Langevin Equations in Coarse-Graining

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1 Introduction

Consider a system where the coarse-grained degrees of freedom $\boldsymbol{x} = \boldsymbol{X}(\boldsymbol{z})$ give rise to a *coarse-grained Hamiltonian* or more correctly a *coarse-grained free energy* defined formally via

$$H(\boldsymbol{x}) = -(k_B T) \ln \int_{\boldsymbol{z}} \delta[\boldsymbol{X}(\boldsymbol{z}) - \boldsymbol{x}] \rho_{\text{eq}}(\boldsymbol{z}) d\boldsymbol{z},$$

where $\boldsymbol{z}$ denotes the microscopic configuration and $\rho_{\text{eq}}(\boldsymbol{z})d\boldsymbol{z}$ is the equilibrium measure for the microscopic dynamics. In some cases the actual Hamiltonian (total energy) may be expressible in terms of the coarse-grained variables and is strictly conserved, but this is not always the case since some of the energy may in fact be incorporated in the coarse-grained free energy as an "entropy". The equilibrium distribution for the coarse variables is the coarse-grained Gibbs distribution

$$P_{\text{eq}}(\boldsymbol{x}) = Z^{-1} \exp\left[-\frac{H(\boldsymbol{x})}{k_B T}\right], \tag{1}$$

and any reasonable coarse-grained dynamics must preserve this distribution as an invariant measure.

In the notation used here, I use a dot to denote an inner product (contraction) and a colon for an inner tensor product (double contraction), which for fields would imply a spatial integration but in any case ultimately the field equations will be discretized anyway. Omitting a symbol will imply an outer product. When $\boldsymbol{x}$ is (formally) infinite dimensional the partial derivatives should be interpreted as functional derivatives, for example,

$$\frac{\partial H}{\partial \boldsymbol{v}} \equiv \frac{\delta H[\boldsymbol{v}(\boldsymbol{r})]}{\delta \boldsymbol{v}}.$$

A more careful notation is developed in [1] but we do not use it here.

1.1 Isolated Systems

In the GENERIC formalism [1] one considers closed systems in which the total energy $E(\boldsymbol{x})$ and entropy $S(\boldsymbol{x})$ can strictly be expressed in terms of the selected variables, and the reversible dynamics is generated from energy gradients while the irreversible dynamics is generated from entropy gradients, as described by the Ito SDE

$$\partial_t \boldsymbol{x} = \boldsymbol{L} \cdot \frac{\partial E}{\partial \boldsymbol{x}} + \boldsymbol{M} \cdot \frac{\partial S}{\partial \boldsymbol{x}} + (2k_B)^{1/2} \boldsymbol{B} \cdot \boldsymbol{W}(t) + k_B \frac{\partial}{\partial \boldsymbol{x}} \cdot \boldsymbol{M}^\star, \tag{2}$$

where $\boldsymbol{W}$ denotes white noise, and we will suppress the explicit dependence on $\boldsymbol{x}$ and usually write $\boldsymbol{L} \equiv \boldsymbol{L}(\boldsymbol{x})$, $\boldsymbol{M} \equiv \boldsymbol{M}(\boldsymbol{x})$, and $\boldsymbol{B} \equiv \boldsymbol{B}(\boldsymbol{x})$. The skew-adjoint operator $\boldsymbol{L} = -\boldsymbol{L}^\star$ generates the

reversible part of the dynamics (e.g., advection), while the irreversible dynamics (e.g., diffusion) is generated from the positive semi-definite operator $\boldsymbol{M}$, and $\boldsymbol{B}$ obeys the fluctuation-dissipation balance principle,

$$\boldsymbol{B}\boldsymbol{B}^{\star} = \boldsymbol{M} \succeq \boldsymbol{0}.$$

The last term in (2) is an additional or "spurious" drift term whose form depends on the particular interpretation of the stochastic equations, and dissappears if one uses an "Klimontovich" or "kinetic" interpretation [2].

