Instanton Calculation of the Escape Rate for Activation over a Potential Barrier Driven by Colored Noise

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In the weak noise limit ($D \to 0$), the escape rate over a one-dimensional potential barrier is $\Gamma \sim \exp(-S/D)$. Here S is calculated exactly by identifying appropriate instanton solutions in a path-integral formulation of the Langevin equation. For the "colored noise" problem, defined by the noise correlator $\langle \xi(t)\xi(t')\rangle = (D/\tau)\exp\{-|t-t'|/\tau\}$, the instanton satisfies a fourth-order, nonlinear, ordinary differential equation which can be readily solved numerically. Analytical results are derived for small and large τ.

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There has been considerable interest over many years[1,2] in physical systems described by the stochastic differential equation

$$\dot{x} = -V'(x) + \xi(t)\,, \tag{1}$$

where $\xi(t)$ is a colored Gaussian noise with zero mean, and correlator

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

In (1), and hereafter, overdots and primes indicate derivatives with respect to t and x, respectively: (1) is a Langevin equation for an overdamped particle moving in a potential $V(x)$ and subject to a noise $\xi(t)$. The quantity of interest to us here is the characteristic time T (e.g., the "mean first passage time"[1,2]) taken for a particle initially located at a minimum of V to escape over a potential barrier. A typical situation is sketched in Fig. 1. The special case of a bistable potential is relevant in many physical applications.[1,2]

In the white noise limit, $\tau = 0$, the problem is well understood. For weak noise (i.e., small D) the escape time is given by the Arrhenius formula $T \sim \exp(\Delta V/D)$,

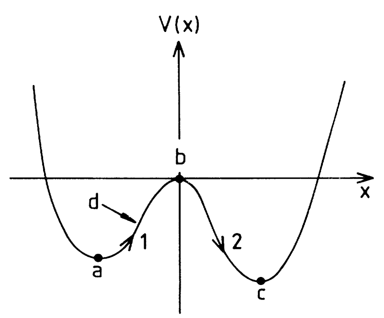

FIG. 1. Typical potential considered in this paper. The rate of escape Γ from the left-hand well is governed by the "action" S of the instanton associated with the "uphill" path 1: $\Gamma \sim \exp(-S/D)$. The instanton associated with the "downhill" path 2 has zero action. The point d is the inflection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

where ΔV [$=V(b)-V(a)$ in Fig. 1] is the height of the barrier, and we ignore preexponential factors. The latter are calculable in principle[3] and will be discussed for general τ elsewhere.[4]

Our goal in this Letter is to generalize the Arrhenius result to arbitrary noise correlation time τ. This problem has generated a mass of papers (see Refs. 1 and 2 for an extensive bibliography), many containing conflicting results, the major difficulty being the absence of a systematic approach. The reason that the colored noise problem is difficult, and has not been solved before, is that for $\tau > 0$ Eq. (1) describes a *non-Markov* process for which there is no simple generalization of the Fokker-Planck equation, the latter being the conventional starting point for studies of the weak noise limit. Here we employ a path-integral formulation[5] which lends itself naturally to a study of the weak noise limit via a steepest-descent approach.[6] The result has the form $T \sim \exp[S(\tau)/D]$. An exact expression for S is derived below: It is simply the minimum over paths $x(t)$ of the generalized Onsager-Machlup functional $S[x]$ [see Eq. (5)]. The extremal path, or "instanton," satisfies the differential equation (7) which may be solved numerically for any given potential $V(x)$. Analytic results are derived, for general potentials, for small and large τ.

We start by observing that the noise probability weight implied by (2) is

$$P(\{\xi(t)\}) \propto \exp\left\{-(1/4D)\int dt\,(\xi^2 + \tau^2\dot{\xi}^2)\right\}. \tag{3}$$

Much of the simplicity of our approach is associated with the "local" nature of the functional in the exponent (i.e., the fact that it contains only one time integral), which is a consequence of the exponential noise correlator (2). Surprisingly, this simplifying feature of exponentially correlated noise does not seem to have been exploited previously. The probability weight for $x(t)$ is obtained by expressing ξ in terms of x using (1):

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

where the Onsager-Machlup functional[5] $S[x(t)]$ is simply

$$S[x(t)] = \tfrac{1}{4}\int dt\{[\dot{x}+V'(x)]^2+\tau^2[\ddot{x}+V''(x)\dot{x}]^2\}\,. \quad (5)$$

We will call S the action by analogy with the path-integral formulation of quantum mechanics (here D plays the role played by $\hbar$ in quantum mechanics). The preexponential factor J in (4) is the Jacobian of the transformation from ξ to x. It has the value[5] $J = \exp\{\frac{1}{2}\int dt\, V''(x(t))\}$ which, being independent of D, will not alter the leading small-D expression in the exponent in (4).

