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Augmented Langevin Description of Multiplicative Noise and Nonlinear Dissipation in Hamiltonian Systems

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The augmented Langevin approach described in a previous article is applied to the problem of introducing multiplicative noise and nonlinear dissipation into an arbitrary Hamiltonian system in a thermodynamically consistent way, so that a canonical equilibrium distribution is approached asymptotically at long times. This approach leads to a general nonlinear fluctuation-dissipation relation which, for a given form of the multiplicative noise (chosen on physical grounds), uniquely determines the form of the nonlinear dissipative terms needed to balance the fluctuations. In addition to the noise and dissipation terms, the augmented Langevin equation contains an additional term whose form depends on the stochastic interpretation rule used. This term vanishes when the Stratonovich rule is chosen and the noise itself is of a Hamiltonian origin. This development provides a simple phenomenological route to results previously obtained by detailed analysis of microscopic system–bath models. The procedure is illustrated by applications to a mechanical oscillator with fluctuating frequency, a classical spin in a fluctuating magnetic field, and the Brownian motion of a rigid rotor.

KEY WORDS: Langevin equation; Fokker–Planck equation; fluctuation-dissipation theorem; multiplicative noise; nonlinear dissipation; Hamiltonian systems; nonlinear dynamics.

1. INTRODUCTION AND SUMMARY

The concept of an isolated Hamiltonian system is a useful idealization upon which much of classical mechanics is based. There are many

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situations, however, in which this idealization is not appropriate because an essential role is played by interactions with the surroundings. For example, the system of interest may be part of a much larger isolated system, the remainder of which serves as a heat bath.[1-3]

A Hamiltonian system in equilibrium with a heat bath is described by the well-established principles of equilibrium statistical mechanics. The dynamical or nonequilibrium behavior of a Hamiltonian system in contact with a heat bath is less easily described, and the various methods that have been proposed for doing so are less well established. One of the oldest and most useful approaches is the phenomenological one of modeling the interaction between the system and heat bath stochastically, in the spirit of the original Langevin theory of Brownian motion. In this approach, one introduces into the dynamical equations for the isolated system an appropriate set of random forcing terms, the form of which is postulated on physical grounds based on one's conception of the nature of the system–bath coupling. These terms will loosely be referred to as "fluctuation" or "noise" terms.

It has not always been recognized that it is simultaneously necessary to introduce corresponding dissipative terms to balance the effects of the fluctuations, for otherwise the model will not be thermodynamically consistent and a canonical equilibrium distribution will not be approached at long times.[3] Unfortunately, the proper form of the required dissipative terms is not always obvious from a phenomenological point of view. In the frequently encountered case of multiplicative noise, the dissipative terms are usually nonlinear and there has been no reliable way to infer them phenomenologically.

This circumstance has motivated a number of investigations of microscopic system–bath models, from which the corresponding stochastic models are obtained by eliminating bath variables. In this way the proper nonlinear fluctuation-dissipation relations for the dissipative terms have been obtained for a variety of systems with multiplicative noise.[3] In these treatments it is very satisfying to see the consistent stochastic model emerge from the microscopic model in a constructive way. Unfortunately, in each analysis of this kind the details are quite different, and one obtains no information of a more general nature. In particular, these treatments have not suggested the existence of the general nonlinear fluctuation-dissipation relation derived in Section 2, which subsumes many of the microscopically derived results as special cases.

Our purpose here is to show that the augmented Langevin approach[4] provides a simple and straightforward phenomenological procedure for consistently introducing multiplicative noise and nonlinear dissipation into an arbitrary classical Hamiltonian system. This approach leads to a general nonlinear fluctuation-dissipation relation which, for a given assumed form of the multiplicative noise, uniquely determines the form of the corresponding nonlinear dissipative terms needed to balance the fluctuations. This way of using the fluctuation-dissipation relation is the converse of the original augmented Langevin reasoning,[4] in which the form of the multiplicative noise was inferred from the given nonlinear dissipation.