In GENERIC, one assumes the degeneracy condition

$$\boldsymbol{M} \cdot \frac{\partial E}{\partial \boldsymbol{x}} = \boldsymbol{0},$$

which can be derived from the microscopic dynamics. One can also show from the microscopic dynamics that

$$k_B \frac{\partial}{\partial \boldsymbol{x}} \cdot \boldsymbol{L} = \frac{\partial S}{\partial \boldsymbol{x}} \cdot \boldsymbol{L} = -\boldsymbol{L} \cdot \frac{\partial S}{\partial \boldsymbol{x}} \text{ and in GENERIC this is } = \boldsymbol{0} \tag{3}$$

but this cannot be derived from the microscopic dynamics. Nevertheless, if one assumes this, it can be shown that (2) preserves the Einstein distribution $P_{\mathrm{eq}}(\boldsymbol{x}) \sim \exp\left[S(\boldsymbol{x})/k_B\right]$. More generally, the microscopic derivation dictates that

$$\frac{\partial}{\partial \boldsymbol{x}} \cdot \left[\boldsymbol{L} \cdot \frac{\partial E}{\partial \boldsymbol{x}} e^{S(\boldsymbol{x})/k_B}\right] = \left(\boldsymbol{L} \cdot \frac{\partial S}{\partial \boldsymbol{x}} + k_B \frac{\partial}{\partial \boldsymbol{x}} \cdot \boldsymbol{L}\right) \cdot \frac{\partial E}{\partial \boldsymbol{x}} e^{S(\boldsymbol{x})/k_B} \sim \frac{\partial E}{\partial \boldsymbol{x}} \cdot \boldsymbol{L} \cdot \frac{\partial S}{\partial \boldsymbol{x}} = 0,$$

which ensures that the equilibrium distribution is the Einstein distribution. While this does not require that

$$-\boldsymbol{L} \cdot \frac{\partial S}{\partial \boldsymbol{x}} = k_B \frac{\partial}{\partial \boldsymbol{x}} \cdot \boldsymbol{L} = \boldsymbol{0}, \tag{4}$$

in general it seems a good modeling practice to try to ensure (4) anyway in order to make the reversible dynamics as close to "Hamiltonian" as possible.

1.2 Isothermal Systems

In the GENERIC formalism it is required that the total energy and entropy be included or at least expressible in terms of the coarse-grained variables. This allows for a strict and meaningful separation between reversible and irreversible dynamics, and there are some stringent conditions imposed on $\boldsymbol{L}(\boldsymbol{x})$ that ensure that the reversible part of the dynamics has a Hamiltonian structure, i.e., that one can form a Poisson bracket using $\boldsymbol{L}$. These assumptions, however, often restrict the choice of the coarse-grained variables too much in practice, and also make the formalism unsuitable for isothermal systems, that is, systems where the canonical distribution $\rho_{\mathrm{eq}}(\boldsymbol{z})$ is maintained by contact with an external heat bath.

As discussed in Ref. [3], a reasonable postulate for extending the Langevin equation to more general Hamiltonian systems is the Ito equation with structure similar to (2),

$$\partial_t \boldsymbol{x} = \boldsymbol{L} \cdot \frac{\partial H}{\partial \boldsymbol{x}} - \boldsymbol{M} \cdot \frac{\partial H}{\partial \boldsymbol{x}} + (2k_B T)^{1/2} \boldsymbol{B} \cdot \boldsymbol{W}(t) + (k_B T) \frac{\partial}{\partial \boldsymbol{x}} \cdot \boldsymbol{M}, \tag{5}$$

where $\boldsymbol{L} = -\boldsymbol{L}^{\star}$ is a skew-adjoint operator that conserves the Hamiltonian (total energy) while the self-adjoint and positive-semidefinite $\boldsymbol{M} \equiv \boldsymbol{M}^{\star} \succeq \boldsymbol{0}$ strictly dissipates it, and $\boldsymbol{B}\boldsymbol{B}^{\star} = \boldsymbol{M}$. Based

on Hamiltonian dynamics, Ref. [3] requires that the reversible dynamics be incompressible in phase space,

$$\frac{\partial}{\partial \boldsymbol{x}} \cdot \boldsymbol{L}(\boldsymbol{x}) = \boldsymbol{0}. \tag{6}$$

This is however not necessarily true for coarse-grained descriptions, and furthermore, it may be destroyed by a simple transformation into (non-canonical) variables, as we will see shortly. It therefore seems necessary to generalize (5).

