defined as $\omega_i = \frac{\partial H(\mathbf{L})}{\partial L_i}$. The group invariant $\sum_i L_i^2$ is clearly a constant of motion.

In summary, we have presented a manifestly canonical-invariant form of the Langevin and Fokker-Planck equations. Within this formulation one can see the effect of thermal noise without losing sight of the structure of the underlying classical mechanics.

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