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Noise-Induced Transitions in a Double-Well Potential at Low Friction

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A new integral representation of the transition rate holds for any friction and is shown to allow a feasible evaluation in a wide friction range. Analytic approximations include the (high-friction) Kramers result with the leading correction, as well as a low-friction case. The method is complementary to a recent one of Melnikov and Meshkov.

KEY WORDS: Fokker–Planck equation; eigenfunction; bistability; transitions at low friction.

1. INTRODUCTION

The mean time for a transition from one metastable state to the other is in fact determined by a partial differential equation of second order, involving the adjoint L^+ of the Fokker–Planck operator L.[1] To solve it in phase space is such a difficult numerical task that approximations are essential. An efficient one is based on the fact that the transition rate is directly related to the smallest nonzero eigenvalue λ of L, L^+, as long as the noise is "moderate" in the sense that the stationary probability density remains concentrated near the potential minima and, equivalently, that the remaining nonzero eigenvalues are of a higher order of magnitude.[2,3] Numerical methods to obtain λ are shown, for example, in Ref. 4. It is of course tempting to search for analytic expressions for λ. Two integral representations of λ are available, both valid for any friction. One of them was put forward in Ref. 5, and a new one, to be presented here, has the advantage of establishing the connection with well-known theories. In fact, for weak noise (thermal energy $\ll$ threshold height) and in a wide friction range

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(reaching from a value of order T to infinity) it reduces to the mean first passage time on the separatrix of the noiseless motion. Only for rather high friction η can the corresponding line integral be evaluated by Laplace's method, leading to the Kramers result.[6] With decreasing η a better approximation of both the potential threshold and the separatrix becomes necessary, resulting in a correction to the Kramers formula; in the general case (within the admitted friction range) a Runge-Kutta method can be used. A specific approximation holds for rather low friction. An advantage of the present approach is that it clearly exhibits some validity limits. It turns out that its results are reliable where a recent method[7] becomes inaccurate.

Excellent reviews of numerous further approaches are given in Refs. 8 and 9; the pioneering work is of course that of Kramers.[10]

We briefly specify the model. The system under consideration is

$$\dot{x} = v, \qquad \dot{v} = -\eta v - U'(x) \tag{1.1}$$

where $U(x)$ is a double-well potential with a smooth threshold at $x = 0$ and with $U(0) = 0$. As in Ref. 10, we set both the mass and Boltzmann's constant equal to unity. Contact with a thermal bath of temperature T leads to fluctuations determined by the Fokker–Planck equation

$$p_{,t} = -vp_{,x} + [(\eta v + U')\, p]_{,v} + \eta T p_{,vv} \tag{1.2}$$

Note that the stationary solution

$$p_0(x, v) = c \exp(-E/T), \qquad E(x, v) = v^2/2 + U(x) \tag{1.3}$$

does not depend on η.

2. SOME GENERAL RELATIONS FOR BISTABLE SYSTEMS

The essential tools for the following discussion apply for any (autonomous) bistable system and are presented for convenience in their general form. With variables $x^1,\dots, x^N$ ($x^1 = x$, $x^2 = v$ in the particular case) the Fokker–Planck operator L and its adjoint, the generator L^+, are

$$\begin{aligned} L &= (\partial/\partial x^i)[-K^i(\mathbf{x}) + (\partial/\partial x^k)\, D^{ik}(\mathbf{x})] \\ L^+ &= K^i(\mathbf{x})\, \partial/\partial x^i + D^{ik}(\mathbf{x})\, \partial^2/\partial x^i\, \partial x^k \end{aligned} \tag{2.1}$$

Here the drift field $\mathbf{K}(\mathbf{x})$ is merely supposed to be bistable, and $\mathbf{D}(\mathbf{x})$ must be symmetric and nonnegative.

2.1. Properties at Moderate Noise

As outlined in Refs. 2 and 3, moderate noise implies that the stationary distribution $p_0(\mathbf{x})$ is concentrated onto two well-separated domains $\mathscr{R}_{A,B}$ of $\mathbf{x}$ space around the attractors A, B of $\mathbf{K}(\mathbf{x})$, so that

$$p_{0A,B} \triangleq \int_{\mathscr{R}_{A,B}} p_0(\mathbf{x})\, d\mathbf{x}, \qquad p_{0A} + p_{0B} \approx 1 \tag{2.2}$$

Furthermore, transitions between $\mathscr{R}_{A,B}$ were shown to form a nearly Markovian jump process, with transition rates

$$r_{A\to B} = \lambda p_{0B}, \qquad r_{B\to A} = \lambda p_{0A} \tag{2.3}$$

λ is the lowest nonzero eigenvalue of L, L^+.