1.3 Augmented Langevin Equation

As discussed at length in the book by Grabert [4] and also in the review article by Pep Espanol [5], a Markovian approximation within the Mori-Zwanzig formalism can be used to obtain a coarse-grained equation of motion for an arbitrary choice of the microscopic ensemble. For generalized sets of coarse-grained variables, it appears one should give up the strict separation between reversible and irreversible dynamics as insisted-upon in (2) and (5), and instead, simply write

$$\partial_t \boldsymbol{x} = -\boldsymbol{N} \cdot \frac{\partial H}{\partial \boldsymbol{x}} + (2k_B T)^{1/2} \boldsymbol{B} \cdot \boldsymbol{W}(t) + (k_B T) \frac{\partial}{\partial \boldsymbol{x}} \cdot \boldsymbol{N}^\star, \tag{7}$$

with the fluctuation-dissipation balance condition

$$\boldsymbol{B}\boldsymbol{B}^\star = \frac{1}{2}(\boldsymbol{N} + \boldsymbol{N}^\star) = \boldsymbol{M} \succeq \boldsymbol{0}.$$

In this picture $\boldsymbol{L} = \frac{1}{2}(\boldsymbol{N}^\star - \boldsymbol{N})$ is the "conservative" part and $\boldsymbol{M}$ is the "dissipative" part of the dynamics,

$$\frac{dH}{dt} = \frac{\partial H}{\partial \boldsymbol{x}} \cdot \boldsymbol{N} \cdot \frac{\partial H}{\partial \boldsymbol{x}} = \mathrm{Re}\left(\frac{\partial H}{\partial \boldsymbol{x}} \cdot \boldsymbol{M} \cdot \frac{\partial H}{\partial \boldsymbol{x}}\right) \leq 0,$$

without placing additional restrictions on the "mobility" operator $\boldsymbol{N} = \boldsymbol{M} - \boldsymbol{L}$ except for time reversibility, as discussed later on.

Note that the Mori-Zwanzig formalism gives explicit expressions for $\boldsymbol{N}(\boldsymbol{x})$ as a sum of a "drift" term, which is the projection of the microscopic Poisson bracket onto the constrained manifold $\boldsymbol{X}(\boldsymbol{z}) = \boldsymbol{x}$, and a "friction" term, which is the integral of the autocorrelation function of the projected microscopic dynamics. This separation seems somewhat arbitrary however, in general. Note that in principle it would seem the formalism gives a way to evaluate $\boldsymbol{N}$ from microscopic simulations but this is not in fact trivial. One recent proposal is to actually constrain the microscopic dynamics to maintain the constraint $\boldsymbol{X}(\boldsymbol{z}) = \boldsymbol{x}$ and thus *enforce* strict separation of time scales between the coarse and full degrees of freedom [6].

1.3.1 Fokker-Planck Description

Note that the "spurious" drift term now involves $\frac{\partial}{\partial \boldsymbol{x}} \cdot \boldsymbol{L}$ as well in cases when the skew-adjoint part of the dynamics is not incompressible in phase space, and in this case one cannot attribute the additional drift to the "noise" and absorb it with a suitable stochastic interpretation. As often observed, the use of a Fokker-Planck Equation (FPE) instead of a stochastic differential equation (SDE) does not suffer from ambiguity, although this is merely a formal statement since eventually in Monte Carlo simulations we will need to convert the FPE to an SDE and make a specific choice for how to generate (interpret) the noise. The FPE can be written mechanically as

$$\frac{\partial P(\boldsymbol{x}, t)}{\partial t} = \frac{\partial}{\partial \boldsymbol{x}} \cdot \left[\boldsymbol{N} \cdot \frac{\partial H}{\partial \boldsymbol{x}} P + (k_B T) \frac{\partial}{\partial \boldsymbol{x}} \cdot (\boldsymbol{M} P) - (k_B T)\left(\frac{\partial}{\partial \boldsymbol{x}} \cdot \boldsymbol{N}^\star\right) P\right],$$

but because $\boldsymbol{L}$ is skew-adjoint and thus

$$\frac{\partial^2}{\partial \boldsymbol{x}^2} : \boldsymbol{L} = 0 \text{ and also } \boldsymbol{L} : \frac{\partial^2 H}{\partial \boldsymbol{x}^2} = 0,$$

we can rewrite the FPE in alternative suggestive forms.

