Properties of the random force in coupled nonlinear Langevin equations

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It is shown that stationarity and causality alone completely determine the second moments of the random forces in a system of coupled nonlinear Langevin equations, and lead to white noise as well as to the appropriate fluctuation dissipation theorems.

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I. INTRODUCTION

In a recent paper [1] with Bedeaux, we discussed the stochastic properties of the random force $f(t)$ in a nonlinear Langevin equation for a stationary random process $\alpha(t)$,

$$\frac{d\alpha(t)}{dt}=-B(\alpha(t))+f(t) . \tag{1.1}$$

The following conditions were assumed to be satisfied.

(i) The random force $f(t)$ is independent of the state $\alpha(t)$ and has zero average.

(ii) The process $\alpha(t)$ is causal in the sense that $\alpha(t)$, or functions thereof, at earlier times t cannot be correlated to the noise $f(t)$ at later times.

(iii) The variable $\alpha(t)$ is either even or odd under time reversal.

It was then shown that (a) it follows from causality that the noise $f(t)$ is white, with

$$\langle f(t)f(t+\tau)\rangle=2\langle \alpha B(\alpha)\rangle\delta(\tau) , \tag{1.2}$$

where $\langle\ \rangle$ denotes a (stationary) ensemble average, and that (b) the noise is Gaussian and white if and only if the function $B(\alpha)$ is related to the stationary (equilibrium) distribution functions $P_0(\alpha)$ by

$$B(\alpha)\sim\frac{d\ \ln P_0(\alpha)}{d\alpha} . \tag{1.3}$$

(c) It follows finally from causality and microscopic reversibility that the noise is necessarily Gaussian so that the possibility to use Eq. (1.1) to describe the dynamical fluctuations of $\alpha(t)$ is restricted to functions $B(\alpha)$ satisfying (1.2), as long as it is required that $f(t)$ be independent of $\alpha(t)$. These rather remarkable results whose proof is somewhat elaborate were obtained for a system described by one variable only.

In this Brief Report we shall show that the result (1.2), which is an expression for the whiteness of the noise and contains a fluctuation-dissipation theorem for the random force in a one-variable nonlinear Langevin equation, not only follows in a simple way from stationarity and causality alone, but can also be generalized to apply to a set of coupled nonlinear Langevin equations. We also show that the requirement that $f(t)$ be independent of $\alpha(t)$, which played a crucial role in our derivation [1], for the one-variable case, of properties (a), (b), and (c), is not essential for obtaining the result (1.2), property (a), and its generalization to the many-variable case.

II. NONLINEAR LANGEVIN EQUATIONS; CAUSALITY

Consider n stationary stochastic processes $\alpha_i(t)$, $i=1,2,\ldots,n$. These processes have a stationary equilibrium distribution function $P_0(\boldsymbol{\alpha})$, where $\boldsymbol{\alpha}$ denotes the n-dimensional vector with components α_i, defined as

$$P_0(\boldsymbol{\alpha})=\langle\delta(\boldsymbol{\alpha}(t)-\boldsymbol{\alpha})\rangle\equiv\left\langle\prod_i\delta(\alpha_i(t)-\alpha_i)\right\rangle . \tag{2.1}$$

$\langle\ \rangle$ denotes a (stationary) ensemble average.

The processes $\alpha_{i(t)}$, which have been chosen, defined in such a way that their average values are zero

$$\langle\boldsymbol{\alpha}(t)\rangle=\int d\boldsymbol{\alpha}\langle\boldsymbol{\alpha}(t)\delta(\boldsymbol{\alpha}(t)-\boldsymbol{\alpha})\rangle=\int d\boldsymbol{\alpha}\,\boldsymbol{\alpha}P_0(\boldsymbol{\alpha})=\mathbf{0} , \tag{2.2}$$