The quantity of interest is the probability density $P(x_1,T\,|\,x_0,0)$ for the particle to be at x_1 at time T given that it was at x_0 at time zero. It is given by the path integral

$$P(x_1,T\,|\,x_0,0) \propto \int dx(t)\, J[x]\exp(-S[x]/D)\,, \quad (6)$$

over all paths satisfying $x(0)=x_0$, $x(T)=x_1$. For $D\to 0$, the path integral can be evaluated by the method of steepest descents, i.e., we require the path $x(t)$ which minimizes $S[x]$. The relevant boundary conditions for the escape process are (see Fig. 1) $x(-\infty)=a$, $x(\infty)=b$. The solution $x_c(t)$ satisfying these conditions is an instanton solution of the theory.[7] Its action $S[x_c]$ determines the escape rate: $\Gamma\sim\exp(-S[x_c]/D)$. Evaluation of the preexponential factor requires integrating over the Gaussian fluctuations around the extremal path[3,7] (and also including multiinstanton contributions,[7] and the Jacobian factor J neglected here), and will be deferred to a future publication.[4]

The extremal condition $\delta S/\delta x=0$ applied to (5) yields a fourth-order nonlinear differential equation for $x_c(t)$:

$$-\ddot{x}+V'(x)V''(x)+\tau^2\{\ddddot{x}+3\dot{x}\ddot{x}V'''(x)+V''''(x)\dot{x}^3-V''(x)V'''(x)\dot{x}^2-V''(x)^2\ddot{x}\}=0\,. \quad (7)$$

For a more general noise correlator than (2), the exponent in (3) would contain higher-order derivatives of ξ, leading to a higher-order (in general, infinite order) differential equation for $x(t)$. Thus the form (2) yields great simplifications.

For a given potential $V(x)$, Eq. (7) can be solved numerically for general τ. However, it is instructive to consider first the small and large τ limits, where analytic results can be obtained for general $V(x)$.

White noise ($\tau=0$).—For $\tau=0$, the first integral of (7) is

$$\dot{x}^2=V'(x)^2\,, \quad (8)$$

where the integration constant vanishes because $\dot{x}=0=V'(x)$ at both end points. Equation (8) is equivalent to the classical mechanics of a particle of unit mass (and zero energy) moving in a potential $\tilde{V}(x)=-\frac{1}{2}V'(x)^2$. Such mechanical analogs are common in instanton physics.[7] The white noise instanton $x_0(t)$ corresponds to the path labeled 1 in Fig. 1. Taking the square root of (8) yields

$$\dot{x}_0=V'(x_0)\,, \quad (9)$$

where the positive square root is appropriate for path 1. Substituting back into the action (5) yields

$$S_0=\int_{-\infty}^{\infty}dt\,\dot{x}_0V'(x_0)=\int_a^b dx_0\,V'(x_0)$$
$$=V(b)-V(a)\equiv\Delta V\,, \quad (10)$$

the Arrhenius result. The negative square root of (8), $\dot{x}=-V'(x)$, describes the path 2 by which the particle descends from the unstable maximum of the potential to the new minimum. Substituting in (5) shows that this solution has zero action, for all τ. This is physically transparent: the downhill path 2 corresponds to a free descent, i.e., it does not require any external noise to drive it. By contrast, the uphill path 1 does require external noise. Specifically (1) and (9) give the critical noise history: $\xi_0(t)=\dot{x}_0+V'(x_0)$. Of all noise histories which take the particle to the top of the barrier, $\xi_0(t)$ is the one with the greatest probability weight. To summarize, the escape rate is determined solely by the uphill path.