We now restate and extend some findings of Ref. 2 about the first nontrivial eigenfunction $q_1(\mathbf{x})$ of L^+: $L^+ q_1 = -\lambda q_1$. It was shown to assume the values Cp_{0B} on $\mathscr{R}_A$ and $-Cp_{0A}$ on $\mathscr{R}_B$. Therefore, with $C=2$, the shifted function

$$\bar{q}(\mathbf{x}) \triangleq q_1(\mathbf{x}) + p_{0A} - p_{0B} \tag{2.4}$$

satisfies

$$\bar{q} = \begin{cases} 1 & \text{on } \mathscr{R}_A \\ -1 & \text{on } \mathscr{R}_B \end{cases} \qquad \text{and} \qquad L^+\bar{q} = -\lambda q_1 \tag{2.5}$$

It is interesting to consider the integral

$$F \triangleq -\int_Z dS_i\, p_0 D^{ik} \bar{q}_{,k} \tag{2.6}$$

taken over the surface Z, where $\bar{q}=0$ ($d\mathbf{S}$ is an element of Z). Clearly, it equals the integral of $-(p_0 D^{ik}\bar{q}_{,k})_{,i}$ over the half-space bounded by Z and containing $\mathscr{R}_A$. This integrand can be rewritten as

$$-(p_0 D^{ik})_{,i}\,\bar{q}_{,k} + p_0(K^i \bar{q}_{,i} + \lambda q_1) = J^i \bar{q}_{,i} + \lambda p_0 q_1$$

where $\mathbf{J}$ is the stationary probability current. Since $J^i_{\ ,i}=0$, the first term equals $(J^i\bar{q})_{,i}$ and does not contribute, as can be seen after retransforming to a surface integral. We are thus left with

$$F = \lambda p_{0A} q_{1A} = 2\lambda p_{0A} p_{0B} \tag{2.7}$$

The eigenvalue λ is thus reduced to F. Moreover, comparison with (2.3) shows that

$$r_{A\to B} = F/2p_{0A}, \qquad r_{B\to A} = F/2p_{0B} \tag{2.8}$$

which denotes an integral representation of the transition rate.

Two important properties of $\bar{q}$ can be derived by setting $L^+\bar{q}\approx 0$, with the values (2.5) on A and B now imposed as boundary conditions (this approximation was discussed in Ref. 2 by means of a Feynman–Kac result). In Ref. 2 it was shown that

$$\bar{q}(\mathbf{x}) = P_A(\mathbf{x}) - P_B(\mathbf{x}) \tag{2.9}$$

where $P_A(\mathbf{x})$ denotes the probability that from the starting point $\mathbf{x}$ the attractor A (in fact, its immediate neighborhood; see Ref. 2) is reached before B (P_B analogously). Note that Z is the "stochastic separatrix," since $P_A = P_B$ there.

Furthermore, $\bar{q}$ gives the mean first passage time $\theta(\mathbf{x})$ on Z from any starting point $\mathbf{x}$, normalized by the values $\theta_{A,B}$ on the respective $\mathscr{R}_{A,B}$:

$$|q(\mathbf{x})| = \theta(\mathbf{x})/\theta_{A,B} \tag{2.10}$$

This follows from the fact that on each side of Z, $L^+\theta = -1$ with $\theta = 0$ on Z,[1] so that $L^+\theta/\theta_{A,B} = -\theta_{A,B}^{-1}\approx 0$, while (2.5) gives the adequate boundary values.

By (2.8) and (2.9) the value of F may be interpreted as the rate of first arrivals on Z of trajectories coming from either of $\mathscr{R}_{A,B}$.

2.2. Low-Noise Approximation

At low noise an important further step consists in introducing the smallness parameter ε of the diffusion

$$D^{ik}(\mathbf{x}) = \varepsilon d^{ik}(\mathbf{x}) \tag{2.11}$$

and in substituting

$$\bar{q}(\mathbf{x}) \triangleq \operatorname{erf}[\rho(\mathbf{x})/(2\varepsilon)^{1/2}] = \left(\frac{2}{\pi\varepsilon}\right)^{1/2} \int_0^{\rho(\mathbf{x})} \exp(-z^2/2\varepsilon)\, dz \tag{2.12}$$

(see also Ref. 11). So far this merely defines $\rho(\mathbf{x})$, which may itself depend on ε. Clearly, ρ also vanishes on Z, and it has the same sign as $\bar{q}$. Inserting (2.12) into $L^+\bar{q}\approx 0$ yields

$$(L^+\rho =)\; K^i\rho_{,i} + \varepsilon d^{ik}\rho_{,ik} = \rho d^{ik}\rho_{,i}\rho_{,k} \tag{2.13}$$