obey the set of coupled stochastic differential equations

$$\frac{d\alpha_i(t)}{dt}=-B_i(\boldsymbol{\alpha}(t))+f_i(t),\quad i=1,\ldots,n , \tag{2.3}$$

where the B_i's are nonlinear functions of the variables $\boldsymbol{\alpha}(t)$ and where the Langevin random forces $f_i(t)$ have, with $\boldsymbol{\alpha}(t=0)=\boldsymbol{\alpha}_0$, conditional mean values zero for positive times

$$\overline{f_i(t)}^{\alpha_0}=\frac{\langle\delta(\boldsymbol{\alpha}(0)-\boldsymbol{\alpha}_0)f_i(t)\rangle}{\langle\delta(\boldsymbol{\alpha}(0)-\boldsymbol{\alpha}_0)\rangle}=0,\quad t>0,\quad i=1,\ldots,n . \tag{2.4}$$

Condition (24) automatically implies that

$$\langle f_i(t)\rangle=0 . \tag{2.5}$$

The converse is, however, not necessarily true. But if causality holds in the sense that, for $t>0$,

$$\langle\delta(\boldsymbol{\alpha}(0)-\boldsymbol{\alpha})f_i(t)\rangle=\langle\delta(\boldsymbol{\alpha}(0)-\boldsymbol{\alpha})\rangle\langle f_i(t)\rangle , \tag{2.6}$$

that is, in the sense that a function of $\boldsymbol{\alpha}$ at a given time t cannot be correlated to the noise, $f_i(t)$, $i=1,2,\ldots,n$ at a later time, then (2.5) implies (2.4): condition (2.4) can therefore be viewed, given (2.5), as a trivial form of the causality requirement. It should be noted that condition

(2.4) is the basic assumption, made by Uhlenbeck and Ornstein [2] concerning the Langevin random force in their theory of Brownian motion. They then supplement, as is usual [3], this first assumption by further assumptions concerning all moments of the random force, thus completely specifying its stochastic properties in order to solve the Brownian motion problem described by the (linear) Langevin equation.

We shall explicitly show in Secs. III and IV that stationarity and the trivial, because almost self-evident, causality requirement (2.4) are sufficient to completely determine the covariances of $f_i(t)$, not only for the linear, but also for a nonlinear set of Langevin equations. Before discussing in the next section the stationarity properties of relevant correlation functions we wish to make one further remark: we note that relation (2.5) describes, without loss of generality, a property of $f_i(t)$. Indeed, if the average of $f_i(t)$ were a constant, this constant could always be subtracted from $f_i(t)$ and thus $f_i(t)$ be redefined to satisfy (2.5) by simultaneously redefining $B_i(\boldsymbol{\alpha})$. However, if (2.5) holds, this also implies that the average of $B_i(\alpha)$ vanishes, since the average of the left-hand side of Eq. (2.3) vanishes due to stationarity.

III. RELEVANT CORRELATION FUNCTIONS AND STATIONARITY

For our analysis of the second moments of the Langevin random forces $f_i(t)$, we consider the following time correlation functions:

$$R_{ij}^{\alpha\alpha}(\tau)\equiv\langle \alpha_i(t)\alpha_j(t+\tau)\rangle \ , \qquad (3.1)$$

$$R_{ij}^{\alpha\mathrm{B}}(\tau)\equiv\langle \alpha_i(t)B_j(\boldsymbol{\alpha}(t+\tau))\rangle \ , \qquad (3.2)$$

$$R_{ij}^{\mathrm{B}\alpha}(\tau)\equiv\langle B_i(\boldsymbol{\alpha}(t))\alpha_j(t+\tau)\rangle \ , \qquad (3.3)$$

$$R_{ij}^{\mathrm{BB}}(\tau)\equiv\langle B_i(\boldsymbol{\alpha}(t))B_j(\boldsymbol{\alpha}(t+\tau))\rangle \ . \qquad (3.4)$$