Small-τ expansion.—A systematic expansion around the white noise limit, in powers of τ^2, is readily developed. Since for $\tau=0$ the solution x_0 is a stationary point of the action functional, to compute the action S to $O(\tau^2)$ one simply substitutes the $\tau=0$ solution into the $O(\tau^2)$ term in (5). To compute S to $O(\tau^4)$, we need $x_c(t)$ to $O(\tau^2)$, and so on. Setting $x_c(t)=\sum_{n=0}^{\infty}x_n(t)\tau^{2n}$ in (7), where x_0 satisfies (9), equating coefficients of τ^{2n}, solving the resulting linear equations for $x_n(t)$ $(n\geq 1)$, and substituting the result into (5) yields

$$x_c=x_0+2\tau^2V'(x_0)V''(x_0)+O(\tau^4)\,, \quad (11)$$

$$S[x_c]=\Delta V+\tau^2\int_a^b dx\,V''(x)^2V'(x)$$
$$-\tau^4\int_a^b dx\,V'''(x)^2V'(x)^3+O(\tau^6)\,. \quad (12)$$

The order τ^2 term was also obtained in Ref. 6(b). We stress that our approach is systematic, and obtaining higher-order terms is straightforward. For the much-studied special case of the quartic bistable potential

$$V(x)=-\alpha x^2/2+\beta x^4/4\,, \quad (13)$$

Eq. (12) becomes

$$S=\Delta V\{1+\tfrac{1}{2}(\alpha\tau)^2-\tfrac{6}{5}(\alpha\tau)^4+O(\tau^6)\}\,. \quad (14)$$

Large-τ limit.— For large τ it is convenient to rescale time, $t \to \tau t$, so that (5) becomes

$$S[x] = \tfrac{1}{4}\tau \int_{-\infty}^{\infty} dt(\{V'(x)^2 + [V''(x)\dot{x}]^2\} + 2\tau^{-1}[V'(x)\dot{x} + V''(x)\dot{x}\ddot{x}] + \tau^{-2}[\dot{x}^2 + \ddot{x}^2]) . \quad (15)$$

The leading large-τ result is obtained by retaining only the terms in the curly brackets. Introducing $U \equiv V'$, the leading action becomes $\frac{1}{4}\tau \int_{-\infty}^{\infty} dt(U^2 + \dot{U}^2)$. The required instanton solution must pass through the inflection point d of the potential (see Fig. 1), and we can choose this to occur at $t=0$, since the origin of time is arbitrary. Splitting the time integral at $t=0$, the two parts of the action can be minimized separately, subject to $x(-\infty)=a$, $x(0)=d$, and $x(\infty)=b$. Varying the action with respect to U yields $U=\ddot{U}$ for $t<0$ and $t>0$. The solution $x_\infty(t)$ satisfying the boundary conditions is given by

$$U \equiv V'(x_\infty) = V'(d)e^{-|t|}, \quad (16)$$

and the associated action is [see also Ref. 6(b)]

$$S_\infty = (\tau/2)V'(d)^2 . \quad (17)$$

For the quartic bistable potential (13), this gives

$$S_\infty = \tfrac{8}{27}\Delta V \alpha\tau , \quad (18)$$

in agreement with the result obtained by simple physical arguments in Ref. 1.

It should be possible to develop a systematic expansion around (17). The leading order correction is naively obtained by setting $x(t) = x_\infty(t)$ in the second set of square brackets in (15). The resulting t integral, however, is found to *diverge*, indicating that no expansion in powers of $1/\tau$ exists. The divergence occurs for $t \to 0$, i.e., for $x \to d$, and is associated with the fact that $\dot{x}_\infty$ diverges at $t=0$, as is clear from (16) since $V''(d)=0$. Preliminary investigations[4] suggest that the leading correction to (17) is a term of order $\tau^{1/3}$.

For intermediate τ, analytical progress is difficult. The first integral of (7) can, however, be obtained analytically by the standard device of multiplying both sides of the equation by $\dot{x}$, and identifying the resulting terms as perfect differentials. This gives

$$\dot{x}^2 - V'(x^2) = \tau^2\{2\dddot{x}\dot{x} - \ddot{x}^2 + 2V'''(x)\dot{x}^3 - V''(x)^2\dot{x}^2\} , \quad (19)$$

where the vanishing of the integration constant follows from the boundary conditions. Further progress requires numerical methods. As an example, we consider again the bistable potential (13). For two of the three boundary conditions needed to specify the solution of (19) we use the behavior for $t \to \mp\infty$, where x approaches its limiting values $a = -(\alpha/\beta)^{1/2}$, $b=0$ at rates determined by linearizing (7) around these limiting values and retaining only the dominant exponential. Specifically, we find $x - a \simeq A\exp(\lambda_a t)$ for $t \to -\infty$, and $x - b \simeq B \times\exp(-\lambda_b t)$ for $t \to \infty$, where $\lambda_a = \min[V''(a), 1/\tau]$ and $\lambda_b = \min[|V''(b)|, 1/\tau]$. As the third boundary condition, we arbitrarily fix $x(0)$ to a value in the interval (a,b). This removes the time translational invariance of the solution {the action $S[x]$ is invariant under $x(t) \to x(t+t_0)$}.