The "boundary layer approximation" (BLA) consists in neglecting the term proportional to ε in (2.13). The legitimation of this step will be discussed in Section 4.4. When $\mathbf{K}$ does not involve ε, it yields an ε-independent ρ, and (2.12) then gives the scaling of $\bar{q}$ with ε, in particular, a layer of a width proportional to $\sqrt{\varepsilon}$, where $\bar{q}$ changes from 1 to -1. As a further consequence, $K^i\rho_{,i}$ vanishes on Z (where $\rho = 0$), so that $\mathbf{K}$ must be tangential to Z. Since $\mathbf{K}$ is bistable, the only tangential surface that does not include an attractor is the separatrix (or boundary) $\partial\Omega$ of the two domains of attraction $\Omega_{A,B}$ of $\mathbf{K}$. Thus

$$Z \equiv \partial\Omega \tag{2.14}$$

For evaluating F one needs the gradient of $\bar{q}$ on Z,

$$\nabla\bar{q}\,|_Z = (2/\pi\varepsilon)^{1/2}\,\nabla\rho\,|_Z \tag{2.15}$$

Still in the BLA, it was shown in Ref. 12 that

$$b \triangleq (\nabla\rho\,|_{\partial\Omega})^{-2} \tag{2.16}$$

is determined by the linear equation

$$K^i b_{,i} - 2gb + 2d = 0 \tag{2.17}$$

where g is the increase of the normal component of $\mathbf{K}$ and d is the scaled diffusion normal to $\partial\Omega$.

3. THE SEPARATRIX

The drift field $\mathbf{K}$, given by the right-hand sides of (1.1), has an unstable equilibrium point (more precisely, a saddlepoint) at $x = 0$, $v = 0$, and the separatrix $v_s(x)$ is the integral line of $\mathbf{K}$ that ends there:

$$v_s' v_s + \eta v_s + U' = 0 \qquad \text{with} \quad v_s(0) = 0 \tag{3.1}$$

The slope at the saddle is

$$\hat{v}_s' = -\eta/2 - [(\eta/2)^2 - \hat{U}'']^{1/2} \tag{3.2}$$

and the next higher derivatives are

$$\begin{aligned} \hat{v}_s'' &= -\hat{U}'''/(3\hat{v}_s' + \eta) \\ \hat{v}_s''' &= -(\hat{U}'''' + 3\hat{v}_s''^2)/(4\hat{v}_s' + \eta) \end{aligned} \tag{3.3}$$

(the caret will denote any quantities referring to the saddle). The turning points $v_s' = \infty$ are on the x axis, and $v_s' v_s = -U'$ there. A plot of $v_s(x)$ is given in Fig. 1. Clearly, for $\eta \to 0$ the spiral becomes arbitrarily tight outside the limiting curve $v_0(x)$ determined by $E = 0$:

$$v_0(x) = [-2U(x)]^{1/2} \tag{3.4}$$

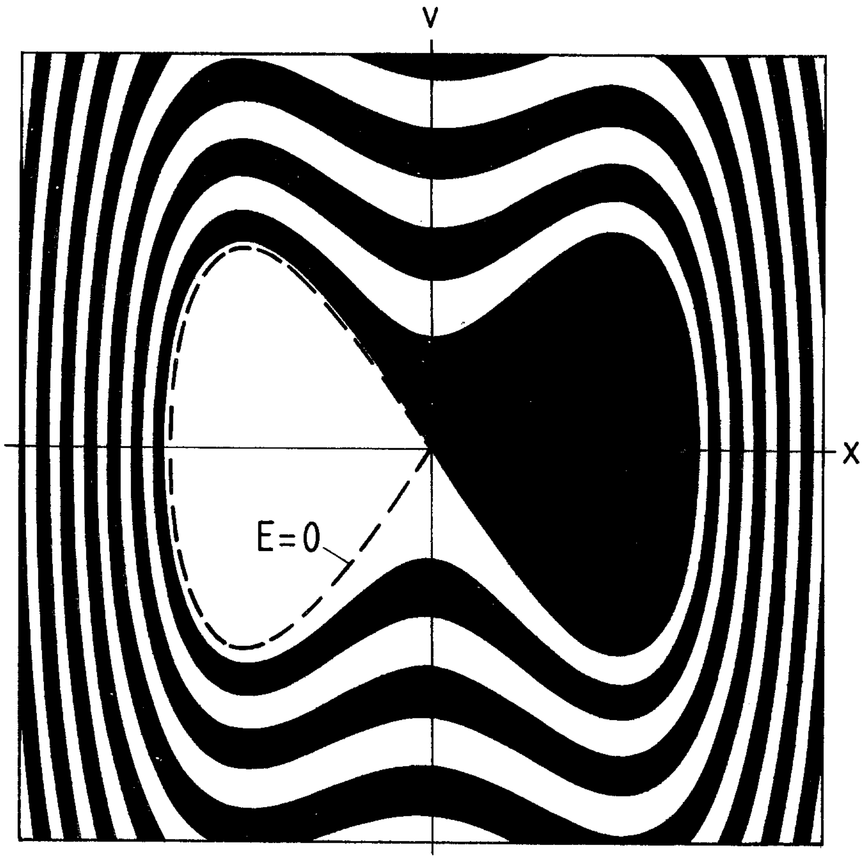

Fig. 1. The separatrix $\partial\Omega$ between the two domains of attraction (white and black) approaches the line $E=0$ (corresponding to the threshold energy) when the friction η becomes small.

