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Inertial Effects on the Escape Rate of a Particle Driven by Colored Noise: An Instanton Approach

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A recent calculation, in the weak-noise limit, of the rate of escape of a particle over a one-dimensional potential barrier is extended by including an inertial term in the Langevin equation. Specifically, we consider a system described by the Langevin equation $m\ddot{x} + \dot{x} + V'(x) = \xi$, where ξ is a Gaussian colored noise with mean zero and correlator $\langle \xi(t)\, \xi(t') \rangle = (D/\tau) \exp(-|t-t'|/\tau)$. A path-integral formulation is augmented by a steepest descent calculation valid in the weak-noise ($D \to 0$) limit. This yields an escape rate $\Gamma \sim \exp(-S/D)$, where the "action" S is the minimum, over paths characterizing escape over the barrier, of a generalized Onsager–Machlup functional, the extremal path being an "instanton" of the theory. The extremal action S is calculated analytically for small m and τ for general potentials, and numerical results for S are displayed for various ranges of m and τ for the typical case of the quartic potential $V(x) = -x^2/2 + x^4/4$.

KEY WORDS: Langevin equation; path integral; colored noise; instanton.

1. INTRODUCTION

The problem of calculating the escape rate for activation over a potential barrier due to colored external noise has been the focus of an explosion of interest (and much controversy) in recent years.[1-10],[2] The difficulties stem from the absence of a simple generalization of the Fokker–Planck equation when the noise is colored (i.e., has nonzero correlation time), which is in turn a consequence of the non-Markov character of the process. Very

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[2] See ref. 1 for recent reviews on the topic of external noise.

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recently, however, a new approach has been introduced,[11] in which a path-integral formulation is combined with a steepest-descent approach to obtain exactly the leading dependence of the escape rate Γ on the noise strength D for $D \to 0$, namely $\Gamma \sim \exp(-S/D)$, where the "action" S reduces to the height of the potential barrier only for white noise. More generally, S is given by the minimum, over paths characterizing escape over the barrier, of a generalized "Onsager–Machlup functional"[12] that plays a role analogous to the action in the path-integral formulation of quantum mechanics (and will be termed such below). The corresponding extremal path is an "instanton" of the theory.[11],[3]

So far, most effort as far as colored noise is concerned has been directed at the overdamped limit, in which the Langevin equation (see below) involves only a first derivative with respect to time. In this paper, we apply the recently developed path-integral methods to derive, for the first time, results for the escape rate when an inertial term (involving a second time derivative) is included in the Langevin equation. The white-noise limit of this problem has been studied extensively, with renewed interest in recent years[14–19] following Kramers's original classic work.[20] Apart from some analogue simulations,[21] however, there seems to have been very little work including both colored noise and inertial effects.

We consider a system described by the Langevin equation

$$m\ddot{x} + \alpha\dot{x} + V'(x) = \xi(t) \tag{1}$$

where $\xi(t)$ is a colored Gaussian noise with zero mean. For definiteness, we will assume that the noise correlator has the standard exponential form

$$\langle \xi(t)\, \xi(t') \rangle = (D/\tau) \exp(-|t - t'|/\tau) \tag{2}$$

corresponding to the simplest non-Markov process.[22] These equations describe the motion of a damped particle of mass m moving in a potential $V(x)$ under the influence of a stochastic force $\xi(t)$. [Note that in (1) and hereafter dots and primes represent derivatives with respect to t and x, respectively.] Henceforth we choose units of time such that $\alpha = 1$. We consider the particle to be initially located at a minimum of V, and are interested in calculating the escape rate Γ over a potential barrier. A typical potential of interest is shown in Fig. 1. The process we are considering is the activation of a particle, initially located at the point a in the left-hand well, over the barrier and into the right-hand well.

In the white noise limit ($\tau = 0$), Eq. (1) describes a Markov process and we may use the Fokker–Planck equation to find the conditional joint

[3] See refs. 13 for a general introduction to instanton methods.

