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LETTER TO THE EDITOR

# Exact solution of the diffusion in a bistable piecewise linear potential

H L Frisch†, V Privman‡, C Nicolis§ and G Nicolis‖

† Department of Chemistry, State University of New York at Albany, Albany, New York 12222, USA
‡ Department of Physics, Clarkson University, Potsdam, New York 13699, USA
§ Institut Royal Météorologique, av. Circulaire 3, 1180 Bruxelles, Belgium
‖ Faculté des Sciences de l'Université de Bruxelles, Campus Plaine, CP 231, Boulevard du Triomphe, 1050 Bruxelles, Belgium

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**Abstract.** An exact solution is obtained for the diffusion in the symmetric bistable W-shaped potential, by using the Laplace transform method. The results thus obtained are used to elucidate the status of the Kramers theory, usually formulated in the limit of large barrier height, as well as to find corrections to the Kramers approximation, and their relation to the pattern of singularities in the complex plane of the Laplace-transformed time variable. The probability mass within a given attraction basin is studied in detail. It is found to satisfy a non-Markovian dynamics in the general case, which reduces to a simple rate equation in the Kramers regime.

Fluctuation induced transitions between simultaneously stable states across a barrier are of great importance in a variety of fields such as chemical kinetics [1, 2], electrical circuits [3], condensed matter [4, 5], laser physics [6], geophysics [7–9]. Following Kramers' seminal work [10] extensive effort has been devoted to the asymptotic properties of a class of Langevin equations and the corresponding Fokker–Planck equations describing simple versions of the problem, particularly overdamped motion in potential systems [11–15]. The Fokker–Planck equation in this case can be solved exactly for the steady state, but not for the time-dependent behaviour. A detailed survey of the Kramers' problem has been published recently [16].

General results are available concerning primarily the mechanisms by which the diffusing particle, moving for a long time in the basin of attraction of one of the stable states associated with potential minima, jumps towards the basin of attraction of another stable state. In the simplest setting of a one-variable system with two stable states separated by a large barrier $\Delta U \gg D$, $D$ being an effective diffusion coefficient (or noise strength), this process is described by an exponential time dependence with the characteristic *Kramers time* [10–16] $\tau \sim \exp[\Delta U/D]$, where the prefactors are determined by the shape of the potential function at the tip of the barrier and at the initial minimum.

In addition to the asymptotic results, the validity of the Kramers approximation has also been tested by analytical (in some cases, exact closed form) solutions for model potentials [12, 17–21]. These potentials include double-square-well, double-parabolic, and certain other shapes. The standard transformation of the Fokker–

  

Planck equation to the Schrödinger form [22] has been generally used to interpret the analytical results thus obtained, in the Kramers regime. Indeed, it appears that the Kramers time is related to the inverse of the leading spectral gap of the Fokker–Planck operator. Specifically, the W-shaped potential considered in this work was studied in the Kramers asymptotic regime within the Schrödinger form approach [19].

Another development, initiated by Gardiner [13], focuses on the time evolution of the total probability mass, $N(t)$, of a given basin of attraction. In this view the Kramers' theory is an *adiabatic approximation*, whereby $N(t)$ varies slowly as compared to the time scales of diffusion within that basin of attraction. One is tempted to deduce that the process of jumping between the attractors could be viewed as a dichotomous noise of the random telegraph signal type. The question then arises to what extent the time variation of $N_j(t)$ for the different basins of attraction (labelled by $j$), can be approximated by the master equations (rate equations)

$$\frac{\mathrm{d}N_j}{\mathrm{d}t} = \sum_{i \neq j} \left( \frac{N_i}{\tau_{i \to j}} - \frac{N_j}{\tau_{j \to i}} \right) \tag{1}$$

where $\tau_{m \to n}$ are the appropriate Kramers time parameters, and $\sum_k N_k(t) = 1$.

In the present work we raise the issue of *corrections* to the Kramers limiting behaviour. This topic has been investigated in the existing literature on the analytical solutions of simple one-variable diffusion equations only for parabolic-like potentials/wells [16, 23–25]. For regular potentials $U(x)$ diverging faster than $\sim|x|$ at both $x = +\infty$ and $-\infty$, these corrections will be controlled by the next-to-leading spectral gaps (provided $\Delta U \gg D$ is satisfied). However, for the W-shaped or any other 1D potential $U(x)$ diverging in at least one of the limits $x \to +\infty$ or $-\infty$ as $|x|^\alpha$, with $\alpha \leq 1$, termed 'soft potentials' [26], calculation of corrections in the Schrödinger form would entail the evaluation of the contribution due to a *continuum of eigenstates* [26] (while the leading Kramers times are associated with the discrete spectrum).