4. CONCLUSIONS FROM THE BOUNDARY LAYER APPROXIMATION

4.1. The Integral for the Transition Rate

In view of (2.14) and of $D^{11}=D^{12}=D^{21}=0$ and $D^{22}=\eta T$, the integral (2.6) reduces to

$$F=\eta T \int dx\, p_0[x, v_s(x)]\, |\bar{q}_{,v}[x, v_s(x)]| \tag{4.1}$$

which is to be continued properly at the turning points.

From (1.1) it readily follows that $\dot{E} = -\eta v^2$, so that

$$E[x, v_s(x)] = -\eta \int_0^x v_s(x')\, dx' \triangleq \eta I(x) \tag{4.2}$$

[note that $I(x)$ increases monotonically from both sides of the saddle]. Thus, with (1.3), the transition rate (2.8) assumes the form

$$r_{A\to B} = (N_A/2)\, \eta \int dx \exp[-(\eta/T)\, I(x)]\, |\bar{q}_{,v}[x, v_s(x)]| \tag{4.3}$$

The factor N_A is easily recognized as not being dependent on η; with the Gaussian approximation of p_0 near the attractor A it becomes

$$N_A = \exp(U_A/T)\, (U''_A)^{1/2}/2\pi \tag{4.4}$$

and involves both the Arrhenius factor and the information about the potential minimum at A.

4.2. The Gradient Term

It remains to work out $|\bar{q}_{,v}|$ on the separatrix. Clearly,

$$|\bar{q}_{,v}| = |\nabla \bar{q}|\, \chi, \qquad \chi(x) \triangleq [v_s'^2(x) + 1]^{-1/2} \tag{4.5}$$

The adequate decomposition (2.11) of $\mathbf{D}$ is $d^{22} = 1$ ($d^{11} = d^{12} = d^{21} = 0$), so that $\varepsilon = \eta T$. Thus, by (2.15), (2.16),

$$(\bar{q}_{,v})^2 = (2/\pi\eta T)\, \chi^2/b \tag{4.6}$$

In the equation (2.17) for b the diffusion term is now $d = \chi^2$. Furthermore, g can be expressed by the normal unit vector $\mathbf{n} \triangleq (v_s', -1)\,\chi$ and by the matrix $\mathbf{B}$ of the derivatives of $\mathbf{K}$: $g = \mathbf{n}^T\mathbf{B}\mathbf{n}$, giving

$$g = [U''v_s' - (v_s' + \eta)]\, \chi^2 = -(v_s' + \eta) + v_s \chi'/\chi \tag{4.7}$$

$$\hat{g} = -(\hat{v}_s' + \eta) = \hat{U}''/\hat{v}_s' \tag{4.7a}$$

where (3.1) and its derivative have been used. Hence

$$v_s b' + 2[(v_s' + \eta) - v_s \chi'/\chi]\, b + 2\chi^2 = 0 \tag{4.8}$$

and

$$\hat{b} = -\hat{\chi}^2/(\hat{v}_s' + \eta) = \hat{v}_s' \hat{\chi}^2/\hat{U}'' \tag{4.8a}$$

A simplification results by setting $b \triangleq \chi^2 \beta$. Then (4.6) and (4.8) become

$$(\bar{q}_{,v})^2 = (2/\pi\eta T)/\beta \tag{4.9}$$

$$v_s \beta' + 2(v_s' + \eta)\,\beta + 2 = 0 \tag{4.10}$$

$$\hat{\beta} = -1/(\hat{v}_s' + \eta) \tag{4.10a}$$

respectively. The only solution of (4.10) that is continuous at the saddle is

$$\beta(x) = -2[v_s(x)]^{-2} \int_0^x dx'\, v_s(x') \exp\left[-2\eta \int_{x'}^x \frac{dx''}{v_s(x'')}\right] \tag{4.11}$$

At the turning points β becomes infinite, but b remains finite and positive, which shows how to continue the integration.

It is readily verified that in the linear part of $v_s(x)$ near the saddle $[v_s(x) \approx \hat{v}_s' x]$ $\beta = \text{const} = \hat{\beta}$.

