Colored Noise and Bistable Fokker-Planck Equations

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The detailed dependence of the smallest nonzero eigenvalue of a bistable periodic Fokker-Planck equation on the external-noise correlation time is determined for the first time numerically to tie down contrasting theoretical predictions. The isospectrality with the Fokker-Planck equation for the metastable system defined by inversion of the bistable potential is proved analytically. This amounts to a generalized supersymmetric transformation between the corresponding non-Hermitean Hamiltonian operators.

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The motivation of the present Letter is twofold. Any one-dimensional Fokker-Planck equation (FPE) is isospectral with a suitably defined Schrödinger equation. Changing the sign of the force term leads to a new isospectral FPE, the related Schrödinger equation being the supersymmetric partner of the old one. This property proved useful in the theory of the FPE[1] as well as for application to field theories.[2] At this point the question arises quite naturally as to what extent the above symmetry survives when the diffusion term of the FPE is to describe a time-correlated (colored) noise instead of the usual delta-correlated (white) one. On the other hand, the problem of the mean first-passage time in bistable potentials is a longstanding topic in nonequilibrium statistical mechanics for its potential application in several fields of physics, chemistry, and engineering.[3] A recent passionate debate[3-12] on the validity of some approximate theories envisaged to account for colored noise effects evidentiated the lack of rigorous results for the theoretical predictions to compare with. Up to now the data available are either plagued by too great an inaccuracy, like in the case of the digital simulation of Ref. 5, or forcibly limited to small potential barriers. Both the analog simulation of Refs. 8 and 9 and the numerical solution discussed in Ref. 10 explore the relaxation process of a particular bistable system, namely the quartic double-well potential, for barrier-height to noise-intensity ratios up to one. In the following, we try to shed light on both problems.

The simplest example of the class of stochastic differential equations under study is given by the two-dimensional problem

$$\dot{x} = -f'(x) + \epsilon(t), \quad \dot{\epsilon} = -(1/\tau)\epsilon + (1/\tau)\eta(t), \tag{1}$$

where $f(x)$ is a binding or periodic potential and the prime denotes derivation with respect to x. $\epsilon(t)$ represents a stochastic Gaussian process with finite correlation time τ, i.e., $\langle \epsilon(t)\epsilon(0)\rangle = (D/\tau)\exp(-|t|/\tau)$, driven by the Gaussian external noise $\eta(t)$ with $\langle \eta(t)\rangle = 0$ and $\langle \eta(t)\eta(0)\rangle = 2D\delta(t)$. The corresponding FPE for the probability distribution function $P(x,\epsilon;t)$ reads

$$\frac{\partial}{\partial t}P = L_{\mathrm{FP}}P, \quad L_{\mathrm{FP}} = \frac{\partial}{\partial x}f'(x) - \epsilon\frac{\partial}{\partial x} + L_\epsilon,$$
$$L_\epsilon = \frac{1}{\tau}\frac{\partial}{\partial \epsilon}\left(\epsilon + \frac{D}{\tau}\frac{\partial}{\partial \epsilon}\right). \tag{2}$$

For the single-variable case it is well established that the mean first-passage time[3,13] in bistable potentials is safely identified with the reciprocal of the smallest nonvanishing eigenvalue λ_1 of the FPE for large barrier heights. For our two-variable case such a connection seems also to be plausible. In any case we calculate the smallest nonvanishing eigenvalue λ_1 of (2). It decreases with τ according to the approximate law

$$\lambda_1(\tau) = \lambda_1(0)e^{-\kappa\tau}. \tag{3}$$

Following some calculations based on the τ expansion in Ref. 4, κ would take on a next-to-leading dependence on the noise intensity proportional to D.[5,6] Elsewhere[7-9,11] approximate estimates for κ are determined which exhibit a linear dependence on the reciprocal of D.