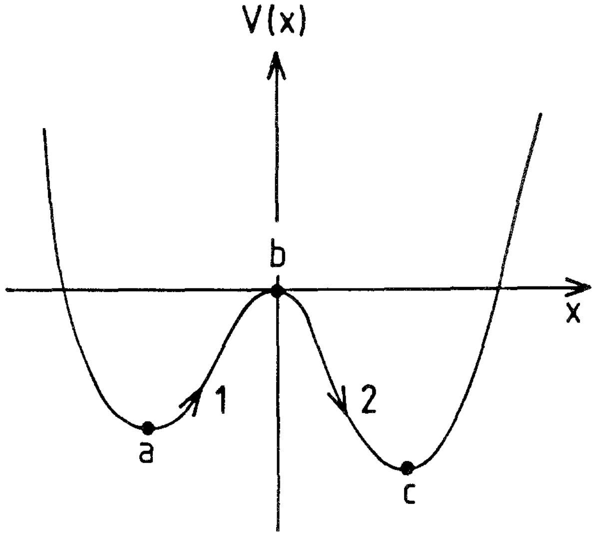

Fig. 1. Typical potential considered in this paper. The rate of escape Γ from the left-hand well is governed by the "action" S of the instanton associated with the "uphill" path labeled 1: $\Gamma \sim \exp(-S/D)$. The instanton associated with the "downhill" path 2 has zero action.

probability distribution $P(\dot{x}, x, t \mid \dot{x}_0, x_0, t_0)$ for the position and velocity of the particle. To deal with the non-Markov process ($\tau > 0$) defined above, we shall use a path-integral formulation of the Langevin equation, which is well suited to the weak noise limit via a steepest descent calculation. A detailed discussion of the path-integral formulation for non-Markov processes is given in ref. 22.

Our principal results are for the extremal "action" S, which determines the escape rate in the weak noise limit via $\Gamma \sim \exp(-S/D)$. The evaluation of the prefactor is beyond the scope of the present paper: it requires the inclusion of small fluctuations around the extremal path, as well as multi-instanton contributions. Analytic results for S are derived, for general potentials, for small m and τ, and also for general m and large τ. For any specified potential, S may be found numerically for arbitrary values of m and τ with the proviso that $\tau > 2m$ for $m > 1/4v''(a)$. [This restriction is a technical one, associated with the requirement (see below) that the instanton solution be nonoscillatory.] In this paper all numerical results are obtained for the quartic potential, $V(x) = -x^2/2 + x^4/4$.

2. THE INSTANTON APPROACH

In this section, a path-integral representation is given for the conditional probability that the particle is in the right-hand well at time T, given that it was at point a of Fig. 1 (with zero velocity and acceleration) at time zero, and the equation which determines the most probable ("instanton") path is derived. The equation is solved, analytically and numerically, in subsequent sections. We shall not dwell on the formal subtleties involved in setting up the path integral, since these have been discussed in detail elsewhere[22]: this paper is concerned with results rather than formalism.

For Gaussian noise with correlator defined by (2), the noise probability weight is given by[11,22]

$$P[\xi] \propto \exp\left[-(1/4D)\int_{-\infty}^{\infty} dt\,(\xi^2+\tau^2\dot{\xi}^2)\right] \tag{3}$$

For a more general correlator, the functional in (3) would contain terms with higher order derivatives of ξ. In this sense, the exponential correlator in (2) represents the simplest non-Markov process.[22] We now use (3) to express the probability weight for the paths $\{x(t)\}$ by expressing ξ in terms of x using (1):

$$P[x] \propto J[x]\exp(-S[x]/D) \tag{4}$$

where the "Onsager–Machlup functional," or "action," $S[x]$ is

$$S[x]=(1/4)\int_{-\infty}^{\infty} dt\,\{[m\ddot{x}+\dot{x}+V'(x)]^2+\tau^2[m\dddot{x}+\ddot{x}+V''(x)\dot{x}]^2\} \tag{5}$$

The Jacobian $J[x]$ of the transformation is independent of D and will not alter the leading small-D expression in the exponent in (4).[11]

The construction of a conditional probability density requires, in general, an adequate specification of the process under consideration.[22] For the system described by (1) and (2) one needs, in principal, to impose three conditions at the earlier time, e.g., the values of x, $\dot{x}$, and $\ddot{x}$ (or, equivalently, of x, $\dot{x}$, and ξ). One way to see this is to observe that the noise correlator (2) is generated by the Ornstein–Uhlenbeck process

$$\tau\dot{\xi} = -\xi+\eta \tag{6}$$

where η is a *white* noise of strength D, i.e.,

$$\langle\eta(t)\,\eta(t')\rangle = 2D\delta(t-t') \tag{7}$$

provided the initial condition on ξ is imposed in the distant past. Eliminating ξ then yields the Langevin equation