In summary, the gradient term becomes

$$|\bar{q}_{,v}[x, v_s(x)]| = (\pi\eta T)^{-1/2}\, |v_s(x)| \left| \int_0^x dx'\, v_s(x') \exp\left(-2\eta \int_{x'}^x \frac{dx''}{v_s(x'')}\right)\right|^{-1/2} \tag{4.12}$$

With the results obtained so far the transition rate is easily computed numerically: this involves solving (3.1) for $v_s(x)$, evaluating $\bar{q}_{,v}$ from (4.12), and, finally, finding $r_{A \to B}$ from (4.3) and (4.4). In practice it might be easier to use (4.10) rather than (4.12), and to integrate it together with (3.1) and (4.3) by a Runge-Kutta method.

4.3. Analytic Results

Explicit formulas hold both for high friction, where the Kramers result and its leading correction in T/η will be found, and for rather low friction, where an η-independent expression gives the maximum rate (provided that the BLA extends so far).

The proper Kramers formula is obtained when the exponential in (4.3) decays so fast that the linear approximation of the separatrix is sufficent.[6] Here we rather consider the cubic approximation, which by (3.3) corresponds to the quartic representation of the potential threshold. With (4.2) and (4.3) this amounts to

$$r_{A \to B} \approx \frac{N_A}{2} \eta \int_{-\infty}^{\infty} dx \exp\left[\frac{\eta}{T}\left(\hat{v}_s' \frac{x^2}{2} + \hat{v}_s'' \frac{x^3}{6} + \hat{v}_s''' \frac{x^4}{24}\right)\right] \times \left| \hat{\bar{q}}_{,v} + \hat{\bar{q}}_{,v}' x + \hat{\bar{q}}_{,v}'' \frac{x^2}{2} \right| \tag{4.13}$$

The saddle values of $\bar{q}_{,v}$ and of its derivatives follow by (4.9) and on expanding (4.10). They will be worked out in the Appendix, together with the evaluation of (4.13) for small T/η. The result is the Kramers formula multiplied by

$$[1+(T/\eta)\,f(\hat{U}'', \hat{U}''', \hat{U}'''', \eta)+O(T/\eta)^2]$$

In particular, for $\hat{U}'''=0$

$$r_{A\to B}\approx N_A(-\hat{U}'')^{-1/2}\left[\left(\frac{\eta^2}{4}-\hat{U}''\right)^{1/2}-\frac{\eta}{2}\right]\left[1-\frac{1}{8}\frac{T}{\eta}\frac{\hat{v}_s'''}{(\hat{v}_s')^2}\left(1-\frac{4\hat{U}''}{\eta^2}\right)^{-1/2}\right] \tag{4.14}$$

Note that for $\hat{U}''''>0$ (so $\hat{v}_s'''>0$) the Kramers value is diminished.

At low friction one may neglect the exponential in (4.12), which leads to

$$\begin{aligned}\bar{q}_{,v}[x, v_s(x)] &\approx -(\pi\eta T)^{-1/2}\, v_s[I(x)]^{-1/2}\\ &= 2(\pi\eta T)^{-1/2}\,\{[I(x)]^{1/2}\}'\end{aligned} \tag{4.15}$$

Inserted into (4.3) this yields

$$r_{A\to B}\approx N_A(\eta/\pi T)^{1/2}\,2\int_0^\infty \exp[-(\eta/T)\,I(x)]\,d[I(x)]^{1/2}=N_A \tag{4.16}$$

Note that this is the Kramers result for $\eta=0$. The approximation (4.15) determines the upper bound for η:

$$1\approx\exp\left[-2\eta\int_{x'}^{x}\frac{dx''}{v_s(x'')}\right]\approx\exp\left(\frac{2\eta}{-\hat{v}_s'}\ln\frac{x}{x'}\right)=\left(\frac{x}{x'}\right)^{2\eta/-\hat{v}_s'}$$

for $x/x'\gg 1$; thus, $2\eta\ll-\hat{v}_s'$ [the divergence at $x'=0$ is of minor importance, as it is integrated over in (4.12)]. Therefore, with (3.2),

$$\eta\ll 2(-\hat{U}'')^{1/2} \tag{4.17}$$

which implies that the separatrix coincides with v_0 at the saddle [note that by (4.17) the correction term in (4.14) is negligible]. The lower bound for η is that given by the BLA and will be specified in Section 4.4.

We mention an interesting consequence of (4.15): the value of $|\bar{q}_{,v}|$ at $x=0$ (after a nonzero number of windings) takes a particularly simple form. With I_0 denoting the accumulated value of $I(x)$ at $x=0$ and v_{s0} the corresponding ordinate $v_s(0)$, (4.2) yields

$$v_{s0}^2/2=\eta I_0$$

thus

$$|v_{s0}| = (2\eta I_0)^{1/2} \tag{4.18}$$

so that

$$|\bar{q}_{,v}(0, v_{s0})| = (\pi\eta T)^{-1/2}\, |v_{s0}|\, I_0^{-1/2} = (2/\pi T)^{1/2} \tag{4.19}$$

which only depends on T.