Our objective here is to derive an exact solution of the diffusion in the W-shaped potential. We employ the *Laplace transform* method which in this case has distinct advantages in evaluating the corrections to the Kramers asymptotic limit. Indeed, we find that these corrections are obtained by the *integration over a branch cut* in the complex plane (while the Kramers type terms are associated with simple-pole singularities), which is a more transparent mechanism than summation over the continuous spectrum in the Schrödinger-form approach. Furthermore, the corrections become comparable to the Kramers contributions when the effective diffusion coefficient is of the order of the barrier height.

Our basic equation is the standard Fokker–Planck equation for the probability density $P(x,t)$ in the 1D diffusion,

$$\frac{\partial P}{\partial t} = D \frac{\partial}{\partial x} \left( \frac{\partial P}{\partial x} + \frac{P}{D} \frac{\mathrm{d}U}{\mathrm{d}x} \right). \tag{2}$$

The potential $U(x)$ is W-shaped, and we consider the symmetric case where all the linear segments have slopes $|U'| = w$, corresponding to the 'drift velocities' $\pm w$. Here $D$ is the diffusion constant (noise strength), while primes will generally denote differentiation with respect to $x$. With these definitions the tip barrier value $U(0)$ and the locations $x = \pm a$ of the minima of the W-shaped potential are related by

$$wa = rD \tag{3}$$

where

$$r \equiv U(0)/D.$$

Thus, the function $U(x)$ is given by $U(x) = \pm wx \pm Dr$, with the obvious choices of signs in the four regions: $(-,-)$ for $x < -a$; $(+,+)$ for $-a < x < 0$; $(-,+)$ for $0 < x < a$; and $(+,-)$ for $x > a$.

The Laplace transform method works for various piecewise linear potentials. However, the expressions obtained are extremely cumbersome. This is the reason for selecting the symmetric case. Furthermore, in order to obtain tractable results we will select the initial conditions exactly at the left minimum ($x = -a$), $P(x, t = 0) = \delta(x + a)$. Even with these assumptions most of the calculations had to be carried out by using the symbolic computer language MACSYMA.

In terms of the Laplace-transformed function

$$F(x,s) = \int_0^\infty e^{-st} P(x,t) dt \tag{4}$$

equation (2) takes the form

$$sF = DF'' + (U'F)' + \delta(x + a). \tag{5}$$

In the four regions between the points $x = -\infty, -a, 0, a, +\infty$, (5) reduces to the differential equations $DF'' \pm wF' - sF = 0$, where the sign is given by the slope of $U(x)$ in the appropriate region. It is convenient to introduce the function $q(s)$ suggested by the appropriate characteristic equations,

$$q \equiv \frac{a}{2D}\left(\sqrt{w^2 + 4Ds} - w\right). \tag{6}$$

Then the general solutions in the four regimes of interest are given by

$$F = A_0(s) e^{-(q+r)x/a} \qquad x > a \tag{7}$$

$$F = B_1(s) e^{(q+r)x/a} + B_2(s) e^{-qx/a} \qquad 0 < x < a \tag{8}$$

$$F = C_1(s) e^{qx/a} + C_2(s) e^{-(q+r)x/a} \qquad -a < x < 0 \tag{9}$$

$$F = E_0(s) e^{(q+r)x/a} \qquad x < -a. \tag{10}$$

The coefficients $A_0, B_{1,2}, C_{1,2}, E_0$ are determined by the conditions of the continuity of $P(x,t)$ and the probability current, at the special points $x = 0, \pm a$. The continuity of $P(x,t)$ implies the continuity of $F(x,s)$ and yields three equations. The continuity of the current is enforced by integrating (5) over the $x$ ranges $-a \pm \epsilon$, $0 \pm \epsilon$, and $a \pm \epsilon$, with an infinitesimal $\epsilon$. This yields the remaining three equations for the six unknown coefficients. For example, integration near $x = -a$ gives

$$(DF' + wF)_{x=-a_+} - (DF' - wF)_{x=-a_-} = -1 \tag{11}$$

where the $-a_+$ expression is calculated by putting $x = -a$ in (9), while the $-a_-$ expression is calculated by using (10). As already mentioned, the actual calculations were programmed in MACSYMA. Only the results are given here:

$$A_0 = r(r+2q)^2 \mathrm{e}^{2r+3q}/\mathcal{H} \tag{12}$$

$$B_1 = r^2(r+2q)\mathrm{e}^{q}/\mathcal{H} \tag{13}$$

$$B_2 = 2qr(r+2q)\mathrm{e}^{r+3q}/\mathcal{H} \tag{14}$$

$$C_1 = -2qr^2\mathrm{e}^{q}\left[\mathrm{e}^{r+2q}-1\right]/\mathcal{H} \tag{15}$$