$$\tau[m\dddot{x}+\ddot{x}+V''(x)\dot{x}]+m\ddot{x}+\dot{x}+V'(x)=\eta(t) \tag{8}$$

from which a conventional Fokker–Planck equation can be derived for the conditional probability $P(x, \dot{x}, \ddot{x}, t \mid x_0, \dot{x}_0, \ddot{x}_0, t_0)$. The "simplest colored noise" (2) effectively enlarges the dimension of the space by one. This Fokker–Planck equation is not, however, a convenient starting point for the calculation of escape rates. The latter emerge cleanly, however, from the path-integral formulation below.

While the above discussion is important for the calculation of general conditional probabilities, the calculation of escape rates is simplified by the fact (see below) that the dominant instanton paths begin and end at turning points of the potential, and have the property that $\dot{x}$ and all higher derivatives vanish at these turning points. Therefore, as far as the calculation of escape rates is concerned, we need only specify the position of the particle. In this connection, the alert reader will have noticed that the probability weight $P[x]$ derived from (7) and (8), using $P[\eta] \propto \exp[-(1/4D) \int dt\, \eta^2]$, would be described by an action $S[x]$ which differs from (5) by the appearance of a "cross term" $2\tau\xi\dot{\xi}$ [where ξ means the left-side of Eq. (1)] in the integrand. This term, however, is a perfect differential, whose integral yields boundary terms which vanish for an instanton path. The manner in which the two forms for $S[x]$ yield equivalent results more generally is discussed in detail in ref. 22.

With the above remarks in mind, the conditional probability density for the particle to be at the point c of Fig. 1 at time $T/2$, given that it was at point a at time $-T/2$, is given by the path integral

$$P(c, T/2 \mid a, -T/2) \propto \int_{x(-T/2)=a}^{x(T/2)=c} d[x]\, J[x] \exp(-S[x]/D) \tag{9}$$

In the weak noise limit ($D \to 0$) the path integral may be evaluated by a steepest descent calculation, i.e., we identify the path $x_c(t)$ that minimizes $S[x]$. This path x_c is the desired instanton solution. The action $S[x_c]$ associated with x_c determines the escape rate, since to leading order for small D, the right-hand side of (9) has the form const $\cdot\, T \exp(-S[x_c]/D)$, the factor T being a consequence of the invariance (for $T \to \infty$) of the action $S[x]$ under time translations.[11,13] Identifying the coefficient of T as the escape rate Γ yields

$$\Gamma \sim \exp(-S[x_c]/D) \tag{10}$$

Evaluation of the prefactor in (10) requires consideration of fluctuations about the extremal path x_c, multi-instanton contributions, and inclusion of the Jacobian factor $J[x_c]$.

We now proceed with the evaluation of $S[x_c]$. To simplify the subsequent calculations, we make a change of variable in the action, Eq. (5), from $x(t)$ to $y(x)$, where $y \equiv \dot{x}$. The action then has the form

$$S[y] = (1/4) \int_a^b (dx/y)\{[myy' + y + V'(x)]^2 + \tau^2 y^2 [m(yy'' + y'^2) + y' + V''(x)]^2\} \tag{11}$$

where a and b are the positions of the local minimum and unstable maximum of the potential, respectively (see Fig. 1). We have fixed the upper limit of the integral as b rather than c, since the escape rate is actually determined from the rate to reach the unstable maximum. The passage of the particle from b to c proceeds by a "free descent," i.e., it is described by Eq. (1) with $\xi = 0$.[11] The relevant instanton for the determination of Γ is thus the "uphill" path, labeled 1 in Fig. 1. The "downhill" path, labeled 2, is also an instanton, but has zero action. Henceforth, therefore, we consider only the instanton associated with the uphill path.

The reasons for using x instead of t as independent variable are twofold: (i) the differential equation that results from extremizing the action is reduced by two orders, and (ii) numerical solution of the equation is now over the finite interval (a, b), whereas in the $x(t)$ variables the solution was over an infinite interval $(-\infty, \infty)$.