In order to sort out this controversy we solved the FPE (2) numerically for a particular choice of the potential,

$$f(x) = -a\cos(x) + b\cos(2x) \tag{4}$$

with $a, b > 0$. The periodicity condition[13]

$$P(x + 2\pi, \epsilon; t) = P(x, \epsilon; t) \tag{5}$$

warrants a good convergence of our numerical algorithm for a wide range of parameter values. Potential (4) combines the advantage of a simple periodic spatial expression (compare with Ref. 10) with the possibility of simulating a bistable binding potential. In Fig. 1, $f(x)$ exhibits its two barriers, a higher one at $x = \pm\pi$ and a lower one at $x = 0$. The barrier heights are $\Delta f(\pi) = 2b + a + a^2/8b$ and $\Delta f(0) = 2b - a + a^2/8b$, respectively. If one chooses a and b so that $\Delta f(\pi) \gg \Delta f(0)$, λ_1 coincides with the mean first-passage time over the barrier at $x = 0$, the escape rate across the boundaries $x = \pm\pi$ being negligible.

In other words, we have a periodic bistable potential.

We outline now the main features of our algorithm —see Ref. 13 for a detailed account. We make the *Ansatz* $P(x,\epsilon;t)=\exp(-\lambda t)P(x,\epsilon)$. The symmetry $L_{\rm FP}(x,\epsilon)=L_{\rm FP}(-x,-\epsilon)$ enables us to separate $P(x,\epsilon)$ into an odd and an even part:

$$P(x,\epsilon)=P_0(x,\epsilon)+P_e(x,\epsilon),$$
$$\begin{pmatrix}P_0(x,\epsilon)\\P_e(x,\epsilon)\end{pmatrix}=\psi_0(\epsilon)\sum_{m,n\geq 0}\left[c^n_{2m}\begin{pmatrix}\sin(nx)\\\cos(nx)\end{pmatrix}\psi_{2m}(\epsilon)+c^n_{2m+1}\begin{pmatrix}\cos(nx)\\\sin(nx)\end{pmatrix}\psi_{2m+1}(\epsilon)\right]. \tag{6}$$

Here $\psi_m(\epsilon)$ are normalized Hermite functions, and $\psi_0(\epsilon)\psi_m(\epsilon)$ are the eigenfunctions of the bath operator $L_\epsilon(2)$ with eigenvalues m/τ. Since only the odd eigenfunctions of the FPE (2) contribute to the escape process, we may leave out $P_e(x,\epsilon)$ in Eq. (6). Substituting Eq. (6) into the FPE and truncating the double sum in $P_0(x,\epsilon)$ at $n=N$ and $m=M$ yields a homogeneous tridiagonal vector recurrence relation[13]

$$\mathbf{Q}^+_m\mathbf{c}_{m+1}+\mathbf{Q}_m\mathbf{c}_m+\mathbf{Q}^-_m\mathbf{c}_{m-1}=0,\quad (\mathbf{Q}^+_m)_{n,n'}=(\mathbf{Q}^-_{m+1})_{n,n'}=[D(m+1)/\tau]^{1/2}n\delta_{n,n'},$$
$$(\mathbf{Q}_m)_{n,n'}=(\lambda-m/\tau)\delta_{n,n'}-\tfrac{1}{2}an\{\delta_{n+1,n'}-\delta_{n-1,n'}\}+bn\{\delta_{n+2,n'}-\delta_{n-2,n'}\}+(-1)^m\delta_{n,1}, \tag{7}$$

and $\mathbf{c}_m=\{c^n_m\}$, with $n,n'=0,1,2,\ldots N$. With the definition of the matrix $\mathbf{K}_m$, $\mathbf{K}_m\mathbf{c}_m=\mathbf{Q}^+_m\mathbf{c}_{m+1}$, Eq. (7) can be cast into the form of a matrix continued fraction (MCF)[13] with the initial condition $\mathbf{K}_M=0$—this corresponds to neglect of $\mathbf{c}_{M+1}$. Computation of λ_1 is reduced to solution of the determinantal equation

$$\det[\mathbf{Q}_0(\lambda)+\mathbf{K}_0(\lambda)]=0. \tag{8}$$

The accuracy of the MCF algorithm has to be tested for a suitable choice of the matrix size N and the iteration number M. In our calculations we used 50×50 matrices and 150 iterations of the MCF. Of course, the present algorithm can be used for determining any eigenvalue of the FPE (2). The corresponding eigenfunction can also be computed by summing up series (6), its coefficients being determined numerically through the recurrence relation (7).[14]

