Complex conjugate eigenvalues in the spectrum of an operator for resonant activation

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We consider the exit problem for an overdamped Brownian particle in a potential undergoing dichotomic fluctuations. The system exhibits resonant activation. We compute the corresponding exit times distribution and show that the resonance is associated with the presence of a finite number of complex conjugate eigenvalue pairs in the spectrum of the evolution equation. The properties of these eigenvalues and their influence on the exit times distribution and on the possible dynamics of the system are discussed in detail.

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I. INTRODUCTION

The phenomenon of resonant activation has been investigated for a number of different systems [1-15]. For a brief review of the various models we refer the reader to Ref. [15]. The simplest model in which resonant activation occurs is probably represented by overdamped diffusion in a potential undergoing dichotomic Markovian fluctuations [1-4]: The escape rate $\kappa = \kappa(\gamma)$ over the fluctuating barrier exhibits a distinct maximum as a function of the potential fluctuation rate γ , and it has been shown [4] that the escape process may then be approximated by the Markovian kinetic equation in the two limits of slow and fast dichotomic fluctuations, $\gamma \ll \kappa$ and $\gamma \gg \kappa$. The resonance phenomenon in the intermediate fluctuation range, however, is non-Markovian, and its exact nature in the various models still remains unclear, despite attempts to model it using nonexponential distributions of the random exit times [5].

The overdamped diffusion in a fluctuating potential is described by a matrix Smoluchowski equation [1,4], which cannot, as opposed to the ordinary equation for a static potential [16], be recast into a self-adjoint form. Its eigenvalues may therefore be complex. We show here by direct calculation that at resonance the lowest nonvanishing eigenvalue is real, and that it is followed by a *finite* number of complex conjugate eigenvalue pairs. The high-order eigenvalues are again real. The finite train of complex conjugate eigenvalues shifts to the left at $\gamma \gg \kappa$ so that in this case the several lowest eigenvalues become real. By contrast, all eigenvalues are real if $\gamma \ll \kappa$.

II. THE SHOOTING METHOD

Our analysis of the escape problem is based on the shooting method of adjoints [17] whose application to the diffusion problem was described in Ref. [3]. The shooting method allows us to compute the missing boundary value conditions in a well-defined boundary value problem. Briefly stated, the method is as follows: Let the set of functions $y_i(x)$ satisfy the linear differential system

$$y'_{i}(x) = \sum_{j=1}^{n} A_{ij}(x)y_{j}(x) + f_{i}(x)$$
(1)

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together with *r* initial conditions at $x = x_1$ and n - r final conditions at $x = x_2$. The remaining n - r conditions at x_1 and *r* conditions at x_2 then satisfy the identity [17]

$$\sum_{j=1}^{2} (-1)^{j} \vec{y}(x_{j}) \cdot \vec{\xi}^{(m)}(x_{j}) = \int_{x_{1}}^{x_{2}} dx \ \vec{\xi}^{(m)}(x) \cdot \vec{f}(x), \qquad (2)$$

where the functions $\vec{\xi}^{(m)}(x)$, m = 1, 2, ..., n, are solutions of the adjoint equation

$$\frac{d\xi_i^{(m)}(x)}{dx} = -\sum_{j=1}^n A_{ji}(x)\xi_j^{(m)}(x)$$
(3)

on which such *n* initial (resp. final) conditions are imposed that the linear system (3) has a solution for the unknown *n* boundary values at x_1 and x_2 . The boundary value problem for Eq. (1) then becomes a more tractable initial value problem.