To minimize $S[y]$, we apply the extremal condition $\delta S[y]/\delta y(x) = 0$. This yields the following fourth-order, nonlinear, ordinary differential equation for $y_c(x)$—the instanton path in $y(x)$ space:

$$\begin{aligned} 0 = {} & 1 - (V'/y)^2 - 2mV'' - m^2(y'^2 + 2yy'') - \tau^2(y'^2 + 2yy'' + 2yV''' - V''^2) \\ & + 2m\tau^2(2yy''V'' + y'^2 V'' + 2yy'V''' + y^2 V'''') \\ & + m^2\tau^2(9y^2 y''^2 + y'^4 + 16yy'^2 y'' + 12y^2 y'y''' + 2y^3 y'''') \end{aligned} \tag{12}$$

Numerical solution of Eq. (12) requires specifying four boundary conditions. Two of these, $y(a) = 0 = y(b)$, follow from the condition that the particle start and finish at rest. For the remaining two, we specify the values of the derivatives at the endpoints, i.e., $y'(a)$ and $y'(b)$. These can be deduced directly from the sixth-order equation for $x(t)$ obtained from the extremal condition $\delta S[x]/\delta x(t) = 0$ for the action $S[x]$ given by (5). Linearizing this equation in $(x - a)$ yields, for small $(x - a)$, a general solution which is a sum of six exponentials, $x - a = \sum_{i=1}^{6} \alpha_i \exp(\lambda_i t)$, with rate constants $\{\lambda_i\}$ given by Eq. (26) below. The boundary condition that $x - a$ vanish for $t \to -\infty$ requires that only the three terms for which λ_i has a positive real part will be present. Furthermore, the λ with the smallest positive real part, say λ_1, will dominate asymptotically. We will work in a regime (see the discussion in Section VI below) where λ_1 is purely real. Then $x-a \sim \exp(\lambda_1 t)$ for $t \to -\infty$ implies $y \equiv \dot{x} \to \lambda_1(x-a)$. This gives the boundary condition $y'(a)=\lambda_1$. A similar linearization for x near b yields the value of $y'(b)$ in terms of the negative eigenvalue with smallest magnitude of the linear equation for $(b-x)$.

With these boundary conditions, Eq. (12) may be solved numerically with a specific choice of potential for general values of m and τ. However, we shall first look at solutions for y_c with a general potential for various limits of m and τ.

3. WHITE NOISE MASSIVE CASE ($m>0$, $\tau=0$)

The differential equation for y_c now has the form

$$1-(V'/y)^2-2mV''-m^2(y'^2+2yy'')=0 \tag{13}$$

and the associated action is

$$S[y]=(1/4)\int_a^b (dx/y)[myy'+y+V'(x)]^2 \tag{14}$$

Now consider the quantity $u(x) \equiv myy'-y+V'(x)$. Inserting this into Eq. (14), we find

$$S[y]=\int_a^b dx\,(y+u)+(1/4)\int_a^b dx\,u^2/y$$

Using the definition of u and the boundary conditions $y(a)=0=y(b)$, we have

$$S[y]=\Delta V+(1/4)\int_a^b dx\,u^2/y$$

where $\Delta V \equiv V(b)-V(a)$ is the height of the potential barrier. Thus, to minimize the action we must set $u=0$, giving us a first-order differential equation for y_c and a simple, mass-independent form for the action, i.e.,

$$my_c y_c'-y_c+V'(x)=0 \tag{15}$$

and

$$S[y_c]=\Delta V(x) \tag{16}$$

The fact that $S[y_c]$ is independent of the mass for white noise can be understood intuitively from the idea that the escape rate should be proportional to the equilibrium probability density to find the particle at the top of the barrier. For white noise, the latter is given by the Boltzmann distribution, and is m independent. The prefactor in Eq. (10) does, however, depend on m.[14–20]

In the next section we shall see that noise color (i.e., $\tau > 0$) introduces mass dependence into the action.

4. SMALL-m EXPANSION FOR GENERAL τ

In this section we wish to write the instanton action in the form

$$S = S_0(\tau) + mS_1(\tau) + O(m^2) \tag{17}$$

The first term corresponds to the action with zero mass and has been extensively studied in ref. 11. For $m = 0$, the instanton path $y_0(x)$ satisfies

$$1 - (V'/y)^2 - \tau^2(y'^2 + 2yy'' + 2yV''' - V''^2) = 0 \tag{18}$$

The solution of this equation, y_0, may be inserted into the $m = 0$ action to give $S_0(\tau)$. Since the action has been extremized with respect to y, we may find $S_1(\tau)$ by inserting the lowest order solution y_0 into the terms of the action, Eq. (11), which are linear in m. Therefore, S_1 is given by

$$S_1(\tau) = (1/2) \int_a^b dx\, [y_0' V' + \tau^2 y_0 V''(y_0 y_0'' + y_0'^2)] \tag{19}$$