The augmented Langevin equation that we obtain contains, in addition to the noise and dissipation terms, an additional term involving the noise coefficient matrix. The form assumed by this term depends upon the choice of a stochastic interpretation rule,[5] which is necessary in order for the corresponding Fokker–Planck equation to be invariant to this choice.[4] Fortunately, if the Stratonovich rule is adopted (which is physically appropriate if the white noise employed in the development is regarded as the limit of colored noise for vanishing autocorrelation time), this additional term vanishes whenever the noise itself is ultimately of a Hamiltonian origin, as is usually the case. This situation obtains, in particular, when the composite system obtained by combining the system of interest with the heat bath is Hamiltonian in nature. The augmented Langevin equation then assumes a simple and intuitive form in which the motion is generated simply by superimposing the noise and dissipation terms upon the Hamiltonian dynamics of the isolated system, just as in the original Langevin theory.

Additional generality is obtained by basing the development upon a generalized formulation of Hamiltonian dynamics in terms of an antisymmetric matrix in state space.[6] This formulation includes canonical Hamiltonian dynamics as a special case, but it also permits the treatment of systems that are essentially Hamiltonian in nature but cannot be cast into canonical form. Certain systems of an odd number of variables may be dealt with in this way; an example is a spin in a magnetic field, which we consider in Section 3. Even when the system of interest is a canonical Hamiltonian system or can be reduced to one by a transformation of variables, the more general formulation has the advantage of greater compactness and transparency. It is therefore more convenient for many purposes, as the present development illustrates.

The general development summarized above is presented in Section 2. Its application to particular systems of interest is illustrated in Section 3, where thermodynamically consistent stochastic equations are obtained for a mechanical oscillator with fluctuating frequency, a classical spin in a fluctuating magnetic field, and a rigid rotor undergoing Brownian motion.

2. GENERAL FORMULATION

We consider an arbitrary Hamiltonian system of the general form[6]

$$\dot{\mathbf{x}} = \mathbf{A}(\mathbf{x}) \cdot \nabla H \tag{1}$$

where $\mathbf{x} = (x_1, x_2,..., x_n)$ is the phase point, $H(\mathbf{x})$ is the Hamiltonian function, $\nabla = \partial/\partial\mathbf{x}$, and $\mathbf{A}(\mathbf{x})$ is an antisymmetric matrix satisfying the condition

$$\nabla \cdot \mathbf{A} = 0 \tag{2}$$

The antisymmetry of $\mathbf{A}$ implies at once that H is a constant of the motion. Equation (2), together with the antisymmetry of $\mathbf{A}$, implies that $\nabla \cdot (\mathbf{A} \cdot \nabla H) = 0$, so that Eq. (1) generates an incompressible or volume-preserving flow in the phase space. Canonical Hamiltonian dynamics is a special case of the above in which n is even, $\mathbf{x} = (q_1, p_1, q_2, p_2,...)$, and $\mathbf{A}$ is the constant matrix whose only nonzero elements are $A_{k,k+1} = -A_{k+1,k} = \frac{1}{2}[1 + (-1)^{k+1}]$.

Equation (1) describes the dynamics of the isolated system. Our objective is to construct a stochastic model of the dynamical behavior when the system is in contact with a heat bath. This will be done by using the augmented Langevin procedure[4] to introduce a multiplicative noise term of the form $\mathbf{G}(\mathbf{x}) \cdot \xi(t)$ into the right member of Eq. (1). Here $\xi(t)$ is an n-dimensional vector whose components are independent zero-mean normalized Gaussian white noises. Thus $\langle \xi(t) \rangle = 0$ and $\langle \xi(t)\, \xi(t+\tau) \rangle = \mathbf{I}\delta(\tau)$, where $\mathbf{I}$ is the unit matrix and the angular brackets denote an appropriately weighted ensemble average over all possible realizations of $\xi(t)$. The appropriate form of $\mathbf{G}(\mathbf{x})$ in any particular situation is to be inferred from the assumed mechanism by which the system and bath are coupled. That is to say, $\mathbf{G}(\mathbf{x})$ is to be chosen by considering the physical origin of the noise. Although it is not explicitly indicated by the notation, $\mathbf{G}$ will in general depend on the bath temperature T as well as on $\mathbf{x}$.