$$C_2 = r\mathrm{e}^{q}\left[r^2+4q(r+q)\mathrm{e}^{r+2q}\right]/\mathcal{H} \tag{16}$$

$$E_0 = r\mathrm{e}^{r+q}\left[2qr+r(r-2q)\mathrm{e}^{r+2q}+4q(r+q)\mathrm{e}^{2(r+2q)}\right]/\mathcal{H} \tag{17}$$

$$\mathcal{H} \equiv 2qw\left[r+2q\mathrm{e}^{r+2q}\right]\left[2(q+r)\mathrm{e}^{r+2q}-r\right]. \tag{18}$$

These expressions yield a complete solution of the time-dependent problem in the Laplace-transformed form. Since the consideration of the $t$-dependence, obtained by the inverse Laplace transform, is in itself non-trivial, we will focus on one quantity: the probability mass $N_+(t)$ that the diffusing particle is found in the basin of attraction of the minimum at $x = a$ (while the initial conditions were $x = -a$), which is the inverse Laplace transform of

$$N_+(s) \equiv \int_0^\infty \mathrm{d}x\, F(x,s) = \frac{ar(r+2q)\mathrm{e}^{q}}{2qw(r+q)\left[r+2q\mathrm{e}^{r+2q}\right]}. \tag{19}$$

The inverse Laplace transform of $N_+(s)$, with the $s$-dependence entering via (6), involves a complex plane integration over a contour $s = \mathrm{Re}(s) + \mathrm{i}\sigma$, with fixed $\mathrm{Re}(s) > 0$, while $\sigma$ is varied in $(-\infty, +\infty)$. As usual, we shift the contour to run counterclockwise around the singularities of $N_+(s)$ on the relevant Riemann sheet, which all are at $\mathrm{Re}(s) \leq 0$. The most obvious singularity is the branch point at

$$s_{\mathrm{B}} = -\frac{w^2}{4D} \tag{20}$$

which suggests that the appropriate Riemann sheet is $\mathrm{Re}[(w^2+4Ds)^{1/2}] \geq 0$, provided the branch cut is selected along the negative real axis, at $-\infty < \mathrm{Re}(s) < s_{\mathrm{B}}$. Another obvious singularity is the simple pole at $s = 0$, due to the factor $q$ in the denominator of (19), the residue of which can be calculated and, as expected, is just $N_+(\infty) \equiv \frac{1}{2}$.

Let us now consider the possible singularities due to other factors in the denominator. First, the term $(r+q)$ yields a simple pole at $s = 0$ on the second Riemann sheet, which is of no consequences in our calculations. Secondly, we consider the equation $r + 2q\mathrm{e}^{r+2q} = 0$. The root corresponding to $2q = -r$ (coinciding in fact with $s = s_{\mathrm{B}}$), is cancelled by the factor $(r+2q)$ in the numerator. In addition, however, this equation has one real root and an infinite number of complex roots. One can establish by graphical analysis of the corresponding equations for $\mathrm{Re}(q)$ and $\mathrm{Im}(q)$ that the complex roots always lie in the second Riemann sheet of the complex-$s$ plane. (This is in fact a non-trivial analysis details of which are not given here.)

The remaining real root $s_{\mathrm{P}}(r)$ is on the correct Riemann sheet only for $r > 1$. For large $r$, we have

$$s_{\mathrm{P}}(r) \simeq -\frac{w^2}{2D}\mathrm{e}^{-r} \qquad (r \gg 1). \tag{21}$$

The residue of the corresponding pole in $N_+(s)$ is given in this limit by $-\frac{1}{2}+\mathrm{o}(\mathrm{e}^{-r})$. However, as $r$ is decreased towards $r=1$, the function $s_\mathrm{P}(r)$ approaches the value $s_\mathrm{B}$. This function cannot be obtained in closed form. Its general trend for $r \geq 1$ is similar to the approximate expression (21) except that near $r=1^+$ the full function has zero slope. The corresponding pole in the complex-$s$ plane approaches and enters the tip of the branch cut as $r \to 1^+$, and emerges on the second Riemann sheet for $0<r<1$.