Specifically, recognizing that the diffusion term can also be written as

$$\frac{\partial}{\partial \boldsymbol{x}} \cdot \left(\frac{\partial}{\partial \boldsymbol{x}} \cdot \boldsymbol{M} P \right) = \left(\frac{\partial^2}{\partial \boldsymbol{x}^2} : \boldsymbol{M} \right) P = \frac{\partial}{\partial \boldsymbol{x}} \cdot \left(\frac{\partial}{\partial \boldsymbol{x}} \cdot \boldsymbol{N} P \right),$$

we can write the FPE in the advection-diffusion form obtained by Grabert [c.f. (4.4.17)] [4]

$$\frac{\partial P(\boldsymbol{x}, t)}{\partial t} = \frac{\partial}{\partial \boldsymbol{x}} \cdot \left\{ \boldsymbol{N} \cdot \left[\frac{\partial H}{\partial \boldsymbol{x}} + (k_B T) \frac{\partial}{\partial \boldsymbol{x}} \right] P \right\} = -(k_B T) \frac{\partial}{\partial \boldsymbol{x}} \cdot (\boldsymbol{N} \cdot \boldsymbol{F} P), \tag{8}$$

where $\boldsymbol{F}$ is a linear operator that acts on distributions,

$$\boldsymbol{F} = \left[\frac{\partial H}{\partial \boldsymbol{x}} + (k_B T) \frac{\partial}{\partial \boldsymbol{x}} \right] = -P_{\text{eq}} \frac{\partial}{\partial \boldsymbol{x}} P_{\text{eq}}^{-1},$$

with adjoint

$$\boldsymbol{F}^\star = P_{\text{eq}}^{-1} \frac{\partial}{\partial \boldsymbol{x}} \cdot P_{\text{eq}}.$$

It is easy to see that $\boldsymbol{F} P_{\text{eq}} = \boldsymbol{0}$ and thus the right hand side of (8) vanishes at equilibrium. This shows that the equilibrium distribution for (7) is (1), as desired, for general $\boldsymbol{N}(\boldsymbol{x})$, at least if one makes the unrestrictive assumption that $\boldsymbol{M} \succ \boldsymbol{0}$.

Equation (8), while formally correct, is not a proper FPE because the diffusive flux (the second term inside the square brackets) must be preceded by a positive semi-definite diffusion matrix, i.e., $\boldsymbol{M}$ and *not* $\boldsymbol{N}$. In particular, $\boldsymbol{N} \cdot \boldsymbol{F} P$ should not be thought of as the phase-space flux. Instead, the FPE should be written as

$$\frac{\partial P(\boldsymbol{x}, t)}{\partial t} = -(k_B T) \frac{\partial}{\partial \boldsymbol{x}} \cdot \{ \boldsymbol{M} \cdot \boldsymbol{F} P - P \boldsymbol{F}^\star \boldsymbol{L} \}, \tag{9}$$

where now the phase-space flux is inside the curly braces and only the first part vanishes at equilibrium.

1.3.2 Transformation of Variables

An important property of the dynamics (7) is that it remains invariant under a change of variables. This is very important since different choices of variables may be easier to work with and it is important to know whether the form of the equation changes. This calculation can either be done at the level of the FPE (private communication with Pep Espanol), or at the level of the SDE. Here we take the second approach, essentially following Ottinger's calculation for the GENERIC equation [1].