According to the augmented Langevin procedure, the introduction of the noise term must be accompanied by the introduction of a correction term $\mathbf{F}(\mathbf{x})$ which vanishes in the limit of zero fluctuations.[4] The correction term is needed to allow for and resolve the inherent phenomenological uncertainty in the application of the conventional Langevin approach to nonlinear problems.[5] The augmented Langevin equation corresponding to Eq. (1) is therefore

$$\dot{\mathbf{x}} = \mathbf{A} \cdot \nabla H + \mathbf{F}(\mathbf{x}) + \mathbf{G}(\mathbf{x}) \cdot \xi(t) \tag{3}$$

which we shall interpret as a Stratonovich equation.[5] We emphasize that this interpretation is a matter of convenience rather than necessity; adoption of the Itô rule (or some other stochastic interpretation rule) would lead to equivalent results.[4]

The augmented Langevin equation (3) is equivalent to the Fokker–Planck equation[4]

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{A} \cdot \nabla H) + \nabla \cdot (\rho \mathbf{V}) = \frac{1}{2} \nabla \cdot (\mathbf{\Gamma} \cdot \nabla \rho) \tag{4}$$

where $\mathbf{\Gamma}(\mathbf{x}) = \mathbf{G}(\mathbf{x}) \cdot \mathbf{G}^T(\mathbf{x})$ (superscript T denotes the transpose), and

$$\mathbf{V}(\mathbf{x}) = \mathbf{F}(\mathbf{x}) - \frac{1}{2} \mathbf{G}(\mathbf{x}) \cdot [\nabla \cdot \mathbf{G}(\mathbf{x})] \tag{5}$$

To ensure that the system approaches a canonical equilibrium distribution at long times, we require that

$$w(\mathbf{x}) = w_0 \exp[-H(\mathbf{x})/kT] \tag{6}$$

be a stationary solution of Eq. (4), where T is the bath temperature and w_0 is a constant determined by the normalization condition $\int d\mathbf{x}\, w(\mathbf{x}) = 1$. By writing the equilibrium distribution in this form, where H is the Hamiltonian of the isolated system, we effectively restrict attention to situations in which the system is weakly coupled to the heat bath. Otherwise $w(\mathbf{x})$ may involve a modified Hamiltonian[7,8] instead of H, and the present phenomenological approach is unable to determine the form of such modifications.

In writing Eq. (6), we have also tacitly assumed that the variables $\mathbf{x}$ are a "natural representation" of the state of the system.[9] Otherwise, a factor of $g^{-1/2}(\mathbf{x})$ would appear in the right member of Eq. (6), where g is the determinant of a metric tensor in state space.[4,9] At the same time, the incompressibility condition of Eq. (2) would have to be replaced by its covariant analog, namely $\nabla \cdot (g^{-1/2}\mathbf{A}) = 0$. Thus, the restriction to "natural" representations is not essential and could easily be lifted. However, in the treatment of particular cases a "natural" choice of the variables $\mathbf{x}$ is usually fairly obvious, so we have streamlined the presentation by restricting attention to this case. Of course, if the variables $\mathbf{x}$ are simply canonical coordinates and momenta, then they automatically constitute a "natural" representation, since Eqs. (2) and (6) then directly apply.

We remark parenthetically that the incompressibility condition of Eq. (2) (or its covariant analog) is not itself mathematically necessary, although it does significantly simplify the development. This condition has been adopted because Hamiltonian systems of physical origin seem invariably to satisfy it. Of course, there are other properties that are commonly associated with Hamiltonian behavior,[10] but they do not interact with the present development, so we need not assume them. Of these, the most fundamental and important is that the generalized Poisson bracket defined by $\{\alpha, \beta\} = (\nabla\alpha) \cdot \mathbf{A} \cdot (\nabla\beta)$ satisfy the Jacobi identity. If in addition the matrix $\mathbf{A}$ is nonsingular (which requires that the number of variables n be even), Darboux' theorem guarantees that the system can be reduced to canonical form by a transformation of variables,[10] and this in turn implies incompressibility of the phase flow. In the present context, however, the incompressibility condition itself is the relevant property, and this condition is satisfied for a wider class of systems than are encompassed by Darboux' theorem. In particular, it can be satisfied for systems of an odd number of variables, as illustrated in Section 3.2.