The action S obtained numerically is shown in Fig. 2. Since one part in 10^6 (or better) accuracy is readily obtainable, these results are essentially exact. For example, for $\alpha\tau = 1$ we obtain $S/\Delta V = 1.2517616(1)$. For presentation purposes, it is convenient to subtract off the white noise limit $S_0 = \Delta V = \alpha^2/4\beta$, and normalize by the large-τ limit S_∞ given by (18). This yields a function which vanishes at $\tau=0$ and saturates to unity for large τ. The broken curve in Fig. 2 is the small-τ form (14), which fits the data well for $\alpha\tau \lesssim 0.25$. By contrast, the large-τ limit of unity is approached only very slowly: The asymptotic limit is still exceeded by $\simeq 8.9\%$ for $\alpha\tau = 100$, and by $\simeq 3.5\%$ for $\alpha\tau = 400$. These results are consistent with the argument[4] that the leading correction to (17) is of order $\tau^{1/3}$.

To summarize, the rate Γ for the escape of a particle over a barrier has been determined for colored noise in the weak noise limit, $D \to 0$. The result is that $\Gamma \sim \exp(-S/D)$. The action S is the minimum over all paths $x(t)$ [with $x(-\infty)=a$, $x(\infty)=b$] of the functional $S[x]$ given by (5). Analytic results for small and large τ are given in (12) and (17), which are valid for *arbitrary* potentials V. For intermediate τ, accurate numerical results can be obtained for any given potential. The preexponential factor in Γ (and higher-order corrections in powers of D) can be systematically calculated in principle by including the effects of fluctuations around the steepest-descent (instanton) path $x_c(t)$.[4]

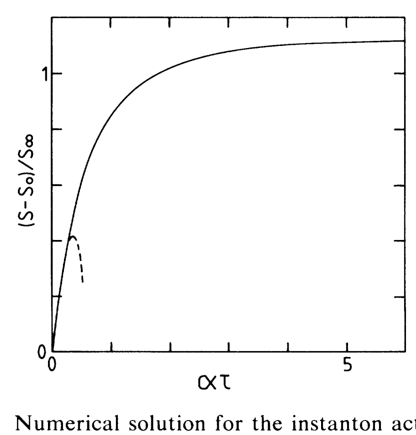

FIG. 2. Numerical solution for the instanton action S, plotted as $(S-S_0)/S_\infty$, for the bistable potential (13), as a function of $\alpha\tau$. The broken curve gives the limiting small-τ form (14).

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[1]G. P. Tsironis and P. Grigolini, Phys. Rev. Lett. **61**, 7 (1988), and references therein.

[2]P. Jung and P. Hänggi, Phys. Rev. Lett. **61**, 11 (1988), and references therein.

[3]See, for example, B. Caroli, C. Caroli, and B. Roulet, J. Stat. Phys. **26**, 83 (1981); U. Weiss, Phys. Rev. A **25**, 2444 (1982); V. F. Baibuz, V. Yu. Zitserman, and A. N. Drozdov, Physica (Amsterdam) **127A**, 173 (1984).

[4]A. J. McKane and A. J. Bray, to be published.

[5]See, for example, R. Graham, *Quantum Statistics in Optics and Solid-State Physics,* Springer Tracts in Modern Physics Vol. 66, edited by G. Höhler (Springer-Verlag, New York, 1973), and in *Fluctuations, Instabilities, and Phase Transitions,* edited by T. Riste (Plenum, New York, 1975).

[6](a) J. F. Luciani and A. D. Verga, Europhys. Lett. **4**, 255 (1987), and (b) J. Stat. Phys. **50**, 567 (1988), have also studied colored noise using a steepest-descent approximation to a functional integral. These authors, however, do not exploit the simplicity of exponentially correlated noise, and their results are mainly restricted to piecewise linear forces.

[7]S. Coleman, in *The Whys of Subnuclear Physics,* edited by A. Zichichi (Plenum, New York, 1979); R. Rajaraman, *Solitons and Instantons* (North-Holland, Amsterdam, 1982); J. Zinn-Justin, in *Recent Advances in Field Theory and Statistical Mechanics,* Proceedings of the 1982 Les Hoches Summer School, Session XXXIX, edited by J.-B. Zuber and R. Stora (North-Holland, Amsterdam, 1984).