The results of Section 3 indicate that $\lim_{\tau \to 0} S_1(\tau) = 0$. We may also see the large-τ behavior of S_1 by considering the physical content of the Langevin equation.[10] For τ large, the noise fluctuates very slowly, and may be viewed as a quasistatic force which has the effect of producing an effective potential that gradually "tilts" with time. The particle then simply adjusts its position at each instant so that it remains in the local minimum of the effective potential. Thus, the position of the particle with time is independent of the mass and we expect $\lim_{\tau \to \infty} S_1(\tau) = 0$. [Strictly, since $S_0(\tau)$ increases linearly with τ for large τ,[9–11] this intuitive argument implies only the weaker result $\lim_{\tau \to \infty} S_1(\tau)/\tau = 0$. However, the numerical results below confirm the stronger result given above.]

To obtain the form of S_1 for general τ, we solve Eq. (19) numerically for the typical case of the quartic potential

$$V(x) = -x^2/2 + x^4/4 \tag{20}$$

for $10^{-2} \leqslant \tau \leqslant 10^4$. Numerical evaluation of the integral in Eq. (19) yields the results shown in Fig. 2. The function $S_1(\tau)$ is small compared to $S_0(\tau)$

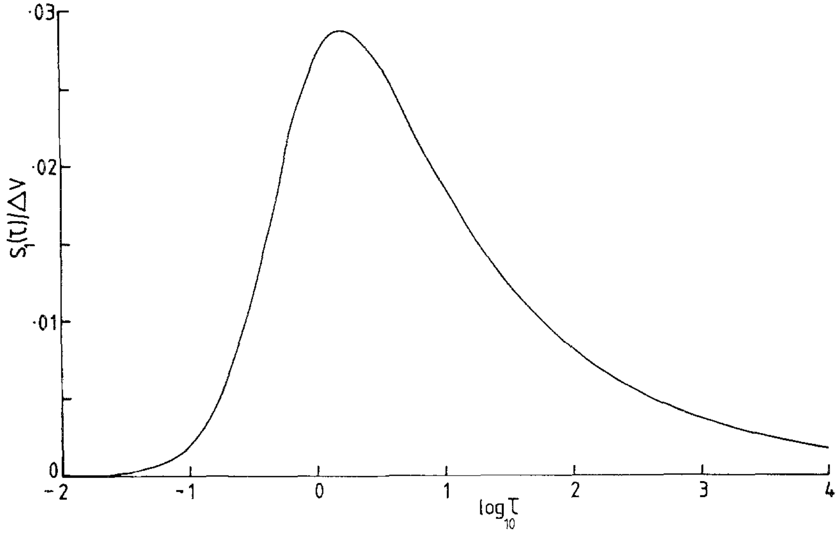

Fig. 2. The function $S_1(\tau)$, defined by the expansion $S = S_0(\tau) + mS_1(\tau) + O(m^2)$ of the instanton action in powers of the particle mass, for the quartic potential given by Eq. (20). The ordinate has been normalized by the white-noise action ΔV ($= 1/4$). S_1 vanishes as τ^2 for $\tau \to 0$, and as $\tau^{-1/3}$ for $\tau \to \infty$.

[which has minimum value $S_0(0) = \Delta V = 1/4$] for the whole range of τ, with a maximum value of $\sim 7.2 \times 10^{-3}$ at $\tau \cong 1.6$. For $\tau \to 0$, S_1 vanishes as $\tau^2/20$ [see Eq. (25)]. The large-τ behavior is consistent with $S_1 \sim \tau^{-1/3}$, suggesting that the m dependence first enters only at the third term of the expansion[11] of $S(\tau)$ in powers of $\tau^{-2/3}$.

