Kramers' rate for systems with multiplicative noise

Alexandre Rosas, Italo'Ivo Lima Dias Pinto, and Katja Lindenberg

Phys. Rev. E **94**, 012101 — Published 1 July 2016

DOI: 10.1103/PhysRevE.94.012101

Kramers' rate for systems with multiplicative noise

Alexandre Rosas*
Departamento de Física, CCEN, Universidade Federal da Paraíba, Caixa Postal 5008, 58059-900, João Pessoa, Brazil

Italo'Ivo Lima Dias Pinto and Katja Lindenberg
Department of Chemistry and Biochemistry, and BioCircuits Institute, University of California San Diego, La Jolla, California 92093-0340, USA

The Kramers' rate for passage of trajectories $X(t)$ over an energy barrier due to thermal or other fluctuations is usually associated with additive noise. We present a generalization of the Kramers' rate for systems with multiplicative noise. We show that the expression commonly used in the literature for multiplicative noise is not correct, and we present results of numerical integrations of the Langevin equation for $dX(t)/dt$ evolving in a quartic bistable potential which corroborate our claim.

I. INTRODUCTION

A key quantity in many problems involving the escape from a metastable state, or the transition between two stable states separated by a high barrier, is the so-called Kramers' escape rate, that is, the inverse of the average time required to cross over the barrier. The most common scenario is that of a potential energy with two minima separated by a high energy maximum that can be overcome by thermal fluctuations alone (for example, "absolute rate theory" for chemical reactions), or together with a weak signal (the "stochastic resonance" problem). There is a vast literature on this subject (see, for example, [1, 2] and references therein).

One common way to formulate Kramers' escape rate problems is as a Langevin equation for the evolution of trajectories, $X(t)$, often in terms of a single variable (i.e., a one-dimensional formulation). Most cases involving Kramers' escape rates in these formulations are restricted to systems with additive noise. If the fluctuations in these Langevin equations are Gaussian and δ-correlated, the problem can easily be transformed to a Fokker-Planck equation (with constant diffusion coefficient D), that is, to a partial differential equation for the probability density $P(x,t)$ such that $P(x,t)dx$ is the probability that a measurement of $X(t)$ yields a result between x and $x+dx$. There are many physical, biological, ecological, economics, etc., problems that admit such a description. In each of these the meaning of $X(t)$ is of course appropriate for that model. In particular, $X(t)$ need not represent the trajectory of a massive particle, although it does in some cases. We explicitly add this remark because this interpretation is often assumed. In this case, the one-dimensional Langevin equation describes the trajectory of an overdamped particle.

In the past two decades or so there have been several attempts to deal with multiplicative noise, often in the context of stochastic resonance. These attempts have dealt with such models theoretically [3–13], numerically [13–17], and experimentally [18, 19]. It is interesting to note that there seems to have been no comparison of any of the theoretical results with experiments or with simulations.

We are interested in exploring the Kramers' escape rate problem in systems with space-dependent diffusion coefficients $D(x)$. For such systems (in one dimension), a suitable change of the variable can map the Fokker-Planck equation into another Fokker-Planck equation with a constant diffusion coefficient, for which the Kramers' escape rate can, in principle, be calculated [20]. However, this change of the variable requires a non-trivial integration of the inverse of the square root of the original space-dependent diffusion coefficient, as well as the calculation of an inverse function, as discussed in the next section. Except for very particular cases, this procedure is in general quite complex and can, in fact, not be completed analytically.

Here we propose an alternative way of obtaining the Kramers' escape rate which does not involve any calculation of inverse functions and can readily be applied to Fokker-Planck equations with space-dependent diffusion coefficients. We call this the "direct approach". Some specific isolated examples that use a direct approach but that do not point to a general method can be found in the literature [10]. In this latter reference, for instance, the discussion starts with a particular example of a system with multiplicative noise. A mean escape time (inverse of the Kramers' rate) is calculated for that example, and the form obtained for this particular case is generalized in an ad hoc way to include all examples of this form. In two other approaches, portions of the multiplicative noise problem are included but others are not.