Consider a change of variables from $\boldsymbol{x}$ to the variables $\tilde{\boldsymbol{x}}(\boldsymbol{x})$, and denote the Jacobian

$$\boldsymbol{J} = \frac{\partial \tilde{\boldsymbol{x}}}{\partial \boldsymbol{x}} = \left(\frac{\partial \boldsymbol{x}}{\partial \tilde{\boldsymbol{x}}} \right)^{-1}, \text{ meaning } \boldsymbol{J}_{ij} = \frac{\partial \tilde{\boldsymbol{x}}_i}{\partial \boldsymbol{x}_j}.$$

This transformation can be carried out on the (7) using Ito's formula, or equivalently, by using the backward Kolmogorov equation,

$$\partial_t \tilde{\boldsymbol{x}} = -\widetilde{\boldsymbol{N}} \cdot \frac{\partial \widetilde{H}}{\partial \tilde{\boldsymbol{x}}} + (2k_BT)^{1/2}\, \widetilde{\boldsymbol{B}} \cdot \boldsymbol{W}(t) + (k_BT)\, \boldsymbol{J} \cdot \frac{\partial}{\partial \boldsymbol{x}} \cdot \boldsymbol{N}^\star + (k_BT) \left(\frac{\partial^2 \tilde{\boldsymbol{x}}}{\partial \boldsymbol{x}^2} : \boldsymbol{M} \right),$$

where the transformed operators are

$$\widetilde{\boldsymbol{N}} = \boldsymbol{J} \cdot \boldsymbol{N} \cdot \boldsymbol{J}^\star \text{ and } \widetilde{\boldsymbol{B}} = \boldsymbol{J} \cdot \boldsymbol{B}.$$

A somewhat tedious but straightforward calculation gives

$$\frac{\partial}{\partial \tilde{\boldsymbol{x}}} \cdot \widetilde{\boldsymbol{N}}^\star = \boldsymbol{J} \cdot \frac{\partial}{\partial \boldsymbol{x}} \cdot \boldsymbol{N}^\star + \frac{\partial^2 \tilde{\boldsymbol{x}}}{\partial \boldsymbol{x}^2} : \boldsymbol{M} + \widetilde{\boldsymbol{N}} \cdot \left(\boldsymbol{J}^{-1} : \frac{\partial \boldsymbol{J}}{\partial \tilde{\boldsymbol{x}}} \right),$$

where we can also rewrite

$$\boldsymbol{J}^{-1} : \frac{\partial \boldsymbol{J}}{\partial \tilde{\boldsymbol{x}}} = \frac{\partial}{\partial \tilde{\boldsymbol{x}}} \left(\ln |\boldsymbol{J}| \right).$$

Defining a transformed free energy as

$$\widetilde{H}\left(\tilde{\boldsymbol{x}}\right) = H\left(\boldsymbol{x}\right) + (k_BT) \ln |\boldsymbol{J}|, \tag{10}$$

we can rewrite the transformed SDE as

$$\partial_t \tilde{\boldsymbol{x}} = -\widetilde{\boldsymbol{N}} \cdot \frac{\partial \widetilde{H}}{\partial \tilde{\boldsymbol{x}}} + (2k_BT)^{1/2}\, \widetilde{\boldsymbol{B}} \cdot \boldsymbol{W}(t) + (k_BT)\, \frac{\partial}{\partial \tilde{\boldsymbol{x}}} \cdot \widetilde{\boldsymbol{N}}^\star, \tag{11}$$

which shows that the form of the SDE (7) is invariant under variable transformations.

The transformation rule for the free energy (10) reflects the fact that what remains invariant is not the free energy itself but the invariant measure $d\mu_{\text{eq}} = \mu_{\text{eq}}\left(d\boldsymbol{x}\right) = P_{\text{eq}}\left(\boldsymbol{x}\right) d\boldsymbol{x}$. Specifically, phase-space averages (observables) must be invariant under a change of variables, and indeed,

$$\left\langle f\left(\boldsymbol{x}\right)\right\rangle_{\text{eq}} = \int f(\boldsymbol{x}) \exp\left(-\frac{H\left(\boldsymbol{x}\right)}{k_BT}\right) d\boldsymbol{x} = \int f(\tilde{\boldsymbol{x}})\, |\boldsymbol{J}|^{-1} \exp\left(-\frac{H\left(\tilde{\boldsymbol{x}}\right)}{k_BT}\right) d\tilde{\boldsymbol{x}} = \int f(\tilde{\boldsymbol{x}}) \exp\left(-\frac{\widetilde{H}\left(\tilde{\boldsymbol{x}}\right)}{k_BT}\right) d\tilde{\boldsymbol{x}}.$$

The result (10) underscores the importance of choosing "natural" coarse-grained variables when writing the coarse-grained free energy [1]. It is important to note that for infinite-dimensional systems (fluctuating field theories) the choice of the appropriate measure is not obvious at all since there is no infinite-dimensional generalization of the Lebesgue measure.