5. SMALL-τ EXPANSION FOR GENERAL *m*

We now perform an analogous expansion to that in Section 4, but for general m and small τ, i.e., we wish to write the action in the form

$$S[y_c] = S_0(m) + \tau^2 S_1(m) + O(\tau^4) \tag{21}$$

The first term is the action for the massive white-noise case and, as shown in Section 3, it has the value ΔV. For $\tau = 0$, the instanton path $y_0(m)$ satisfies Eq. (15). (Note that the subscript zero indicates $\tau = 0$ in this section, not $m = 0$.) Since the action has been extremized, we may find $S_1(m)$ by inserting the lowest order solution y_0 into the terms of the action, Eq. (11), which have a coefficient of τ^2. After some manipulation using (15), one finds

$$S_1(m) = \int_a^b dx\, y_0\, y_0'^2 \tag{22}$$

We may find the form of $S_1(m)$ by solving Eq. (15) numerically for given m, inserting the solution into (22), and evaluating the integral numerically. Figure 3 shows the results of this procedure for the quartic potential (20). Note that in practice the range of m for which this procedure works well is restricted. This is because the instanton solution has an oscillatory component in the (x, t) plane for $m > m_c = 1/4V''(a) = 1/8$ for the potential (20). This oscillatory behavior, which is associated with complex rate constants $\{\lambda_i\}$ in the solution for $x(t)$ linearized near $x = a$ (see the discussion at the end of Section 2, and Section 6 below), implies a path in the (x, y) plane that spirals out from the initial point, $x = a$, $y = 0$, i.e., the instanton solution $y(x)$ becomes multivalued. In principle, one can circumvent this difficulty by working with the original (x, t) variables. In practice, however, the COLSYS package[23] which was used to solve the differential equation does not converge well in the oscillatory regime.

The function $S_1(m)$, Eq. (22), may be evaluated analytically as a power series in m. Inserting $y = \sum_{n=0}^{\infty} m^n y_n$ into (15) and equating coefficients order by order in m gives

$$y = V' + mV'V'' + m^2(V'^2 V''' + 2V'V''^2) + O(m^3) \tag{23}$$

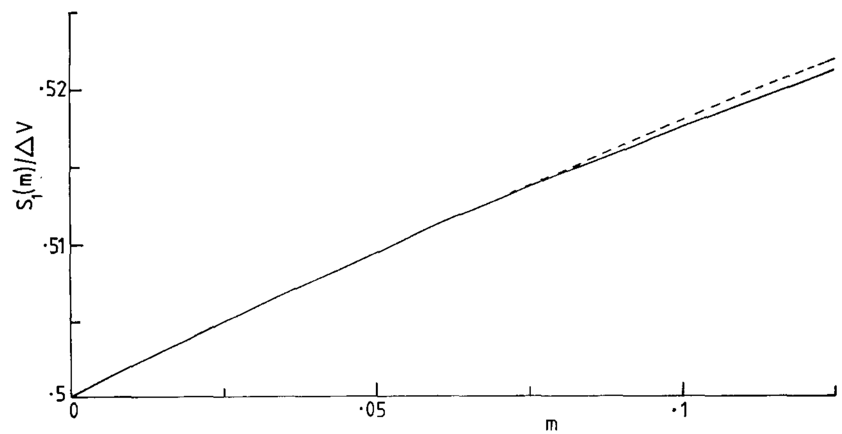

Fig. 3. The function $S_1(m)$ (solid curve), defined by the expansion $S = S_0(m) + \tau^2 S_1(m) + O(\tau^4)$, for the quartic potential (20). The ordinate has been normalized by the white-noise action ΔV $(=1/4)$. The broken curve shows the result obtained from the first three terms of the small-m expansion, given by Eq. (25). For reasons discussed in the text, the results are limited to $m < m_c = 1/8$.

Substituting this expansion for y_0 in (22) yields

$$S_1(m) = \int_a^b dx\, [V'V''^2 + mV'V''^3 + (1/2)\, m^2 V'^2 V''(2V'V'''' + V''V''') + O(m^3)] \tag{24}$$

For the quartic potential (20) this becomes

$$S_1(m) = \Delta V(1/2 + m/5 - m^2/5 + O(m^3)) \tag{25}$$

The expansion (25) is included in Fig. 3 along with the numerical results. The first three terms in the m expansion provide a very good approximation over the whole range $m < m_c = 1/8$.

6. RESULTS FOR GENERAL m AND τ

In the above sections we have calculated the action in the form of various expansions, i.e., we have taken one or both of the parameters m and τ to be small. However, we may solve the full differential equation (12) numerically for more general values of the parameters. In practice, as discussed above, numerical solution requires restrictions on the relative sizes of the two parameters, such that in (x, t) space the instanton path is nonoscillatory. Oscillations only occur for $m > m_c$, but even if this condition pertains, they may be "damped out" if τ is large enough.