In this paper we derive the general form of the Kramers' rate associated with systems driven by multiplicative noise. In Sec. II we start with a general one-dimensional Fokker-Planck equation with space-dependent diffusion and first show in detail why conversion (by change of variables) to a Fokker-Planck equation for additive noise is not a practical way to pro-

*Electronic address: arosas@fisica.ufpb.br

ceed. Instead, we directly formulate a direct approach to calculate the Kramers' rate associated with the original Fokker-Planck equation. In Sec. III we implement this approach and arrive at an explicit form of the Kramers' rate. We also exhibit two other rates used for the same problems in the literature that we assert are not the correct Kramers' rates. In Sec. IV we then consider the example of a bistable system with both additive and multiplicative noise. We calculate the Kramers' rate for passage from one well to the other using our formula, one of the incorrect formulas, and the result obtained by numerical simulations. That our result is the correct one is incontrovertible. Finally, we end with a short summarizing conclusion in Sec. V.

II. THE FOKKER-PLANCK EQUATION

Our starting point is the Fokker-Planck equation with space-dependent drift and diffusion,

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left[F(x)P(x,t)\right] + \frac{\partial^2}{\partial x^2}\left[G(x)P(x,t)\right]. \quad (1)$$

This Fokker-Planck equation is associated with the Langevin equation

$$\dot{X} = -U'(X) + g(X)\xi(t) + \eta(t), \quad (2)$$

where $U(X)$ is the "deterministic" potential, the prime denotes a derivative with respect to the argument, $\xi(t)$ and $\eta(t)$ are mutually uncorrelated Gaussian δ-correlated noises of zero mean,

$$\begin{aligned} \langle \xi(t)\xi(t')\rangle &= 2D_M\delta(t-t'), \\ \langle \eta(t)\eta(t')\rangle &= 2D_A\delta(t-t'), \end{aligned} \quad (3)$$

and the space-dependent diffusion coefficient $G(x)$ (called $D(x)$ in the Introduction) is given by

$$G(x) \equiv D_M g^2(x) + D_A. \quad (4)$$

With the Stratonovich interpretation for multiplicative noise, which we subsequently use, we have

$$F(x) = -U'(x) + \frac{1}{2}G'(x). \quad (5)$$

With the Itô interpretation, $F(x) = -U'(x)$. The Fokker-Planck equation yields the probability density $P(x,t)$ that at time t a measurement of the random variable $X(t)$ yields the value x.

The multiplicative noise problem can be transformed to one associated with additive noise via a change of variables from x to y and correspondingly from $X(t)$ to $Y(t)$. The change of variables is (see, for example, [20])

$$y(x) = \int^x \left[\frac{D}{G(x')}\right]^{1/2} dx', \quad (6)$$

where the lower limit and D can both be chosen arbitrarily. One can then write the Fokker-Planck equation for the probability distribution

$$\widetilde{P}(y,t) = \left[\frac{G(x)}{D}\right]^{1/2} P(x,t) \quad (7)$$

as follows:

$$\frac{\partial \widetilde{P}(y,t)}{\partial t} = -\frac{\partial}{\partial y}\left[\widetilde{F}(y)\widetilde{P}(y,t)\right] + D\frac{\partial^2}{\partial y^2}\left[\widetilde{P}(y,t)\right]. \quad (8)$$

D can thus be identified as the diffusion constant in the additive noise version. The explicit definition of D is obtained from Eq. (6) as

$$D = \left(\frac{dy}{dx}\right)^2 G(x). \quad (9)$$

The new drift term is given by

$$\widetilde{F}(y) = \sqrt{\frac{D}{G(x)}}\left[F(x) - \frac{1}{2}G'(x)\right], \quad (10)$$

and the new Langevin equation is

$$\dot{Y} = \widetilde{F}(Y) + \zeta(t), \quad (11)$$

where $\zeta(t)$ is another Gaussian δ-correlated noise with zero mean and

$$\langle \zeta(t)\zeta(t')\rangle = 2D\delta(t-t'). \quad (12)$$

The problem with this approach is that in order to write the new drift term $\widetilde{F}$ explicitly as a function of y we need to perform the integral in Eq. (6) and calculate the inverse function in order to obtain $x(y)$ and use it in Eq. (10). Except for very simple cases, this task is analytically impossible. We therefore follow an alternative route.

Our approach is to directly calculate the Kramers' rate associated with the original Fokker-Planck equation, Eq.(1), with the space-dependent diffusion term. We follow a path similar to that used in Ref. [20], but allow the diffusion contribution to vary in space. We will later compare our results with two others that have appeared in the literature and that we assert are incorrect, as confirmed in at least one of the two cases by numerical simulations (the other case has a fundamental flaw and does not need to be compared, as will be discussed later).