Due to stationarity, i.e., invariance for translation in time, these functions depend only on τ and have the properties (replace t by $t-\tau$)

$$R_{ij}^{\alpha\alpha}(\tau)=R_{ji}^{\alpha\alpha}(-\tau) \ , \qquad (3.5)$$

$$R_{ij}^{\alpha\mathrm{B}}(\tau)=R_{ji}^{\mathrm{B}\alpha}(-\tau) \ , \qquad (3.6)$$

$$R_{ij}^{\mathrm{BB}}(\tau)=R_{ji}^{\mathrm{BB}}(-\tau) \ . \qquad (3.7)$$

Stationarity furthermore also implies that $[dg(t)/dt=\dot{g}(t)]$

$$\langle \dot{\alpha}_i(t)\dot{\alpha}_j(t+\tau)\rangle=-\ddot{R}_{ij}^{\alpha\alpha}(\tau) \ , \qquad (3.8)$$

$$\langle \dot{\alpha}_i(t)B_j(t+\tau)\rangle=-\dot{R}_{ij}^{\alpha\mathrm{B}}(\tau) \ . \qquad (3.9)$$

Using the stochastic differential equations (1.3), as well as the last two relations, one may express the time correlation functions (second moments) of the random forces in terms of the correlation functions defined above [cf. (3.1)–(3.4)] and their time derivatives

$$\langle f_j(t)f_i(t+\tau)\rangle=-\ddot{R}_{ji}^{\alpha\alpha}(\tau)+\dot{R}_{ji}^{\mathrm{B}\alpha}(\tau)-\dot{R}_{ji}^{\alpha\mathrm{B}}(\tau)+R_{ji}^{\mathrm{BB}}(\tau) \ . \qquad (3.10)$$

In the special case of a one-variable linear system $[B(\alpha)=M\alpha,\ M$ constant], the corresponding equation takes the form

$$\langle f(t)f(t+\tau)\rangle=-\ddot{R}^{\alpha\alpha}(\tau)+M^2R^{\alpha\alpha}(\tau) \ . \qquad (3.11)$$

Equation (3.10) will enable us to derive a simple expression for the second moments of the processes $f_i(t)$.

IV. RANDOM-FORCE SECOND MOMENTS AND FLUCTUATION-DISSIPATION THEOREM

Let us as a first step in this derivation multiply both members of the Langevin equation (2.3) for $t=\tau$ by $\alpha_j(0)$ and then average. Using condition (2.4), that is the causality requirement in its simplest most obvious form, we then obtain, with the definitions (3.1) and (3.2) for positive time, the following relation between correlation functions:

$$\dot{R}_{ji}^{\alpha\alpha}(\tau)=-R_{ji}^{\alpha\mathrm{B}}(\tau), \quad \tau>0 \ . \qquad (4.1)$$

Similarly multiplying Eq. (2.3) by $B_j(\boldsymbol{\alpha}(0))$ one obtains, with Eqs. (3.3) and (3.4), the relation

$$\dot{R}_{ji}^{\mathrm{B}\alpha}(\tau)=-R_{ji}^{\mathrm{BB}}(\tau), \quad \tau>0 \ . \qquad (4.2)$$

Both relations may be extended with the stationary conditions (3.5)–(3.7) to hold for all times. Thus, relation (4.1) becomes for positive and negative τ,

$$\frac{d\,R_{ji}^{\alpha\alpha}(\tau)}{d\tau}+U(\tau)R_{ji}^{\alpha\mathrm{B}}(\tau)-U(-\tau)R_{ij}^{\alpha\mathrm{B}}(-\tau)=0 \ , \quad i,j=1,2,\ldots,n \ . \qquad (4.3)$$

Here $U(\tau)$ is the Heaviside function defined as

$$U(\tau)=\begin{cases}0 & \text{for } \tau<0\\ 1 & \text{for } \tau>0 \ .\end{cases} \qquad (4.4)$$

One easily convinces oneself, using condition (3.5), that the set of equations (4.3) is invariant under the transformation $\tau\rightarrow-\tau$.