We now return to the main development. The requirement that the canonical distribution $w(\mathbf{x})$ of Eq. (6) be a stationary solution of Eq. (4) will be met by imposing the potential conditions

$$\nabla \cdot (w\mathbf{A} \cdot \nabla H) + \nabla \cdot (w\mathbf{V}_R) = 0 \tag{7}$$

$$w\mathbf{V}_I = \tfrac{1}{2}\mathbf{\Gamma} \cdot \nabla w \tag{8}$$

where $\mathbf{V}_R + \mathbf{V}_I = \mathbf{V}$. These conditions are equivalent to detailed balance, and must therefore be satisfied in a true thermodynamic equilibrium.[4] By virtue of Eq. (2), the term $\nabla \cdot (w\mathbf{A} \cdot \nabla H)$ in Eq. (7) is identically zero, so that Eq. (7) reduces simply to $\nabla \cdot (w\mathbf{V}_R) = 0$. This is the simplification that results from adoption of the incompressibility condition.

The quantities $\mathbf{V}_R$ and $\mathbf{V}_I$ respectively represent reversible and irreversible fluctuation-induced modifications to the dynamics of the isolated system. The irreversible term $\mathbf{V}_I$ is uniquely determined by Eq. (8), whereas the condition $\nabla \cdot (w\mathbf{V}_R) = 0$ constrains $\mathbf{V}_R$ but does not determine it uniquely. A thermodynamically consistent stochastic model results from any choice of $\mathbf{V}_R$ that satisfies this constraint and vanishes properly in the limit of zero fluctuations.

Of course, $\mathbf{V}_R$ is in principle determined by the nature of the heat bath and the detailed microscopic form of the system–bath coupling. (In particular, $\mathbf{V}_R$ may itself be Hamiltonian in form, thereby effectively modifying H[7,8] and/or $\mathbf{A}$, or it may have a more general form.) These microscopic details cannot be accommodated in the present phenomenological approach, and if they are important to the behavior of interest, this approach is not likely to be useful. The present procedure is therefore effectively limited to cases in which the features of interest are relatively insensitive to the choice of $\mathbf{V}_R$. It is then permissible to adopt the simplest thermodynamically consistent choice, and in the present formulation this is clearly $\mathbf{V}_R = 0$. With this choice Eq. (7) is trivially satisfied and $\mathbf{V} = \mathbf{V}_I$ becomes purely irreversible in nature.

The assumed insensitivity to $\mathbf{V}_R$ may be expected to be quite common in the weakly coupled systems to which our attention is restricted. The weak system–bath coupling implies that $\mathbf{V}_R$ represents a small correction to the dominant reversible dynamics of the isolated system. In contrast, the dissipative term $\mathbf{V}_I$ is *not* a small correction to the dissipative dynamics; it is in fact the *entire* dissipative contribution, since there is no dissipation in the isolated system. The dissipative term is needed to balance the effects of the noise, as shown by Eq. (8). Thus, although we have in effect simply neglected $\mathbf{V}_R$, in doing so we have nevertheless retained the lowest order nonvanishing contributions of both reversible and irreversible character, and in this sense the formulation is consistent.

Equation (8) may be directly solved for $\mathbf{V}_I = \mathbf{V}$, and we thereby obtain

$$\mathbf{V} = -\frac{1}{2kT} \mathbf{\Gamma} \cdot \nabla H \tag{9}$$

where use has been made of Eq. (6). Combining Eqs. (3), (5), and (9), we obtain

$$\dot{\mathbf{x}} = \mathbf{A} \cdot \nabla H - \frac{1}{2kT} \mathbf{\Gamma} \cdot \nabla H + \frac{1}{2} \mathbf{G} \cdot (\nabla \cdot \mathbf{G}) + \mathbf{G} \cdot \xi(t) \tag{10}$$

which is the appropriate augmented Langevin equation for a Hamiltonian system of the form of Eq. (1) in contact with a heat bath at temperature T, the dynamical effect of the bath being modeled by the multiplicative noise term $\mathbf{G} \cdot \xi(t)$. We remind the reader that Eq. (10) is a Stratonovich equation. The equivalent Fokker–Planck equation, obtained by combining Eqs. (4) and (9), is