As in the constant diffusion case, we want to calculate the escape rate from a deep well over a high barrier, so that the probability current over the top of the barrier is very small and the probability density in the well is almost time-independent. In other words, the system behaves as if it were in a steady state. Consequently, the probability density inside the well is well described by the steady state probability density

$$P_{ss}(x) = \frac{K}{G(x)}\exp\left[\int^x \frac{F(x')}{G(x')}dx'\right] = Ke^{-U_{eff}(x)}, \quad (13)$$

where K is a normalization constant, the lower limit of the integral is arbitrary, and the upper limit x is deep inside the well. We have defined the effective potential $U_{eff}(x)$ as

$$U_{eff}(x) = \ln\left[G(x)\right] - \int^{x} \frac{F(x')}{G(x')}dx'. \tag{14}$$

The condition that the well is deep is contained in the inequality

$$U_{eff}(x_{max}) \gg U_{eff}(x_{min}), \tag{15}$$

where x_{max} (x_{min}) is the position of the maximum (minimum) of $U_{eff}(x)$, that is, the top of the barrier (bottom of the well).

The flow of probability outward across a point x at time t, $\partial S(x,t)/\partial x$, is related to the rate of change of the probability at that point, $\partial P(x,t)/\partial t$, by the continuity equation:

$$-\frac{\partial S(x,t)}{\partial x} = \frac{\partial P(x,t)}{\partial t}. \tag{16}$$

In terms of the effective potential, the probability current is given by

$$S(x,t) = -G(x)e^{-U_{eff}(x)}\frac{\partial}{\partial x}\left[e^{U_{eff}(x)}P(x,t)\right]. \tag{17}$$

Since we are considering a quasi-steady state regime, we have

$$-\frac{\partial S(x,t)}{\partial x} = \frac{\partial P(x,t)}{\partial t} \simeq 0 \quad \Rightarrow \quad S(x,t) \simeq S_0. \tag{18}$$

Therefore, rearranging Eq.(17) and integrating from x_{min} to a given point $x = q$ on the other side of the high potential barrier, we have

$$S_0 \int_{x_{min}}^{q} \frac{e^{U_{eff}(x')}}{G(x')}dx' = -\Big[e^{U_{eff}(q)}P(q,t) - e^{U_{eff}(x_{min})}P(x_{min},t)\Big]. \tag{19}$$

Note that once a trajectory crosses the barrier, the time it takes to arrive anywhere in the other well is very short. Hence the precise location of q does not matter. Assuming that at time t most of the probability is still in the initial well so that $P(q,t)$ is small, we have

$$S_0 = \frac{e^{U_{eff}(x_{min})}P(x_{min},t)}{\int_{x_{min}}^{q}\frac{e^{U_{eff}(x')}}{G(x')}dx'}. \tag{20}$$

The probability p of finding the system in the initial well is

$$p = \int_{x_1}^{x_2} P(x',t)dx', \tag{21}$$

where x_1 and x_2 are two points around x_{min} such that the probability of finding the system outside of the interval $[x_1, x_2]$ is vanishingly small. Since for weak noise the system rapidly decays to the bottom of the well, the probability of finding the system far away from x_{min} is exponentially small, and x_1 and x_2 need not be carefully specified. Deep in the well the probability density is quasi-stationary, so we can use Eq. (13),

$$P(x,t) \simeq P_{ss}(x) = P_{ss}(x_{min})e^{[U_{eff}(x_{min})}e^{-U_{eff}(x)]}. \tag{22}$$

Here we have explicitly exhibited the normalization constant $K = P_{ss}(x_{min})e^{U_{eff}(x_{min})}$. We can then write the probability p as

$$p = P(x_{min},t)e^{U_{eff}(x_{min})}\int_{x_1}^{x_2} e^{-U_{eff}(x')}dx'. \tag{23}$$

Equations (20) and (23) are the main results of this section and will be used in the next section to calculate the Kramers' rate.

III. THE KRAMERS' RATE

The characteristic time T_K that the system spends in the initial well is given by the ratio of the probability of the system being in the well over the probability flow over the barrier away from the well. This time is the inverse of the escape rate r_K from the well:

$$T_K = \frac{1}{r_K} = \frac{p}{S_0} = \int_{x_1}^{x_2} e^{-U_{eff}(x')}dx' \int_{x_{min}}^{q} \frac{e^{U_{eff}(x')}}{G(x')}dx'. \tag{24}$$