The above analysis suggests that for $r>1$ we can generally write $N_+(t)-\frac{1}{2}=N_\mathrm{P}(t)+N_\mathrm{B}(t)$, were the notation is self-explanatory. The pole contribution, which has the exponential time dependence, dominates for long times when $r \gg 1$, corresponding to $U(0) \gg D$. In this limit it is given by

$$N_\mathrm{P}(t)=\mathrm{residue}(r)\exp(-|s_\mathrm{P}(r)|t) \simeq -\frac{1}{2}\exp\left(-\frac{w^2\mathrm{e}^{-r}}{2D}t\right). \tag{22}$$

The contribution due to the branch cut, obtained by integrating the discontinuity along it in a standard fashion, can be evaluated for long times. We only quote the result of this lengthy calculation

$$N_\mathrm{B} \approx -\frac{a\sqrt{D}\mathrm{e}^{-r/2}}{\sqrt{\pi}w^2(r-1)^2}t^{-3/2}\exp\left(-\frac{w^2}{2D}t\right) \qquad (r \neq 1, t \to \infty). \tag{23}$$

Note that $N_\mathrm{B}$ becomes comparable to $N_\mathrm{P}$ when $r>1$ is of O(1).

For $r \leq 1$, there is no pole contribution so that formally one can put $N_\mathrm{P} \equiv 0$. The branch cut contribution is then the only time dependence present. It turns out that the long-time limiting form for $r<1$ is still given by (23). However, at $r=1$ a special behaviour is found

$$N_\mathrm{B} \approx -\frac{2\sqrt{a}}{\sqrt{\pi w\mathrm{e}}}t^{-1/2}\exp\left(-\frac{w^2}{2D}t\right) \qquad (r=1, t \to \infty). \tag{24}$$

Finally, we note that the short-time behaviour of $N_+(t)$ can be calculated by a different approach not detailed here. The leading order result is

$$N_+(t \to 0) \approx \frac{\mathrm{e}^{-r}\sqrt{t}}{\sqrt{\pi}aD^{3/2}}\exp\left(-\frac{a^2D}{2t}\right) \tag{25}$$

illustrating the expected essential singularity at $t=0$.

It is instructive to compare the explicit expressions with the results available in the literature. First, we note that the complex plane pattern of singularities in the Laplace transform formulation is reminiscent of the eigenvalue spectrum in the Schrödinger form [19]. Indeed, $|s_\mathrm{P}(r)|$ corresponds to the gap due to the discrete excited state, while $|s_\mathrm{B}(r)|$ equals the gap value of the edge of the continuous spectrum.

Next consider the case of large $r$. Turning to eq. (1), we note that in the present case, due to the symmetry of the potential, the two time parameters $\tau$ are equal. By using the relation $N_- = 1-N_+$, we can reduce the two equations ($\pm$) to the form

$$\frac{\mathrm{d}}{\mathrm{d}t}N_+(t)=-\frac{2}{\tau}\left(N_+(t)-\frac{1}{2}\right). \tag{26}$$

Thus in the symmetric case there is an extra factor of 2 relating the Kramers time and the decay rate in, e.g., (22). Our calculations thus suggest $\tau=(4D/w^2)\mathrm{e}^r$.

The original Kramers formulation [10], when put in our notation, suggests the relation

$$\tau = D^{-1}\left[\int_{-a}^{a} \mathrm{d}x \exp\left(\frac{\Delta U(x)}{D}\right)\right]\left[\int_{-\infty}^{\infty} \mathrm{d}x \exp\left(\frac{-\Delta U_{-}(x)}{D}\right)\right] \tag{27}$$

where $\Delta U(x) \equiv U(x) - U(-a) = U(x)$; see also [26] for a discussion of relations of this kind. The first integral here is over the barrier region and is usually approximated by the quadratic expansion near the tip. In our case the barrier is not quadratic. However, the potential is simple enough to calculate the exact value, $(2D/w)\mathrm{e}^{r} + \mathrm{O}(1)$. The second integral is about the minimum at $x = -a$, and $\Delta U_{-}(x)$ is a *single-minimum potential* which describes the shape of $\Delta U(x)$ at $-a$. Again, the usual quadratic approximation does not apply here. We take, instead, $\Delta U_{-}(x) = w|x + a|$. The second integral in (27) then yields $2D/w$. Collecting the results, we obtain the $\tau$ value consistent with the exact solution and with the Markovian character of the process governing the transitions between the two attractors. When on the other hand $r$ is of the order of unity, the dynamics is non-Markovian.

In summary, this work illustrates by exact calculations for the W-shaped potential how the Kramers regime emerges as the leading order in some approximate limit, and how the corrections to this result can be associated with the complex plane singularities in the Laplace transform formulation—which is particularly useful in cases when the Schrödinger formulation involves a continuous eigenspectrum—and can even dominate the long-time behaviour in certain conditions.

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