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{A} \cdot \nabla H) - \frac{1}{2kT} \nabla \cdot (\rho \mathbf{\Gamma} \cdot \nabla H) = \frac{1}{2} \nabla \cdot (\mathbf{\Gamma} \cdot \nabla \rho) \tag{11}$$

The term $-(2kT)^{-1} \mathbf{\Gamma} \cdot \nabla H$ in Eq. (10) is simply the dissipative term required to balance the effect of the noise. This term is of the form $\mathbf{D} \cdot \nabla H$, where $\mathbf{D} = -(2kT)^{-1} \mathbf{\Gamma} = -(2kT)^{-1} \mathbf{G} \cdot \mathbf{G}^T$ is symmetric and negative definite. It follows that the dissipative term makes a negative contribution to $\dot{H}$, so it does indeed dissipate energy as the terminology implies. The dissipative term is usually nonlinear for multiplicative noise because of the $\mathbf{x}$ dependence contained in $\mathbf{G}$ and therefore in $\mathbf{D}$. The above relation between the dissipative matrix $\mathbf{D}$ and the noise coefficient matrix $\mathbf{G}$ is the general nonlinear fluctuation-dissipation relation referred to in Section 1. It should be noted that this relation is unaffected by the choice of $\mathbf{V}_R$.

The term $\frac{1}{2}\mathbf{G} \cdot (\nabla \cdot \mathbf{G})$ in Eq. (10) does not appear to possess any simple physical interpretation, which is perhaps just as well in view of the fact that its form depends on the choice of a stochastic interpretation rule. In particular, use of the Itô rule would have led to the Itô equation equivalent to Eqs. (10) and (11), in which $\frac{1}{2}\nabla \cdot \mathbf{\Gamma}$ appears instead of $\frac{1}{2}\mathbf{G} \cdot (\nabla \cdot \mathbf{G})$. Fortunately, however, our adoption of the Stratonovich rule has the beneficial side effect that the term in question vanishes identically in the case of greatest interest, namely when the noise term $\mathbf{G} \cdot \xi(t)$ is itself of a Hamiltonian nature. In this case $\mathbf{G} \cdot \xi(t)$ must be of the form $\mathbf{A} \cdot \nabla H'$, where $H'(\mathbf{x}, t)$ is a stochastic Hamiltonian. But $\nabla \cdot (\mathbf{A} \cdot \nabla H') = 0$ by virtue of Eq. (2), so $\nabla \cdot \mathbf{G}$ must vanish as well. The augmented Langevin equation (10) then assumes the simple and intuitive form

$$\dot{\mathbf{x}} = \mathbf{A} \cdot \nabla H - \frac{1}{2kT} \mathbf{\Gamma} \cdot \nabla H + \mathbf{G} \cdot \xi(t) \tag{12}$$

A sufficient condition for the noise to be Hamiltonian is that a composite Hamiltonian system be obtained when the system of interest is combined with the heat bath. Of course, this is ordinarily true by construction for the microscopic system–bath models.[3] Even when the noise is not Hamiltonian and $\nabla \cdot \mathbf{G} \neq 0$, it may be possible to find a different but stochastically equivalent $\mathbf{G}$ with vanishing divergence. [Since $\mathbf{G}$ enters into the Fokker–Planck equation (11) only through $\mathbf{\Gamma} = \mathbf{G} \cdot \mathbf{G}^T$, two noise coefficient matrices $\mathbf{G}_1$ and $\mathbf{G}_2$ are stochastically equivalent if $\mathbf{G}_1 \cdot \mathbf{G}_1^T = \mathbf{G}_2 \cdot \mathbf{G}_2^T$.] Indeed, one expects on general grounds that an equivalent divergenceless $\mathbf{G}$ can ordinarily be found in systems of three or more variables.[11]

There is a close connection between the present general formulation and the phenomenological equations for "mixed canonical and dissipative dynamics" in the presence of noise, which have been used by Enz to discuss critical dynamics.[12] Since Enz implicitly adopts the Itô rule, the connection is most easily established via the Fokker–Planck equation. To this end, we rewrite the Fokker–Planck equation (11) of the present development in the equivalent form