To see this, we linearize the differential equation for $x(t)$ obtained from Eq. (9) via the substitution $y = \dot{x}$ [or directly from (5) via $\delta S[x]/\delta x(t) = 0$] around the stable fixed point $x = a$. As discussed at the end of Section 2, this equation is sixth order, and therefore has six independent solutions (for $x - a$) of the form $\exp(\lambda_i t)$ $(i = 1,..., 6)$, with rate constants

$$\lambda_i = \pm\frac{1}{\tau}, \pm\frac{1}{2m}\{1 \pm [1 - 4mV''(a)]^{1/2}\} \tag{26}$$

For $t \to -\infty$, the instanton will be a linear combination of the three terms for which λ_i has positive real part, and the term with smallest positive real part will dominate asymptotically. In the overdamped regime $4mV''(a) < 1$, all three λ's are real, and $x(t)$ is nonoscillatory for all τ. Even in the underdamped regime, however, where two of the three relevant λ's are complex, the real one $(1/\tau)$ still dominates for $\tau > 2m$, giving (asymptotically) nonoscillatory behavior. We emphasize that the reason for the above discussion is a technical limitation of our differential-equation-solving package,[23] which finds difficulty in converging onto oscillatory solutions:

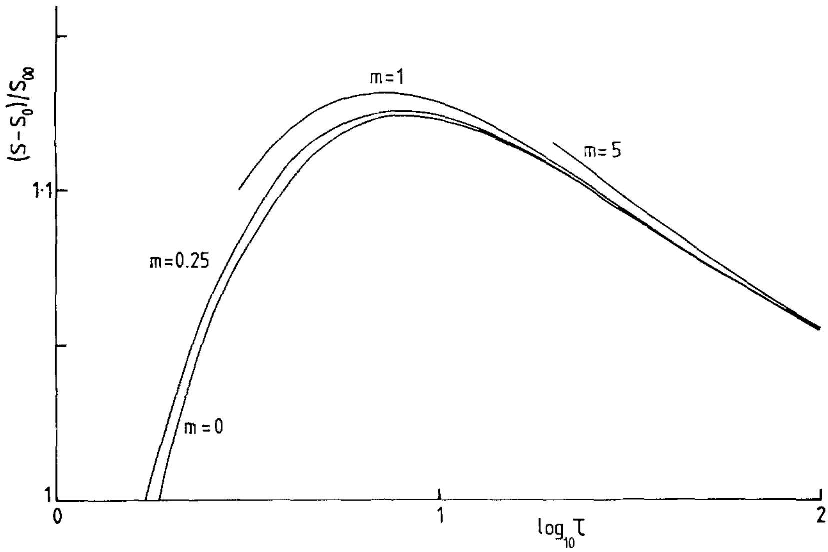

Fig. 4. The instanton action S, as a function of τ for various m, plotted as $(S-S_0)/S_\infty$ versus $\log_{10}\tau$. The results pertain to the quartic potential (20). $S_0 = \Delta V = 1/4$ and $S_\infty = (2/27)\tau$ are the white-noise and large-τ limits of S, respectively.

this discussion does not imply any fundamental difficulties in the physics of the underdamped regime.

Figure 4 contains representative results for the action as a function of τ for various m. All results are for the quartic potential (20), and are plotted in the form $(S-S_0)/S_\infty$ versus $\log_{10}\tau$, where $S_0 = \Delta V = 1/4$ is the white-noise action, and $S_\infty = (2/27)\tau$ is the large-τ form of the action.[9-11] The range of τ presented for larger m is limited for the reasons given above. The most striking feature of the results is once more the relative insensitivity of the action to the mass m.

7. SUMMARY

By using a path-integral formulation of the Langevin equation, the escape rate of a massive particle, driven by colored noise, over a potential barrier has been calculated for the first time. In the weak noise limit, the escape rate has the form $\Gamma \sim \exp(-S/D)$. For white noise, the action S has the value ΔV, independent of m. Expansions of S for one or both of m and τ small have been derived for general potentials, while numerical results have been obtained for more general situations for one specific potential. We find that a non-Markov process ($\tau > 0$) brings mass dependence into the action S, but the effect is numerically quite small for the range of m which we have been able to probe. An interesting open problem is to devise a technique for exploring the regime of extreme light damping.

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