In the same way relations (4.2) $i,j=1,2,\ldots,n$, become for positive and negative τ,

$$U(\tau)\frac{d\,R_{ji}^{\mathrm{B}\alpha}(\tau)}{d\tau}-U(-\tau)\frac{d\,R_{ij}^{\mathrm{B}\alpha}(-\tau)}{d\tau}+R_{ji}^{\mathrm{BB}}(\tau)=0 \ . \qquad (4.5)$$

For the one-variable linear case, $B(\alpha)=M\alpha$, both relations (4.3) and (4.5) reduce to the simple differential equation for $R^{\alpha\alpha}(\tau)$

$$\frac{d\,R^{\alpha\alpha}(\tau)}{d\tau}=S(\tau)MR^{\alpha\alpha}(\tau) \ , \qquad (4.6)$$

where $S(\tau)\equiv U(\tau)-U(-\tau)$, $S^2(\tau)=1$. For use below note also that $U(\tau)+U(-\tau)=1$ and that $\dot{U}(\tau)=\delta(\tau)$.

We proceed now by taking the time derivative of Eq. (4.3) and by subtracting the resulting equation from Eq. (4.5). Using also relation (3.6), one thus gets

$$-\ddot{R}_{ji}^{\alpha\alpha}(\tau)+\dot{R}_{ji}^{B\alpha}(\tau)-\dot{R}_{ji}^{\alpha B}(\tau)+R_{ji}^{BB}(\tau)$$
$$=\{\langle\alpha_j B_i(\boldsymbol{\alpha})\rangle+\langle\alpha_i B_j(\boldsymbol{\alpha})\rangle\}\delta(\tau)\ , \quad (4.7)$$

since $R_{ij}^{\alpha B}(\tau=0)=\langle\alpha_i B_j(\boldsymbol{\alpha})\rangle$, etc.

If we then substitute this equation into Eq. (3.10) we obtain for the second moments of the random force $f_i(t)$,

$$\langle f_j(t)f_i(t+\tau)\rangle=\{\langle\alpha_j B_i(\boldsymbol{\alpha})\rangle+\langle\alpha_i B_j(\boldsymbol{\alpha})\rangle\}\delta(\tau)\ , \quad (4.8)$$

and this result follows therefore from the obvious condition (1.4) (causality requirement), which is a condition for the conditional first moment of $f_i(t)$, *and from stationarity alone.* Equation (4.8) represents a generalized fluctuation-dissipation theorem for the random forces $f_i(t)$. In the linear case,

$$B_i(\boldsymbol{\alpha})=\sum_k M_{ik}\alpha_k\ , \quad (4.9)$$

Eq. (4.8) takes the usual form

$$\langle f_j(t)f_i(t+\tau)\rangle=(L_{ij}+L_{ji})\delta(\tau)\ , \quad (4.10)$$

where the Onsager coefficients L_{ij}, defined as

$$L_{ij}=\sum_k M_{ik}\langle\alpha_k\alpha_j\rangle\ , \quad (4.11)$$

characterize the system's entropy production.

V. DISCUSSION AND CONCLUSION

It has been argued above that for a system described by a set of variables obeying coupled nonlinear Langevin equations, the second moments of the random forces can be determined in a simple way and need not be postulated independently. It is in fact shown that stationarity and causality lead to white (δ correlated in time) noise and to the appropriate fluctuation-dissipation theorems. The above proof generalizes to more than one variable, but for the second moments alone, the more elaborate derivation previously given, for one variable only, but yielding expressions for all moments, or cumulants, of the random force.

It should perhaps be stressed at this point that there is of course no fundamental, nontrivial difference between the multivariable and the single-variable case: only technical, notational difficulties have prevented us from generalizing to more than one variable the proof for *all* the results stated in the Introduction and given in [1]. It is, however, quite easy to guess what the corresponding analogous results would be.