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{A} \cdot \nabla H) - \frac{1}{2} \nabla \cdot [\rho(\mathbf{\Gamma} \cdot \nabla H - \nabla \cdot \mathbf{\Gamma})] = \frac{1}{2} \nabla\nabla : (\rho \mathbf{\Gamma}) \tag{13}$$

where we have temporarily switched to units in which $kT = 1$ in accordance with the convention used by Enz. The corresponding Fokker–Planck equation in the Enz theory is obtained by combining his Eqs. (4.1), (4.2), and (4.26), and imposing the incompressibility condition of our Eq. (2). When allowance is made for the differences in notation, the result is precisely Eq. (13). It follows that the general nonlinear fluctuation-dissipation relation of the present development is equivalent to the "generalized Einstein relations" of the Enz theory.[12] In the applications considered by Enz, however, much of the generality is discarded by restricting attention to additive noise, for which $\mathbf{G}$ is independent of $\mathbf{x}$ and the fluctuation-dissipation relation becomes linear. In contrast, our interest here centers specifically on the fact that the general fluctuation-dissipation relation is fully nonlinear and may therefore be used to treat multiplicative noise and nonlinear dissipation. It is also noteworthy that in the present development, the $\nabla \cdot \mathbf{\Gamma}$ term in the left member of Eq. (13) arises automatically, along with the dissipation term $\mathbf{\Gamma} \cdot \nabla H$, as a consequence of the augmented Langevin correction term $\mathbf{F}$.

3. EXAMPLES

3.1. Mechanical Oscillator with Fluctuating Frequency

Consider a one-dimensional harmonic oscillator described by the equations

$$\dot{x} = v \tag{14}$$

$$\dot{v} = -\omega_0^2 x \tag{15}$$

where x is the position, v is the velocity, and ω_0 is the natural frequency. This system may be written in the Hamiltonian form of Eq. (1) by letting $\mathbf{x} = (x, v)$, $H = \frac{1}{2}(v^2 + \omega_0^2 x^2)$, and

$$\mathbf{A} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{16}$$

Since $\mathbf{A}$ is independent of $\mathbf{x}$ here, Eq. (2) is trivially satisfied.

Now if the oscillator frequency is random, the restoring force becomes $-\omega^2(t)\, x$ instead of $-\omega_0^2 x$. We shall suppose that $\omega^2(t) = \omega_0^2 + \gamma\xi(t)$, where $\xi(t)$ is zero-mean normalized Gaussian white noise. Of course, the frequency modulation has no effect on the kinematic equation (14). Thus the noise term we wish to introduce into $\dot{\mathbf{x}}$ is simply $(0, -\gamma x \xi(t))$. This is of the form $\mathbf{G}(\mathbf{x}) \cdot \boldsymbol{\xi}(t)$ if we take

$$\mathbf{G} = \begin{pmatrix} 0 & 0 \\ 0 & -\gamma x \end{pmatrix} \tag{17}$$

Here the noise term is also of Hamiltonian form, with the stochastic Hamiltonian given by $H' = \frac{1}{2}\gamma x^2 \xi(t)$, so $\nabla \cdot \mathbf{G}$ must be zero. This is easily verified by direct calculation from Eq. (17). It follows from Eq. (17) that

$$\mathbf{\Gamma} = \begin{pmatrix} 0 & 0 \\ 0 & \gamma^2 x^2 \end{pmatrix} \tag{18}$$

so that $\mathbf{\Gamma} \cdot \nabla H = \mathbf{\Gamma} \cdot (\omega_0^2 x, v) = (0, \gamma^2 x^2 v)$. The augmented Langevin equation (12) for this example, in component form, is therefore given by

$$\dot{x} = v \tag{19}$$

$$\dot{v} = -\omega_0^2 x - \frac{\gamma^2}{2kT} x^2 v - \gamma x \xi(t) \tag{20}$$

in which the noteworthy feature is the cubic damping term. This result is in precise agreement with that of a microscopic system–bath model analysis by Lindenberg and Seshadri.[13]