III. THE EXIT PROBLEM

We define the evolution equation [4]

$$\frac{\partial}{\partial t} \begin{pmatrix} P_1 \\ P_2 \end{pmatrix} = \begin{pmatrix} \mathcal{L}_+ + \gamma & -\gamma \\ -\gamma & \mathcal{L}_- + \gamma \end{pmatrix} \begin{pmatrix} P_1 \\ P_2 \end{pmatrix}$$
(4)

for dichotomic fluctuations between the two symmetric potentials $\pm V(x)$, V(x) = V(-x). The probability distributions $P_i = P_i(x,t)$, where *t* is time and *x* position, and the Smoluchowski operator [16]

$$\mathcal{L}_{\pm} = \frac{\partial}{\partial x} \bigg[\pm V'(x) + \frac{\partial}{\partial x} \bigg], \tag{5}$$

where V'(x) = dV(x)/dx, and γ is the rate of the random fluctuations. The distributions $P_i(x,t)$ satisfy absorbing boundary conditions at $x = \pm 1$, but making use of the symmetry of the problem it is possible to impose the mixed boundary conditions, $P_i(1,t) = 0$ and $P'_i(0,t) = 0$, and to solve the exit problem on the interval $\langle 0, 1 \rangle$. The extremal property somewhat simplifies the problem, as can be seen by analyzing Eq. (6) below. The normalized total probability distribution P = $P_1 + P_2$ defines the time-dependent occupation probability W(t|-1,1), W(0|-1,1) = 1 by assuming that the diffusing particle is located within the interval $\langle -1,1 \rangle$ at time t. Given

$$\frac{dW(t)}{dt} = \frac{d}{dt} \int_{-1}^{1} dx \ P(x,t) = P'(1,t)$$
(6)

$$= -Q(t|-1,1).$$
 (7)

The last relation defines the distribution Q of exit times out of the interval $\langle -1,1\rangle$.

The shooting method of adjoints [3,17] allows us to numerically compute the Laplace transform $\hat{Q}(p)$ of the distribution (7) for an arbitrary potential V = V(x). For comparison with the numerical results for a fluctuating potential shown below we cite here some archetypal analytic results representing the exit out of a static potential. The Laplace transform of the diffusion equation may in this case be rewritten in the form (1), with n = 2, $\vec{y} = [\hat{P}'(x, p), \hat{P}(x, p)]$,

$$A = \begin{pmatrix} -V' & p - V'' \\ 1 & 0 \end{pmatrix}, \tag{8}$$

and $\overline{f} = -P(x,0)[1,0]$. According to the identity (2) the adjoint equation (3) is then to be solved with the initial (resp. final) conditions $\overline{\xi}^{(m)}(x_m) = [0,1]$, m = 1 and 2. For a piecewise constant symmetric potential with V(x) = 0 for |x| < a and $V(x) = V_0$ for $a < |x| \leq 1$ there is

$$\hat{Q}(p) = \frac{1}{\xi(1,p)} \int_{-1}^{1} dx \ P(x,0)\xi(x,p), \tag{9}$$

where $\xi(x,p) = A(x,p) \cosh(p^{1/2}x)$ and the discontinuous factor $A^{-1}(x,p) = 1$ if |x| < a and

$$A^{-1}(x,p) = 1 - (1-a)(e^{V_0} - 1)p^{1/2}\sinh(p^{1/2}a)$$

if $a < |x| \le 1$. Similarly, assuming that $P(x,0) = \delta(x)$, we obtain for the piecewise linear asymmetric potential, $V(x) = -2\omega_1 x$ on $\langle -x_1, 0 \rangle$ and $V(x) = 2\omega_2 x$ on $\langle 0, x_2 \rangle$, $x_i > 0$, the expression

$$D(p)\hat{Q}(p) = 2\sum_{i=1}^{2} \Omega_{i} e^{-\omega_{i} x_{i}} \sinh \Omega_{i} x_{i},$$

$$D(p) = (\omega_{1} + \omega_{2}) [\cosh \Omega_{-} - \cosh \Omega_{+}] + (\Omega_{1} - \Omega_{2}) \sinh \Omega_{-} - (\Omega_{1} + \Omega_{2}) \sinh \Omega_{+},$$
(10)

with $\Omega_i = (\omega_i^2 + p)^{1/2}$, $\Omega_{\pm} = x_1 \Omega_1 \pm x_2 \Omega_2$. Obviously, in this case of an asymmetric potential, the simplified Eq. (6) is no longer applicable.