The numerical results for $\lambda_1(\tau)$ are displayed in Fig. 2. In both cases some important features are immediately recognizable: (i) $\lambda_1(\tau)$ decreases almost exponentially with τ for the whole interval of τ explored, in close agreement with formula (3). (ii) The slopes of the curves drawn in Fig. 2 exhibit a strong dependence on D. An increasingly stronger τ dependence shows up for higher potential barriers, i.e., $\Delta f(0)\gg D$, whereas for small potential barriers the curves obtained are almost parallel (therefore, in good agreement with the results of

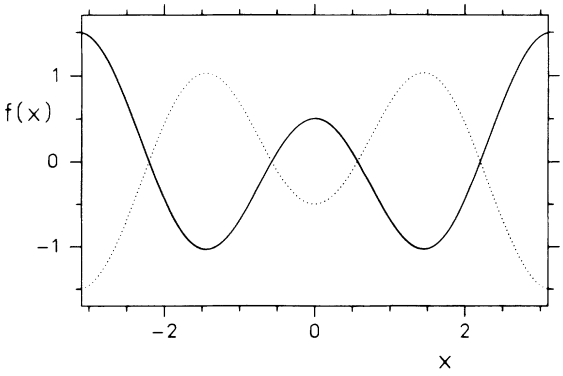

FIG. 1. Solid curve: Bistable periodic potential (4) with $a=0.5$ and $b=1$. Dotted curve: Metastable periodic potential (4) with $a=-0.5$ and $b=-1$.

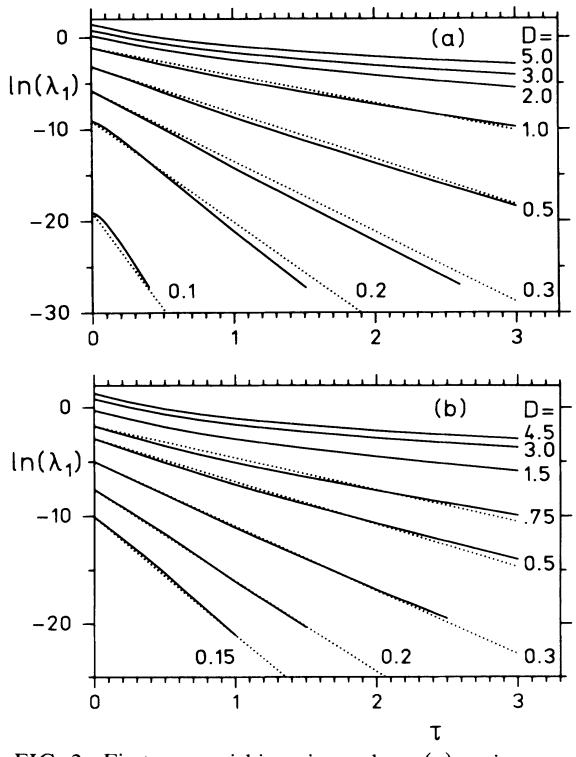

FIG. 2. First nonvanishing eigenvalue: (a) cosine potential, Eq. (4) with $a=0$ and $b=1$, i.e., $\Delta f(0)=\Delta f(\pi)$; (b) bistable periodic potential, Eq. (4) with $a=0.5$ and $b=1$, i.e., $\Delta f(\pi)/\Delta f(0)\approx 1.65$. Solid curves: numerical results; dotted curves: approximated predictions of the decoupling *Ansatz*.

analog simulation[8,9]). (iii) $\lambda_1(0)$ fits very closely the theoretical predictions available in the literature for both $\Delta f(0) \gg D$ (Kramers theory) and $\Delta f(0) \ll D$ (see, e.g, Ref. 13, Chap. 11) provided that the symmetry of the system is taken into account explicitly.[15]