4.4. Validity of the Boundary Layer approximation

A crucial difference in the role of the two factors η and T of the smallness parameter ε lies in the fact that the drift $\mathbf{K}$ does not involve T, whereas it depends on η, even in such a way that the bistability disappears for $\eta = 0$. While it is rather obvious that for given η there always exists a $T > 0$ small enough that the BLA holds, the converse is not true: when T is fixed at some value $\ll \min(-U_A, -U_B)$, a too small η entails such a tight spiraling of $\partial\Omega$ that the boundary layer cannot develop any more.

More specifically, a necessary condition for the BLA to hold is that the spacing between consecutive windings of the separatrix, i.e. the tails of the domains of attraction $\Omega_{A,B}$, be wider than the boundary layer itself, at least where the exponential in (4.3) is appreciable. This condition can easily be checked by (4.18) and (4.19) at the first return of the separatrix to the v axis: the requirement that $|\bar{q}_{,v}(0, v_{s0})\, v_{s0}| \gg 1$ amounts to

$$\eta I_{A,B} \gg T \qquad \text{or} \qquad \eta \gg T/\min(I_A, I_B) \tag{4.20}$$

where $I_{A,B}$ are the values of I after the first surrounding of the attractor A or B, respectively. For their evaluation it is usually sufficient to take the action of the frictionless oscillation with $E = 0$. Physically, (4.20) means that the energy loss of an oscillation starting at $x = 0$ (with velocity v_{s0}) and ending there with velocity zero exceeds T. It is important to note that (4.20) implies at the same time that the exponential in (4.3), which determines the part of $\partial\Omega$ where transitions actually take place, decays before the separatrix reaches the v axis again.

As is natural to expect, a tail of $\Omega_{A,B}$ thinner than the boundary layer implies an appreciable magnitude of the term $\eta T\rho_{,vv}$ neglected in (2.13), more precisely, a magnitude comparable with $\rho(\rho_{,v})^2$: with Δv denoting the width of the tail in v direction, the critical situation is $\bar{q}_{,v} \approx 1/\Delta v$; thus, by (2.15), $\rho_{,v} \approx (\eta T)^{1/2}/\Delta v$. Then, on one hand, $\rho(\rho_{,v})^2 \approx \Delta v(\rho_{,v})^3 \approx (\eta T)^{3/2}\,(\Delta v)^{-2}$; on the other hand, $\eta T\rho_{,vv} \approx \eta T\rho_{,v}/\Delta v \approx (\eta T)^{3/2}\,(\Delta v)^{-2}$ as well.

The validity of the BLA is also related to the question of how a particle starting at the saddle continues to move after one oscillation (clearly, it enters either of the wells with probability $\frac{1}{2}$): when the BLA holds, it typically thermalizes in the well initially chosen, and only reattains the threshold energy after a time of order r^{-1}. In contrast, when (4.20) is not met, the boundary layer along one loop of the separatrix includes the saddle itself, which means that the particle has a good chance of escaping again from the well after the first oscillation. For an asymmetric potential this may hold in one well only, in which case it is easily seen that the saddle does not belong to Z; in particular, this shows that Z and $\partial\Omega$ no longer coincide in general.

At very low friction a particle with initial energy zero is thus even likely to cross both wells several times before thermalizing in one of them.

5. LOWEST FRICTION

Below the limit (4.20) the evaluation of (2.6) becomes unfeasible, as the separatrix $\partial\Omega$ of $\mathbf{K}$ and the "stochastic separatrix" Z need not coincide any more. A simple method for calculating Z, or even the gradient of $\bar{q}$ on Z, is not available.

In the lowest friction range the final remark of Section 4.4 gives another possibility for evaluating the transition rate: since a particle with energy $E \approx 0$ typically crosses both wells several times before thermalizing, it is sufficient to know the mean times $\Theta_{\mathrm{A,B}}$ for reaching the threshold energy $E=0$ from $\mathscr{R}_{\mathrm{A,B}}$, as well as the probabilities $P_{A,B}$ for rethermalization in $\mathscr{R}_{A,B}$. These probabilities do not vary along the $E=0$ curve in this case, and they are determined by

$$r_{A \to B} = \Theta_A^{-1} P_B \qquad (\text{and } A \leftrightarrow B) \tag{5.1}$$

and by the stationarity condition

$$p_{0A} r_{A \to B} = p_{0B} r_{B \to A}$$

as

$$P_A = p_{0A} \Theta_B (p_{0A} \Theta_B + p_{0B} \Theta_A)^{-1} \qquad (\text{and } A \leftrightarrow B) \tag{5.2}$$

Inserted into (5.1), this gives

$$r_{A \to B} = p_{0B} (p_{0A} \Theta_B + p_{0B} \Theta_A)^{-1} \tag{5.3}$$

and (2.3) reveals that

$$\lambda = (p_{0A} \Theta_B + p_{0B} \Theta_A)^{-1} \tag{5.4}$$

which is symmetric in A and B, as is natural to expect.