The subscript K stands for Kramers. The integrand of the second integral can be rewritten as

$$\frac{e^{U_{eff}(x)}}{G(x)} = \exp\left[U_{eff}(x) - \ln G(x)\right] = e^{\widehat{U}_{eff}(x)}, \tag{25}$$

where we have defined

$$\widehat{U}_{eff}(x) = -\int^{x} \frac{F(x')}{G(x')}dx'. \tag{26}$$

Hence, we have that,

$$T_K = \frac{1}{r_K} = \int_{x_1}^{x_2} e^{-U_{eff}(x')}dx' \int_{x_{min}}^{q} e^{\widehat{U}_{eff}(x')}dx'. \tag{27}$$

Each of the potentials $U(x)$ and $\widehat{U}(x)$ has a deep well where most of the probability distribution resides and a high barrier crossed due to thermal fluctuations. It follows that the integrand of the leftmost integral is highly peaked around the minimum of U_{eff}, already labeled x_{min}, and that of the rightmost integrand around the maximum of $\widehat{U}_{eff}$, defined as $\widehat{x}_{max}$. It is therefore valid to expand each of the potentials around the appropriate

extremum and retain terms up to second order, respectively, yielding

$$U_{eff}(x) \approx U_{eff}(x_{min}) + \frac{U''_{eff}(x_{min})}{2}(x - x_{min})^2,$$
$$\widehat{U}_{eff}(x) \approx \widehat{U}_{eff}(\widehat{x}_{max}) + \frac{\widehat{U}''_{eff}(\widehat{x}_{max})}{2}(x - \widehat{x}_{max})^2. \tag{28}$$

Using these expansions in Eq. (27), and extending the limits of integration to go from $-\infty$ to $+\infty$ (which can safely be done because the integrands are highly peaked), we arrive at Gaussian integrals that can readily be performed analytically, leading to the Kramers' rate

$$r_K = (2\pi)^{-1}\sqrt{-\widehat{U}''_{eff}(\widehat{x}_{max})U''_{eff}(x_{min})} \times \exp\left[-\widehat{U}_{eff}(\widehat{x}_{max}) + U_{eff}(x_{min})\right]. \tag{29}$$

If a more accurate result is desired, one can easily keep terms up to fourth order in the expansion (28). Equation (29) is the principal result of this paper.

Several papers in the literature have presented incorrect calculations of the Kramers' rate (or the average escape time) over a barrier for systems with multiplicative noise. For instance, [4–9, 17] present the following expression for the Kramers' rate (the notation is adapted to ours for comparison):

$$r^*_K = (2\pi)^{-1}\sqrt{-U''(x_+)U''(x_0)} \times \exp\left[-U_{eff}(x_+) + U_{eff}(x_0)\right], \tag{30}$$

where x_+ and x_0 are the maximum and minimum of the deterministic potential $U(x)$ of Eq. (2). We will show in a particular example that the inverse of the mean escape time obtained by performing an average over realizations of the direct integration of the Langevin equation, Eq. (2), for that example does not agree with this expression, but is well approximated by Eq. (29).

The other expression we found in the literature appears in Ref. [13], where it is said that the escape rate can be calculated using the effective potential U_{eff} instead of the deterministic potential that appears in the additive noise case,

$$r^\dagger_K = (2\pi)^{-1}\sqrt{-U''_{eff}(x_{max})U''_{eff}(x_{min})} \times \exp\left[-U_{eff}(x_{max}) + U_{eff}(x_{min})\right]. \tag{31}$$

This expression has an additional fundamental flaw: it does not reduce to the additive noise result when one has both additive and multiplicative noise, and the multiplicative noise is allowed to vanish at the end of the calculation. Instead, in this limit the escape rate appears divided by the additive noise diffusion constant. Therefore, we will not discuss this case any further.

IV. A PARTICULAR EXAMPLE

As a test case, consider a simple bistable system under the influence of both additive and multiplicative noise, described by the Langevin equation

$$\dot{X} = aX - bX^3 + X\xi(t) + \eta(t), \tag{32}$$

where a and b are positive constants, and $\xi(t)$ and $\eta(t)$ are mutually uncorrelated Gaussian fluctuations with zero mean and correlations given in Eq. (3). Using the Stratonovich formalism, the functions F and G in the Fokker-Planck equation, Eq. (1), now are

$$F(x) = ax - bx^3 + D_M x, \tag{33}$$

$$G(x) = D_M x^2 + D_A. \tag{34}$$

For this simple model, the escape rate expressions Eqs. (29) and (30) can be calculated analytically, leading to

$$r_K = \sqrt{\frac{[D_M(a-D_M)+bD_A]\,(a^2-D_M^2)}{2\pi D_A b}} \times \exp\left[\frac{D_M(a-D_M)-(D_M(a+D_M)+bD_A)\log\left(\frac{D_M(a-D_M)}{bD_A}+1\right)}{2D_M^2}\right] \tag{35}$$

and

$$r_K^* = \frac{a}{\sqrt{2}\pi}\exp\left[-\frac{(D_M(a+D_M)+bD_A)\log\left(\frac{aD_M}{bD_A}+1\right)-aD_M}{2D_M^2}\right]. \tag{36}$$