Figure 2 confirms the D dependence of coefficient κ —see Eq. (3)— predicted in Refs. 8–12. We want now to compare our numerical results with a recent determination of κ based on the decoupling *Ansatz*.[8,9] For a binding bistable potential κ is approximated by[12]

$$\kappa = \Delta f(0) f''(x_m)/D + \tfrac{1}{2}\{f''(x_m) + |f''(x_M)|\}, \quad (9)$$

where $\Delta f(0)$ is the barrier height and $\pm x_m$ and x_M denote the position of the minima and the barrier of the potential, respectively. For our potential $f''(x_m) = 4b - a^2/4b$, $|f''(x_M = 0)| = 4b - a$. However, the boundary conditions of the two systems are different: absorbing walls at $x = \pm\infty$ in Ref. 12, periodicity condition (5) for any x in the present analysis. For the sake of comparison $\lambda_1(\tau)$ determined numerically by means of the MCF algorithm has to be related to the smallest nonvanishing eigenvalue obtainable for the same potential but with periodic boundary conditions $P(-\pi, \epsilon; t) = P(\pi, \epsilon; t)$. In view of Floquet's theorem this can be achieved by simply doubling the spatial period of condition (5), 4π instead of 2π. The two problems are equivalent provided that τ is replaced with $\tau/4$ in the initial problem (1), (4), and (5), or equivalently κ with 4κ on the left-hand side of Eq. (9).[14] The comparison of our numerical results with the corresponding predictions based on the decoupling *Ansatz* is illustrated in Fig. 2 and looks very encouraging indeed.

Let us now address the question posed at the very beginning of this Letter. Inverting potential (4), $f(x) \rightarrow -f(x)$ corresponds to studying a *periodic metastable potential* (see Fig. 1). The MCF algorithm applies to the new problem too, with the only difference that $P_e(x, \epsilon)$ in Eq. (6) solely contributes to the calculation of λ_1, while $P_0(x, \epsilon)$ may be released. As a result we found that λ_1 for $f(x)$ and $-f(x)$ coincide for any value of the noise correlation time and potential parameters to within the numerical precision employed. This finding suggests that *the two FPE's are isospectral.*

In fact, this is a rigorous result. FPE (2) is equivalent to the eigenvalue problem

$$-\lambda\phi(x, \epsilon) = L(x, \epsilon)\phi(x, \epsilon), \quad (10)$$

where $L(x, \epsilon) = \phi_0^{-1} L_{\mathrm{FP}} \phi_0$ and $\phi(x, \epsilon) = \phi_0^{-1} P(x, \epsilon)$ with $\phi_0(x) = \exp\{-f(x)/(2D)\}$. $L(x, \epsilon)$ is given a simple expression in terms of creation and annihilation operators,

$$L(x, \epsilon) = -a^\dagger a - (a^\dagger)^2 + a^\dagger \epsilon + L_\epsilon, \quad (11)$$

with

$$a^\dagger = -\sqrt{D}\,\partial/\partial x + f'(x)/2\sqrt{D},$$

$$a = \sqrt{D}\,\partial/\partial x + f'(x)/2\sqrt{D}.$$

In the case of white noise ($\tau = 0$), $L(x, \epsilon)$ would be Hermitean and Eq. (10) a Schrödinger-type equation,[13] whereas $L(x, \epsilon)$ in Eq. (11) is non-Hermitean. Analogously for the inverted potential Eq. (10) must be replaced by

$$-\bar{\lambda}\bar{\phi}(x, \epsilon) = \bar{L}(x, \epsilon)\bar{\phi}(x, \epsilon), \quad (12)$$

$$\bar{L}(x, \epsilon) = -aa^\dagger - a^2 - a\epsilon + L_\epsilon \quad (13)$$

(note that $\bar{a} = -a^\dagger$, $\bar{a}^\dagger = -a$). $\bar{L}(x, \epsilon)$ is easily related to the adjoint of $L(x, \epsilon)$ with respect to the variable x

$$aL^\dagger(x, -\epsilon) = \bar{L}(x, \epsilon)a. \quad (14)$$

Because λ does not depend on the sign of ϵ we have

$$aL^\dagger(x, -\epsilon)\phi^\dagger(x, -\epsilon) = -\lambda a\phi^\dagger(x, -\epsilon)$$

$$= \bar{L}(x, \epsilon)a\phi^\dagger(x, -\epsilon). \quad (15)$$

Comparing Eqs. (12) and (15), we immediately recognize that $L^\dagger$ and $\bar{L}$ are isospectral with eigenfunctions