The times $\Theta_{A,B}$ were evaluated in Ref. 6 as

$$\Theta_A^{-1} = N_A \eta I_A / T \qquad (\text{and } A \leftrightarrow B) \tag{5.5}$$

where I_A is the area enclosed by the curve $E = 0$ around A; see also the remark after (4.20). This result holds for every $\eta > 0$ and for $T \ll -U_{A,B}$.

With $p_{0A} = N_B/(N_A + N_B)$ (and $A \leftrightarrow B$) it now follows that

$$r_{A \to B} = N_A \eta T^{-1} (I_A^{-1} + I_B^{-1})^{-1} \tag{5.6}$$

$$\lambda = (N_A + N_B) \eta T^{-1} (I_A^{-1} + I_B^{-1})^{-1} \tag{5.7}$$

6. DISCUSSION, RELATED WORK, AND CONCLUDING REMARKS

The present approach is based on the eigenvalue λ, which refers to the whole phase space. As it turns out, an essential line in phase space is the "stochastic separatrix" Z, from which both metastable states are approached with probability $\frac{1}{2}$: the integral (2.6) along Z gives λ in the whole friction range, and thus also the transition rates. The practical determination of both Z and the integrand depends on an approximation (the BLA), which primarily consists in neglecting a term in the transformed backward equation (2.13). Under the BLA, Z is shown to coincide with the separatrix of the noiseless motion; moreover, a well-known method for evaluating the integrand can be invoked. In this situation the transition rate is just half of the inverse mean first passage time on the (deterministic) separatrix. A closer inspection of the integrand reveals that the region where the transitions actually occur strongly depends on the friction η; for high η it is such a narrow part of the separatrix that a saddlepoint integration of second order (Laplace method) is sufficient, leading to the Kramers result. With decreasing η this region widens, so that an increasing part of the potential becomes important. For a quartic approximation of the potential threshold, corresponding to a cubic approximation of the separatrix, a higher saddlepoint integration results in a T/η correction of the Kramers formula. For lower η a Runge-Kutta evaluation is possible. Still lower η [see (4.17)] allows a specific approximation, which yields an η-independent result, namely the value of the (high-friction) Kramers formula with $\eta = 0$. When the transition region extends over a full loop of the separatrix, the BLA breaks down. Physically, this situation means that a particle starting on top of the threshold with $v = 0$ has an appreciable chance of crossing the threshold after one oscillation, since the thermal energy may compensate for the friction loss.

These findings are to be related with existing work. Among the approaches that claim to cover the whole friction range without an explicit ad hoc ansatz, we mainly consider those of Matkovsky *et al.* (MST)[6] and of Mel'nikov and Meshkov (MM)[7]; but we also point to an interesting integral representation for λ by Dekker,[5] for which a systematic construction of trial functions might be found.

The MST work is based on mean first passage times: τ_1 on the curve of the threshold energy E_c and τ_2 on the (deterministic) separatrix; starting points are either at the metastable state A or somewhere on the E_c curve. It is shown that $\tau_2(A)=\tau_1(A)+\tau_2(E_c)$. The second contribution is represented as $\tau_2(E_c)=V\tau_2^*(A)$, where $\tau_2^*(A)$ is the high-friction value of $\tau_2(A)$ and where V $(0<V<1)$ is given by an integral that accounts for the fact that for low friction the separatrix and the E_c curve become very close. The expression $[\tau_1(A)+2\tau_2(E_c)]^{-1}$ for the rate actually interpolates between the results for extreme friction. However, the first correction to the high-friction case, which can be obtained by expanding V, differs from (4.14) in its dependence on the potential: instead of a higher derivative at the threshold, it involves the surface enclosed by the E_c curve, which is a nonlocal functional of the potential well.

The MM theory uses action and energy rather than x and v, and it establishes an integral equation with a kernel that is approximated for the low-friction case. Indeed, for lowest η, the solution agrees with (5.6) and confirms the $\eta^{3/2}$ correction of Ref. 13, and it increases monotonically with η. To cover also the higher friction domain, the authors simply multiply their result by a factor that is approximately one for small η and reproduces the Kramers result for large η. Yet this procedure is merely a crude approximation, as can be seen from the fact that it accounts for the potential only by the action of the frictionless motion and by the curvature at the threshold, while already (4.14) shows a different dependence (the Arrhenius factor and the contribution from the potential minima are not concerned by this argument).

Actually, the MM theory and the present one are complementary, as the former describes the increasing part and the latter the (slowly) decreasing part of the transition rate as a function of η.