3.2. Classical Spin in a Fluctuating Magnetic Field

Consider next a classical spin of magnetic moment $\mathbf{M}$ in an external magnetic field $\mathbf{H}_0$. The equations of motion for the isolated system are

$$\dot{\mathbf{M}} = \gamma \mathbf{M} \times \mathbf{H}_0 \tag{21}$$

where γ is the gyromagnetic ratio. These equations can be written in the Hamiltonian form of Eq. (1) by letting $\mathbf{x} = \mathbf{M} = (M_x, M_y, M_z)$, $H = -\mathbf{M} \cdot \mathbf{H}_0$, and $\mathbf{A} = \gamma \boldsymbol{\epsilon} \cdot \mathbf{M}$, where $\boldsymbol{\epsilon}$ is the Levi-Civita antisymmetric third-order tensor. Here $\mathbf{A}$ is not constant, but one readily verifies that $(\partial/\partial \mathbf{M}) \cdot \mathbf{A} = 0$, so that Eq. (2) is satisfied.

We now wish to introduce into Eq. (21) a noise term corresponding to a fluctuating magnetic field $\mathbf{h}(t)$; i.e., a term of the form $\gamma \mathbf{M} \times \mathbf{h}(t) = -\mathbf{A} \cdot \mathbf{h}(t)$. We shall assume the components of $\mathbf{h}(t)$ to be independent zero-mean Gaussian white noises of identical amplitude, so that $\mathbf{h}(t) = \eta \boldsymbol{\xi}(t)$. The desired noise term then becomes $-\eta \mathbf{A} \cdot \boldsymbol{\xi}(t) = \mathbf{G} \cdot \boldsymbol{\xi}(t)$, where $\mathbf{G} = -\eta \mathbf{A}$. It follows that $\nabla \cdot \mathbf{G} = 0$, as indeed it must since here again the noise is of a Hamiltonian nature. [In this case the stochastic Hamiltonian is just $H' = -\mathbf{M} \cdot \mathbf{h}(t)$.] The dissipative matrix $\mathbf{\Gamma}$ is given by

$$\mathbf{\Gamma} = \eta^2 \mathbf{A} \cdot \mathbf{A}^T = \gamma^2 \eta^2 (|\mathbf{M}|^2 \mathbf{I} - \mathbf{M}\mathbf{M}) \tag{22}$$

Since $\nabla H = -\mathbf{H}_0$, the augmented Langevin equation (12) for this example is therefore

$$\dot{\mathbf{M}} = \gamma \mathbf{M} \times \mathbf{H}_0 - \frac{\gamma^2 \eta^2}{2kT} [(\mathbf{M} \cdot \mathbf{H}_0) \mathbf{M} - |\mathbf{M}|^2 \mathbf{H}_0] + \gamma \eta \mathbf{M} \times \boldsymbol{\xi}(t) \tag{23}$$

in which the noteworthy feature is the quadratic dissipative term. In contrast to the preceding example, the proper form of the nonlinear dissipative term in this case could hardly have been obtained by intuition alone. Equation (23) confirms, in the classical case, the results of a microscopic system–bath model analysis by Seshadri and Lindenberg.[14]

3.3. Brownian Motion of a Rigid Rotor

Our final example concerns the stochastic dynamics of a rigid rotor immersed in a heat bath. The dynamical effect of the bath on the rotor will be modeled as a random torque.

The center of mass of the rotor is held fixed, and the rotor is free to rotate about it. The rotor is taken to be axisymmetric, so its orientation may be specified by a unit vector **R** collinear with the symmetry axis. The problem is further simplified by assuming that the principal moment of inertia for rotation about the symmetry axis is negligible. The other two principal moments of inertia are equal; their common value is taken to be unity.

The equations of motion for the isolated rotor are

$$\dot{\mathbf{R}} = \boldsymbol{\omega} \times \mathbf{R} \tag{24}$$

$$\dot{\boldsymbol{\omega}} = 0 \tag{25}$$

where $\boldsymbol{\omega}$ is the angular velocity of the rotor. These equations can be cast into the Hamiltonian form of Eq. (1) by letting $\mathbf{x} = (\mathbf{R}, \boldsymbol{\omega})$, $H = \frac{1}{2} |\boldsymbol{\omega}|^2$, and

$$\mathsf{A} = \begin{pmatrix} \mathbf{0} & \mathsf{a} \\ \mathsf{a} & \mathbf{0} \end{pmatrix} \tag{26}$$

where $\mathbf{0}$ is the 3×3 zero matrix and a is the antisymmetric 3×3 matrix defined by $\mathsf{a} = \boldsymbol{\epsilon} \cdot \mathbf{R}$. One readily verifies that $\nabla \cdot \mathsf{A} = 0$, so that Eq. (2) is satisfied.