Equation (9) qualitatively represents the decay over a symmetric potential, while Eq. (10), which represents decay over two unequal barriers, may approximately be regarded as a superposition of the two unbiased results. The functions $\hat{Q}(p)$ have poles along the negative real axis of the complex p plane, and in the limit of small p they assume the Markovian form [18]

$$1/\hat{Q}(p) = 1 + p\langle \tau \rangle + o(p). \tag{11}$$

where

$$\langle \tau \rangle = \int_0^\infty dt \ W(t|-x_1, x_2) \tag{12}$$

is the mean first passage time [18] from within the static potential well. For reference we also note that for $V_0 = 0$ Eq. (9) admits analytic Laplace inversion [19]: For the singular initial distribution $P(x,0) = \delta(x)$ we obtain

$$W(t) = \frac{4}{\pi} \sum_{k=0}^{\infty} \frac{(-1)^k}{1+2k} e^{p_k t},$$
(13)

 $p_k = -\pi^2 (2k+1)^2/4$ and $\langle \tau \rangle = 1/2$, while for the uniform distribution P(x,0) = 1/2 there is

$$W(t) = \frac{8}{\pi^2} \sum_{k=0}^{\infty} \frac{1}{(1+2k)^2} e^{p_k t}$$
(14)

with $\langle \tau \rangle = 1/3$. The poles p_k are the eigenvalues of the diffusion equation. Remarkably, numerical studies show that the relation $p_k \propto k^2$ is preserved also for high-order eigenvalues of more general static and fluctuating potentials.

For a fluctuating potential the distribution $\hat{Q}(p)$ must be sought numerically. We set n = 4, $\vec{y} = [\hat{P}'_1, \hat{P}_1, \hat{P}'_2, \hat{P}_2]$,

$$A = \begin{pmatrix} -V' & p + \gamma - V'' & 0 & -\gamma \\ 1 & 0 & 0 & 0 \\ 0 & -\gamma & V' & p + \gamma + V'' \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad (15)$$

and $\vec{f} = -[P_1(x,0),0,P_2(x,0),0]$. For the initial conditions $2P_i(x,0) = \delta(x)$ the shooting method then yields the soughtafter values $y_1(1) = \hat{P}'_1(1,p)$ and $y_3(1) = \hat{P}'_2(1,p)$ in the form

$$2\sum_{i=0}^{1} y_{2i+1}(1)\xi_{2i+1}^{(m)}(1) = -1,$$
(16)

m = 1 and 2, where the four functions $\xi_j^{(m)}$ satisfy the Volterratype integral equations

$$\xi_{1}^{(m)}(x) = \xi_{1}^{(m)}(0) + \int_{0}^{x} dx_{1} \ e^{V(x_{1})} \int_{0}^{x_{1}} dx_{2} \ e^{-V(x_{2})} \\ \times \left[(p+\gamma)\xi_{1}^{(m)}(x_{2}) - \gamma\xi_{3}^{(m)}(x_{2}) \right], \tag{17}$$

$$\xi_{3}^{(m)}(x) = \xi_{3}^{(m)}(0) + \int_{0}^{m} dx_{1} \ e^{-V(x_{1})} \int_{0}^{m} dx_{2} \ e^{V(x_{2})} \\ \times \left[(p+\gamma)\xi_{3}^{(m)}(x_{2}) - \gamma\xi_{1}^{(m)}(x_{2}) \right], \tag{18}$$

with $\xi_1^{(1)}(0) = \xi_3^{(2)}(0) = 1$ and $\xi_1^{(2)}(0) = \xi_3^{(1)}(0) = 0$. The solutions of these equations vary exponentially fast and are therefore best sought using the Piccard iterations [3].