In the limit of vanishing multiplicative noise, $D_M \to 0$, both expressions give the same familiar result for the average escape rate, $[a/\sqrt{2}\pi]e^{-a^2/4bD_A}$, but when the multiplicative noise increases, so does the difference between r_K and r_K^*. In Fig. 1, we show an example of how the two results differ, and compare these with the outcome of the numerical integration of the Langevin equation Eq. (32). This numerical integration was performed as follows. The initial condition in all the integrations was set at one of the minima of the effective potential $U_{eff}(x)$, and the trajectory was allowed to evolve according to the Langevin equation until it reached the other minimum. We recorded the time it took the trajectory to arrive at the other minimum as the escape time. We repeated this process for 1,000 runs and calculated the average time it took the system to go from one minimum to the other. We equated the Kramers' rate with the inverse of this mean escape time. Since the potential is symmetric, the time it takes from either minimum to the other is the same.

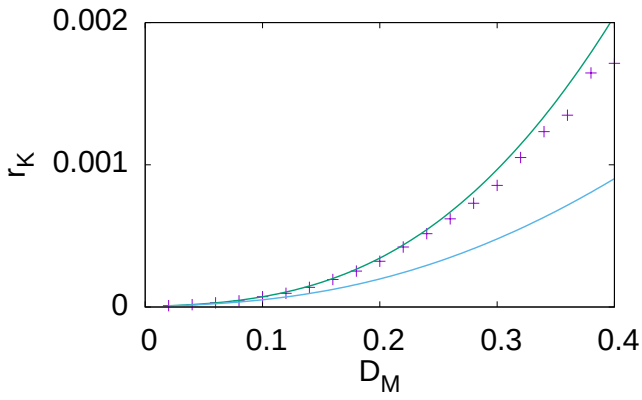

FIG. 1: Transition rates vs multiplicative noise strength parameter D_M, calculated directly from the integration of the Langevin equation (averaged over 1000 samples), crosses; from Eq. (35), top curve; and from Eq. (36), bottom curve. The values of the other parameters are $a = 5.0$, $b = 1.0$, and $D_A = 0.5$.

It is clear from the figure that the agreement of our result, Eq. (35), and the result of the integration of the Langevin equation, is excellent, and that both differ from the result (36). The difference between our results and the direct integration at high values of D_M is a consequence of the fact that here the multiplicative fluctuations are large, or, correspondingly, the barrier is no longer so high. We note that for this example the analytic transition rates obtained in Ref. [10] also fall essentially on top of our analytic curve in Fig. 1 (result not shown), but that our analytic result (29) differs from theirs. Specifically, direct comparison leads to the conclusion (in our notation) that instead of using the minimum of $U_{eff}(x)$ and the maximum of $\widehat{U}_{eff}(x)$, the potentials shifted from the deterministic potential by the multiplicative noise, in their steepest descent implementation they work with the extrema of the deterministic potential. We expect the differences in the results not to be major not only for this particular example but more generally when the shifts are small, which is the case when the barrier is high relative to the fluctuations.

V. CONCLUSION

In this paper we have derived an explicit expression for the Kramers' transition rate from one potential well over a potential barrier for systems with multiplicative noise. Our starting point was a one-dimensional Fokker-Planck equation, and our basic assumptions were similar to the two hypotheses usually made in the purely additive noise case, namely, that the system is in the adiabatic limit (that is, the relaxation to equilibrium is much faster than any other process), and that the (effective) potential barrier is high. We explained why our result differs from one that has been incorrectly used in the literature. We have shown via an explicit example that the integration of the Langevin equation corroborates our result. Our

findings can be used to explain existing numerical results in a variety of escape problems involving multiplicative noise. One particularly interesting problem that we are now able to reproduce with our theory is that of stochastic resonance in the presence of multiplicative noise [21].

Acknowledgments

AR acknowledges Capes for its support (No. 99999.000296/2015-05). ILDP acknowledges the CNPq for financial support. KL acknowledges the support of the US Office of Naval Research (ONR) under Grant No. N00014-13-1-0205.

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