For Hamiltonian dynamics canonical variables provide natural coordinates, but in many cases non-canonical variables may be appropriate. A transformation of variables applied to eq. (5) would have shown that that form of the dynamics is not invariant under a change of coordinates. In particular, assume that $\boldsymbol{L}(\boldsymbol{x})$ is divergence free for some choice of variables, which means that the reversible (Hamiltonian) dynamics preserves the Lebesgue measure. A coordinate transformation can then make $\widetilde{\boldsymbol{L}}\left(\tilde{\boldsymbol{x}}\right)$ non-divergence free, meaning that the reversible dynamics would not preserve the Lebesgue measure and thus a term proportional to $(k_BT)\, \frac{\partial}{\partial \tilde{\boldsymbol{x}}} \cdot \widetilde{\boldsymbol{L}}$ would be necessary in the transformed equation in order for the transformed dynamics to preserve the equilibrium measure.

1.3.3 Time Reversal

It is also useful to look at the time reversed dynamics at equilibrium. It is well known that the time-reversed SDE is also an SDE, with the same stochastic forcing term as the original equation, but with a modified drift

$$\boldsymbol{N} \cdot \frac{\partial H}{\partial \boldsymbol{x}} - (k_B T) \frac{\partial}{\partial \boldsymbol{x}} \cdot \boldsymbol{N}^\star + (2k_B T) P_{\mathrm{eq}}^{-1} \frac{\partial}{\partial \boldsymbol{x}} \cdot (\boldsymbol{M} P_{\mathrm{eq}}) .$$

An explicit calculation for the coarse-grained Gibbs distribution gives

$$(2k_B T) P_{\mathrm{eq}}^{-1} \frac{\partial}{\partial \boldsymbol{x}} \cdot (\boldsymbol{M} P_{\mathrm{eq}}) = (2k_B T) \left(\frac{\partial}{\partial \boldsymbol{x}} \cdot \boldsymbol{M} \right) - 2\boldsymbol{M} \cdot \frac{\partial H}{\partial \boldsymbol{x}},$$

which shows that the time-reversed SDE has the same form as the original equation but with the adjoint of the mobility matrix (which implies reversal of the sign of the skew-adjoint part $\boldsymbol{L}$),

$$\partial_t \boldsymbol{x} = -\boldsymbol{N}^\star \cdot \frac{\partial H}{\partial \boldsymbol{x}} + (2k_B T)^{1/2} \boldsymbol{B} \cdot \boldsymbol{W}(t) + (k_B T) \frac{\partial}{\partial \boldsymbol{x}} \cdot \boldsymbol{N}. \tag{12}$$

The time-reversed SDE (11) shows what the Markovian dynamics is if one reads the evolution at equilibrium backward in time. Now we want to write this in terms of time-reversed variables, so that we see what SDE describes the physical system under a time-reversal transformation. The different coarse-grained variables will transform differently under time-reversal,

$$\tilde{\boldsymbol{x}}_k = \epsilon_k \boldsymbol{x}_k,$$

where the parity $\epsilon_k = 1$ for positional variables and $\epsilon_k = -1$ for velocity variables. If the free-energy is time-reversal invariant, $\widetilde{H}(\tilde{\boldsymbol{x}}) = H(\boldsymbol{x})$, and the mobility satisfies the reciprocal relations [4]

$$\widetilde{\boldsymbol{N}}_{kj}(\tilde{\boldsymbol{x}}) = \boldsymbol{N}_{kj}[\tilde{\boldsymbol{x}}(\boldsymbol{x})] = \epsilon_k \epsilon_j \left[\boldsymbol{N}^\star_{jk}(\boldsymbol{x}) \right], \tag{13}$$

then in the time-reversed variables the reversed evolution (12) becomes the SDE (11). Therefore, the reversed evolution has exactly the same form as the forward evolution (7), that is, the process is time reversible at equilibrium (obeys detailed balance). We may therefore stipulate that it is important for coarse-grained equations to obey the reciprocity conditions (13). This implies that for pairs of variables for which $\epsilon_k \epsilon_j = 1$, the corresponding part of $\boldsymbol{L}$ should change sign upon time reversal, while the corresponding part of $\boldsymbol{M}$ should not. For pairs of variables for which $\epsilon_k \epsilon_j = -1$, the corresponding part of $\boldsymbol{L}$ should not change sign upon time reversal, while the corresponding part of $\boldsymbol{M}$ should.