Now a crucial element of the more complete (one-variable) analysis was the requirement that the Langevin random force be independent of the fluctuating variable itself. Stationarity, causality, and microscopic reversibility then lead to Gaussian white noise and moreover the restriction that $B(\alpha)$ must be of the form

$$B(\alpha)=-\gamma\frac{d\ln P_0(\alpha)}{d\alpha}\ , \quad (5.1)$$

where γ is constant.

On the other hand, the requirement that $f_i(t)$ be independent of $\boldsymbol{\alpha}(t)$ has not explicitly played a role in the simple derivation of an expression for the second moments of the random forces. For this derivation to go through it is sufficient that condition (2.4) holds. It was shown that (2.4) is valid in particular if causality holds in the form (2.6), which indeed would imply that $f_i(t)$ is independent of $\boldsymbol{\alpha}$.

But suppose that, e.g., in the one-variable case, which we consider here solely for brevity's sake,

$$B(\alpha)=M(\alpha)\alpha\ , \quad (5.2)$$

with $M(\alpha)=M(-\alpha)$ an α-dependent kinetic coefficient, and $P_0(\alpha)$ a Gaussian function. For Brownian motion this corresponds to the situation of a momentum-dependent friction coefficient. Then $B(\alpha)$, which has an average value zero, is not of the form (5.1), so that according to the theorem referred to above and in the Introduction, $f(t)$ *cannot* be independent of $\alpha(t)$. (It is assumed that the variables α considered are either even or odd under time reversal.)

Suppose then that $f(t)$ is of the form

$$f(t)=\sqrt{C(\alpha(t-\epsilon))}\tilde{f}(t)\ , \quad (5.3)$$

where $C(\alpha)$ is an undetermined function of α, ϵ an infinitesimally small positive quantity, and where we now take $\tilde{f}(t)$ to be independent of $\alpha(t)$. [It should be noted that Eq. (5.3) then corresponds to Ito's choice of interpretation [3,4] for the product $C^{1/2}(\alpha(t))\tilde{f}(t)$.] Causality now implies that

$$\langle f(t)\rangle=\langle C^{1/2}(\alpha)\rangle\langle\tilde{f}(t)\rangle=0 \quad (5.4)$$

and therefore also that for $t>0$,

$$\bar{f}^{\,\alpha_0}(t)=P_0^{-1}(\alpha)\langle\delta(\alpha(0)-\alpha_0)\sqrt{C(\alpha(t-\epsilon))}\rangle\langle\tilde{f}(t)\rangle$$
$$=0\ , \quad (5.5)$$

or, in other words, that condition (2.4) holds. Consequently, one finds according to Eq. (4.8),

$$\langle f(t)f(t+\tau)\rangle=2\langle\alpha^2 M(\alpha)\rangle\delta(\tau)\ , \quad (5.6)$$

and using Eq. (5.3) and once more causality,

$$\langle\tilde{f}(t)\tilde{f}(t+\tau)\rangle=2\langle C(\alpha)\rangle^{-1}\langle\alpha^2 M(\alpha)\rangle\delta(\tau)\ . \quad (5.7)$$

A plausible choice for $C(\alpha)$ would seem

$$C(\alpha)=M(\alpha)\ . \quad (5.8)$$

When M is a constant, the random force $f(t)$ is then automatically independent of $\alpha(t)$, as it should be, while the autocorrelation function of $\tilde{f}(t)$ becomes independent of M.

It remains of course an open question whether the assumed form (5.3) with (5.8) for $f(t)$ is correct and what the complete stochastic properties of $\tilde{f}(t)$ then are. Nevertheless, the discussion given illustrates the fact that the result (4.8) for the second moments of the random force can be obtained *without* imposing the restrictive condition on the random forces that they may not depend on the fluctuating variables obeying the coupled nonlinear Langevin equations.

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