The properties of the mean first passage time for the symmetric fluctuating potential are well known [1–4]: The function τ decreases with small γ till it reaches a local minimum, and then it increases toward an asymptotic value corresponding to the average potential [4] $V_{av} = 0$. The rate of the initial decrease and the depth of the local minimum increase rapidly with increasing strength of the fluctuating potential, i.e., with the amplitude of the driving dichotomic fluctuations.

We find that for the sample fluctuating harmonic potential $V(x) = \pm \omega x^2/2$ the properties of the function $\hat{Q}(p)$ are as follows: If the dichotomic fluctuations are slow, then the Laplace transformed exit times distribution is approximately given by a superposition of the two static cases, and the decay is governed by the slower of the two [4]. All poles



FIG. 1. Distribution of the poles of the function $\hat{Q}(p|-1,1)$ in the second quadrant of the complex p plane, with $p = p_{(1)} + ip_{(2)}$, $p_{(1)} \leq 0$, and $p_{(2)} \geq 0$. We consider dichotomic fluctuations between the two harmonic potentials $V_{\pm}(x) = \pm \omega x^2/2$, with fluctuation rate $\ln \gamma = 2.5$ close to the maximum of resonant activation. The amplitude of the potential is $\omega = 3$, 4 (\circ), 5, 7 (\circ), 8, 9 (\circ), 10, 11 (\circ), 12, 13 (\circ), 15, 17 (\circ), and 19. The connecting lines [labeled for selected values of ω] merely guide the eye, and the alternating full (\bullet) and open (\circ) symbols are used for easier reading of the figure.

are real, and, as expected, at sufficiently large ω the poles satisfy the relation $|p_1^{(1)}| \ll |p_1^{(2)}|$, Im $p^{(i)} = p_2^{(i)}i = 0$. Apart from rapidly decaying transients the decay is here exponentail. With increasing γ the first pole p_1 shifts along the real negative axis to the *left*, and, at the same time, a *finite* number of poles, beginning with the second one, splits into complex conjugate pairs. The number of the complex conjugate pairs, and the magnitude of their imaginary parts, increase with increasing strength of the potential as discussed below. On further increase of the fluctuation rate the train of complex poles gradually shifts to the left, leaving behind a pattern of real eigenvalues corresponding to the asymptotic average potential [4]. In all three cases the process described by the evolution equation (4) is Markovian by construction.

We depict a sample distribution of the complex poles of the function $\hat{Q}(p) = \hat{Q}^*(p^*)$ in Fig. 1. The selected value of the fluctuation rate $\ln \gamma = 2.5$ is close to the maximum amplitude of the resonant activation. As stated, the resonant amplitude rapidly increases [3] with increasing strength of the potential V, but a striking feature of the plot of Fig. 1 is the fact that with increasing ω the first nonzero poles (which govern the Markovian exponential decay) shift slightly to the *left* along the real axis. In the Markov case this would imply a slight decrease of the resonant amplitude rather than the observed strong increase. We therefore conclude that the rapid variation of the mean first passage time with the potential amplitude ω is due to a contribution of a large number of poles. At $\ln \gamma = 2.5$ we have numerically computed the residues [20] of the first four poles and found them to be alternating in sign, similar to Eq. (13); the very slow convergence of the series, however, makes it all but impossible to compute the real time decay probability W(t) with sufficient precision.

IV. SUMMARY

In summary, we find that the resonant enhancement of activation rate by dichotomic fluctuations is associated with the presence of a finite number of complex conujugate eigenvalue pairs in the spectrum of the evolution equation (4). We also find that the resonant decay cannot be described by a single (first nonzero) exponent.

The presence of the complex conjugate eigenvalue pairs suggests the possibility of resonant response to an applied periodic field. Of particular interest here would be the ac susceptibility of a fluctuating system with reflecting boundary conditions at $x = \pm 1$. The infinitesimal ac field does not disrupt the property of resonant activation, but it would be necessary to compute first the stationary state of the fluctuating system and the time required to reach it. However, no solvable system of this kind is as yet known to us.

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