APPENDIX

The evaluation of (4.13) involves the expansion of

$$\int_{-\infty}^{\infty} dx \exp[-(Ax^2+Bx^3+Cx^4)/\delta^2]\,(a+bx+cx^2) \qquad \text{(A.1)}$$

for small $\delta^2 = T/\eta$. Clearly, $A = -\hat{v}_s'/2 > 0$; moreover, $C > 0$ is supposed for the present. Substituting $x = \delta y$ and expanding

$$\exp(-\delta By^3 - \delta^2 Cy^4) \approx 1 - \delta By^3 - \delta^2 Cy^4 + \delta^2 B^2 y^6/2$$

to order δ^2 yields

$$\delta \int_{-\infty}^{\infty} dy \exp(-Ay^2)\{a + \delta^2[cy^2 - (aC + bB)\, y^4 + (aB^2/2)\, y^6]\}$$

With

$$\int_{-\infty}^{\infty} dy \exp(-Ay^2)\, y^{2k} = \sqrt{\pi}\, \frac{1 \cdot 3 \cdot \cdots \cdot (2k-1)}{2^k A^{k+1/2}}$$

this results in

$$\left(\frac{\pi}{A}\right)^{1/2} \delta \left[a + \delta^2 \left(\frac{c}{2A} - \frac{3}{4}\frac{aC + bB}{A^2} + \frac{15}{16}\frac{aB^2}{A^3}\right)\right] \tag{A.2}$$

The assumption $C > 0$ can now be dropped by analytic continuation.

We briefly work out the coefficients. While A, B, and C are evident, the a, b, and c are to be obtained from (4.9) and (4.10). By (4.9) and its first and second derivatives it follows that

$$a = (2/\pi\eta T\hat{\beta})^{1/2}, \qquad b = -\tfrac{1}{2}a\hat{\beta}'/\hat{\beta}, \qquad c = -\tfrac{1}{4}a[\hat{\beta}''/\hat{\beta} - \tfrac{3}{2}(\hat{\beta}'/\hat{\beta})^2] \tag{A.3}$$

Furthermore, (4.10) yields

$$\begin{aligned} \hat{\beta}^{-1} &= -(\hat{v}_s' + \eta) = [(\eta/2)^2 - \hat{U}'']^{1/2} - \eta/2 \\ \hat{\beta}'/\hat{\beta} &= -2\hat{v}_s''/(3\hat{v}_s' + 2\eta) \\ \hat{\beta}''/\hat{\beta} &= -[\hat{v}_s''' - 5(\hat{v}_s'')^2/(3\hat{v}_s' + 2\eta)]/(2\hat{v}_s' + \eta) \end{aligned} \tag{A.4}$$

By taking a out of the curly bracket, we obtain for (A.2)

$$\frac{2}{\eta}\frac{[(\eta/2)^2 - \hat{U}'']^{1/2} - \eta/2}{(-\hat{U}'')^{1/2}} \left\{1 + \frac{T}{\eta}\left[\frac{c/a}{2A} - \frac{3}{4}\frac{C + (b/a)\,B}{A^2} + \frac{15}{16}\frac{B^2}{A^3}\right]\right\} \tag{A.5}$$

where c/a and b/a are given by (A.3) and (A.4).

The case $\hat{U}''' = 0$ entails a substantial simplification, since, by $\hat{v}_s'' = 0$, B vanishes and c/a reduces to $\hat{v}_s'''/4(2\hat{v}_s' + \eta)$.

REFERENCES

1. E. B. Dynkin, *Markov Processes* (Springer, New York, 1965).
2. D. Ryter, *Physica* **142A**: 103 (1987).
3. D. Ryter and H. Meyr, *Physica* **142A**:122 (1987).
4. H. Risken, *The Fokker–Planck Equation* (Springer, Berlin, 1983).
5. H. Dekker, *Physica* **135A**:80 (1986).
6. B. J. Matkovsky, Z. Schuss, and C. Tier, *J. Stat. Phys.* **35**:443 (1984).
7. V. I. Mel'nikov and S. V. Meshkov, *J. Chem. Phys.* **85**:1018 (1986).
8. G. H. Weiss, *J. Stat. Phys.* **42**:3 (1986).
9. P. Hänggi, *J. Stat. Phys.* **42**:105 (1986).
10. H. A. Kramers, *Physica* **7**:284 (1940).
11. P. Talkner and D. Ryter, in *Noise in Physical Systems and 1/f Noise* (North-Holland, Amsterdam, 1983).
12. D. Ryter, *Physica* **130A**:205 (1985).
13. M. Büttiker, E. Harris, and R. Landauer, *Phys. Rev. B* **28**:1268 (1983); H. Risken and K. Voigtlaender, *J. Stat. Phys.* **41**:825 (1985).