1.3.4 Linearization

In a linear approximation, which will be useful for analyzing numerical discretizations, $H(\boldsymbol{x})$ is approximated by its second-order Taylor series,

$$H(\boldsymbol{x}) \approx H(\boldsymbol{x}_0) + \frac{\partial H(\boldsymbol{x}_0)}{\partial \boldsymbol{x}} \cdot (\delta \boldsymbol{x}) + \frac{1}{2} (\delta \boldsymbol{x}) \cdot \frac{\partial^2 H(\boldsymbol{x}_0)}{\partial \boldsymbol{x}^2} \cdot (\delta \boldsymbol{x})$$

where $\delta \boldsymbol{x} = \boldsymbol{x} - \boldsymbol{x}_0$ and the mean or reference state $\boldsymbol{x}_0$ is a steady-state for the deterministic dynamics,

$$\boldsymbol{N}(\boldsymbol{x}_0) \cdot \frac{\partial H(\boldsymbol{x}_0)}{\partial \boldsymbol{x}} = \boldsymbol{0}.$$

Usually $\boldsymbol{x}_0$ is a (metastable) minimum of the coarse-grained free energy,

$$\frac{\partial H\left(\boldsymbol{x}_0\right)}{\partial \boldsymbol{x}} = \boldsymbol{0},$$

so that the fluctuations around $\boldsymbol{x}_0$ are Gaussian with equilibrium covariance

$$\left\langle \left(\delta\boldsymbol{x}\right)\left(\delta\boldsymbol{x}\right)^{\star}\right\rangle = \boldsymbol{C}_{\mathrm{eq}} = \left[\frac{\partial^2 H\left(\boldsymbol{x}_0\right)}{\partial \boldsymbol{x}^2}\right]^{-1}.$$

For notational simplicity we will hereafter denote $\delta\boldsymbol{x}$ with $\boldsymbol{x}$, and use a subscript zero to denote evaluation at $\boldsymbol{x}_0$. The linear Langevin equation is

$$\dot{\boldsymbol{x}} = -\boldsymbol{A}\cdot\boldsymbol{x} + \left(2k_BT\right)^{1/2}\boldsymbol{B}\cdot\boldsymbol{W}(t),$$

where $\boldsymbol{A} = \boldsymbol{N}_0\cdot\boldsymbol{C}_{\mathrm{eq}}^{-1}$ is now a constant linear operator and the fluctuation-dissipation theorem takes the familiar form

$$2\boldsymbol{B}\boldsymbol{B}^{\star} = \boldsymbol{A}\cdot\boldsymbol{C}_{\mathrm{eq}} + \boldsymbol{C}_{\mathrm{eq}}\cdot\boldsymbol{A}^{\star}.$$

The fluctuation-dissipation relation can simply be thought of as a definition of $\boldsymbol{B}$, assuming that the linearized deterministic dynamics $\boldsymbol{A}$ and the covariance matrix of the fluctuations $\boldsymbol{C}_{\mathrm{eq}}$ are known. More generally, if the system is not at equilibrium the steady-state covariance of the linearized fluctuations $\boldsymbol{C}_{n\mathrm{eq}}$ can be found by solving the system of linear equations [7]

$$\boldsymbol{A}\cdot\boldsymbol{C}_{\mathrm{neq}} + \boldsymbol{C}_{\mathrm{neq}}\cdot\boldsymbol{A}^{\star} = 2\boldsymbol{B}\boldsymbol{B}^{\star},$$

where it is usually assumed that $\boldsymbol{B}$ is well-approximated by its equilibrium value (more generally, by envoking a local equilibrium assumption).

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