We now wish to introduce a random torque $\mathbf{N}(t)$ into Eq. (25). Since we have neglected the moment of inertia for rotation about the symmetry axis, we must for consistency require that **N** is always normal to **R**. Thus we take $\mathbf{N} = \mathbf{F}(t) \times \mathbf{R}$, where $\mathbf{F}(t)$ is a random force whose components are independent zero-mean Gaussian white noises of equal amplitude λ. An equivalent but more convenient form is $\mathbf{N} = (\boldsymbol{\epsilon} \cdot \mathbf{R}) \cdot \mathbf{F} = \mathsf{a} \cdot \mathbf{F}$. Thus, the noise term we wish to introduce into $\dot{\mathbf{x}}$ is just $(\mathbf{0}, \mathsf{a} \cdot \mathbf{F})$, and this is of the standard form $\mathsf{G}(\mathbf{x}) \cdot \boldsymbol{\xi}(t)$ if we take

$$\mathsf{G} = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \lambda \mathsf{a} \end{pmatrix} \tag{27}$$

One readily verifies that $\nabla \cdot \mathbf{G} = 0$. Once again this reflects an underlying Hamiltonian structure of the noise, with the stochastic Hamiltonian given by $H' = \mathbf{R} \cdot \mathbf{F}$.

It follows from Eq. (27) that the dissipation matrix $\mathbf{\Gamma}$ is given by

$$\mathbf{\Gamma} = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \lambda^2 \mathbf{a} \cdot \mathbf{a}^T \end{pmatrix} \tag{28}$$

and one readily verifies that

$$\mathbf{a} \cdot \mathbf{a}^T = |\mathbf{R}|^2 \mathbf{I} - \mathbf{RR} = \mathbf{I} - \mathbf{RR} \tag{29}$$

where $\mathbf{I}$ is the 3×3 unit matrix. Since $\nabla H = (\mathbf{0}, \boldsymbol{\omega})$, we find that $\mathbf{\Gamma} \cdot \nabla H = (\mathbf{0}, \lambda^2 \mathbf{a} \cdot \mathbf{a}^T \cdot \boldsymbol{\omega})$. The absence of rotation about the symmetry axis implies that $\mathbf{R} \cdot \boldsymbol{\omega} = 0$, so that $\mathbf{a} \cdot \mathbf{a}^T \cdot \boldsymbol{\omega} = \boldsymbol{\omega}$ and $\mathbf{\Gamma} \cdot \nabla H = (\mathbf{0}, \lambda^2 \boldsymbol{\omega})$. The augmented Langevin equations (12) for this example are therefore

$$\dot{\mathbf{R}} = \boldsymbol{\omega} \times \mathbf{R} \tag{30}$$

$$\dot{\boldsymbol{\omega}} = -\frac{\lambda^2}{2kT} \boldsymbol{\omega} + \mathbf{F}(t) \times \mathbf{R} \tag{31}$$

in which the dissipative term is seen to be linear. As usual, this result is in precise agreement with that of a corresponding microscopic system–bath model analysis.[15]

The occurrence of a linear dissipative term may seem curious in view of the multiplicative nature of the noise term $\mathbf{F}(t) \times \mathbf{R}$. In a sense, however, this noise term is not really multiplicative. The vector $\mathbf{R}$ is of unit length, and its presence merely serves to enforce the constraint that the random torque be normal to the rotor axis. If it were convenient to directly generate random torques satisfying this constraint, the noise term would be linear in them. Such subtleties are the price we pay for the convenience of considering $\mathbf{R}$ and $\boldsymbol{\omega}$ as three-dimensional vectors, even though each of them really represents only two degrees of freedom.

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