$$\bar{\phi}(x, \epsilon) = a\phi^\dagger(x, -\epsilon). \quad (16)$$

Equation (16) is valid provided that $a\phi^\dagger$ does not vanish identically. That occurs for $\lambda_0 = 0$. For binding potentials this implies deleting the steady state, whereas for periodic boundary conditions the two steady-state distributions $\phi_0(x, \epsilon)$ and $\bar{\phi}_0(x, \epsilon)$ can be determined numerically as solutions to the homogeneous equations $L\phi = 0$, and $\bar{L}\bar{\phi} = 0$, respectively.[14] The proof above can be extended to any noise statistics represented by a tridiagonal linear thermal bath operator L_ϵ according to Mori's expansion [$(\epsilon = (\epsilon, \epsilon_1, \epsilon_2, \ldots, \epsilon_N)$, N arbitrary, is a vector of auxiliary variables].[14] This proves our statement.

The proof above suggests a simple supersymmetric interpretation. $L_{\mathrm{FP}}(x, \epsilon)$ was associated with a non-Hermitean Hamiltonian operator $L(x, \epsilon)$ which defines two complete sets of orthogonal functions $\{\Phi_n\}$ and $\{\Phi_n^+\}$. Inverting the potential in the FPE left the eigenvalue spectrum unchanged—apart from possibly deleting the zero eigenvalue. This operation corresponds to transforming $L(x, \epsilon)$ according to the generalized supersymmetry description $a \rightarrow -a^\dagger$ and $a^\dagger \rightarrow -a$. The eigenfunctions of the non-Hermitean supersymmetric partner $\bar{L}(x, \epsilon)$ are given by $a\Phi_n^\dagger$. The similarity to ordinary supersymmetry for Hamiltonian operators is evident.[1,2]

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[1]M. Bernstein and L. S. Brown, Phys. Rev. Lett. **52**, 1933 (1984).

[2]C. M. Bender, F. Cooper, and B. Freedman, Nucl. Phys. **B219**, 61 (1983).

[3]For a review see P. Hanggi, J. Stat. Phys. **42**, 105 (1986); T. Fonseca, J. A. N. F. Gomes, P. Grigolini, and F. Marchesoni, Adv. Chem. Phys. **62**, 389 (1985).

[4]J. M. Sancho, M. San Miguel, S. L. Katz, and J. D. Gunton, Phys. Rev. A **26**, 1589 (1982); A. Hernández-Machado, M. San Miguel, and J. M. Sancho, Phys. Rev. A **29**, 3388 (1984).

[5]P. Hanggi, F. Marchesoni, and P. Grigolini. Z. Phys. B **56**, 333 (1984).

[6]K. Lindenberg and B. J. West, Physica (Amsterdam) **119A**, 485 (1983); J. Masoliver, B. J. West, and K. Lindenberg, Phys. Rev. A **35**, 3086 (1987).

[7]R. F. Fox, Phys. Rev. A **33**, 467 (1986); R. F. Fox and R. Roy, Phys. Rev. A **35**, 1838 (1987).

[8]P. Hanggi, T. J. Mroczkowski, F Moss, and P. V. E. McClintock, Phys. Rev. A **32**, 695 (1985).

[9]L. Fronzoni, P. Grigolini, P. Hanggi, F. Moss, R. Mannella, and P. V. E. McClintock, Phys. Rev. A **33**, 3320 (1986).

[10]P. Jung and H. Risken, Z. Phys. B **61**, 367 (1985).

[11]J. M. Sancho, F. Sagues, and M. San Miguel, Phys. Rev. A **33**, 3399 (1986).

[12]F. Marchesoni, Phys. Rev. A (to be published).

[13]H. Risken, *The Fokker-Planck Equation,* Springer Series in Synergetics Vol. 18 (Springer-Verlag, Berlin, 1984).

[14]Th. Leiber, F. Marchesoni, and H. Risken, to be published.

[15]In the case of Fig. 2(a), for instance, $\lambda_1(0)$ is 8 times the Kramers rate of escape out of the corresponding one-side metastable potential well as a result of the symmetry of the potential (4) under parity $x \rightarrow -x$ and its spatial period halving for $a=0$.