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Time Oscillations of Escape Rates in Periodically Driven Systems

V. N. Smelyanskiy,[1,2] M. I. Dykman,[1] and B. Golding[1]
[1]*Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824*
[2]*Caelum Research Company, NASA Ames Research Center, MS 269-2, Moffett Field, California 94035-1000*
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We provide an explicit solution of the problem of activation escape from a metastable state of a periodically driven Brownian particle, including both the exponent and the prefactor. We find the instantaneous and time-average escape rates, and a crossover in their field dependence, from weak to exponentially strong, with amplitude and period of the driving field. The results apply for an arbitrary ratio between the field amplitude and the noise intensity, and between the field period and the relaxation time of the system. [S0031-9007(99)08926-7]

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The problem of fluctuation-induced escape from a metastable state, and of activated processes in general, is central to many areas of physics, from diffusion in crystals to nucleation at phase transitions. It was first considered quantitatively in a seminal paper by Kramers [1] using a model of a Brownian particle that escapes from a potential well. In many cases of current interest, escape is studied for systems away from thermal equilibrium, such as trapped electrons which display bistability in a strong periodic field [2], or spatially periodic nonequilibrium systems (ratchets) that display unidirectional current [3]. Whereas for equilibrium systems the exponent in the escape rate can be found, at least in principle, as the height of the free-energy barrier, for nonequilibrium systems there are no universal relations from which it can be obtained [4], and the situation with the prefactor is even more complicated [5].

In the present paper, we develop a theory of escape rates for periodically driven systems, one of the most important classes of nonequilibrium systems. The problem has attracted a great deal of attention in several contexts, most recently in the area of phenomena related to stochastic resonance [6]. For the most part, prior theory has explored the case of slowly varying driving fields, where the system remains in thermal equilibrium. The present analysis, however, does not rely on this approximation. For *arbitrary* ratios of field period and system relaxation time, we are able to determine the time-dependent escape rate, including both the exponent and prefactor, find the time-average rate, and investigate its nonanalytic dependence on the field intensity.

Let us consider a simple model of a driven system: an overdamped Brownian particle in a potential $U(q)$ driven by a periodic force $F(t) = F(t + \tau_F)$ (see Fig. 1),

$$\dot{q} = -U'(q) + F(t) + \xi(t), \tag{1}$$

where $\xi(t)$ is white Gaussian noise, $\langle \xi(t)\xi(t')\rangle = 2D\delta(t - t')$ (for thermal noise, the noise intensity $D = k_B T$).

The motion of the system (1) is characterized by three times: the typical relaxation time t_r in the absence of noise and driving, the period of the force τ_F, and the reciprocal escape rate $1/\overline{W}$ averaged over the period τ_F. We assume that the noise intensity D is small (the small parameter of the theory), so that $\overline{W} \ll 1/t_r, 1/\tau_F$.

In the limit of very small t_r/τ_F, the escape rate $W(t)$ adiabatically follows the instantaneous potential $U(q) - F(t)q$,

$$W(t) \approx W_0 \exp[-\delta U(t)/D], \qquad \delta U(t) = F(t)(q_a - q_b), \tag{2}$$

where q_a and q_b are the positions of the potential minimum and the barrier top, respectively (see Fig. 1), and

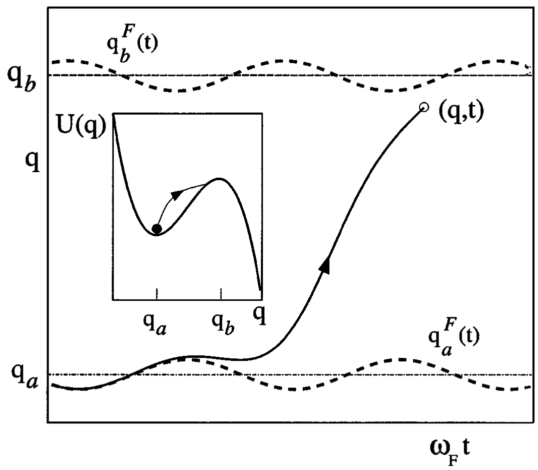

FIG. 1. Optimal fluctuational path (solid line) that arrives at the point q at the instant t in a periodically driven system. The path starts at $t \to -\infty$ at the periodic attractor $q_a^F(t)$. The attractor and the boundary of the attraction basin $q_b^F(t)$ are shown dashed. The horizontal lines show the positions of the minimum and local maximum of the potential $U(q)$ (shown in the inset) in which the particle is fluctuating.

$W_0 \propto \exp(-\Delta U/D)$ is the Kramers escape rate for $F = 0$ [$\Delta U = U(q_b) - U(q_a)$ is the barrier height]. We assume that the force $F(t)$ is *dynamically weak*, so that the modulation of the barrier height $|\delta U| \ll \Delta U$. Yet $|\delta U|$ may largely exceed the noise intensity D, and then $W(t)$ is *exponentially strongly* modulated in time: Escape is most likely to occur where the barrier is at its lowest, generically once per period of the field.

The escape problem becomes much more complicated for higher field frequencies where Eq. (2) no longer applies [7]. Nevertheless the field-induced change of the escape rate may still be exponentially strong. Whereas for small F/D the change of W is known, theoretically [8] and experimentally [9], to be quadratic in F/D, for large F/D (but still relatively small F) it becomes nonanalytic in $F(t)$, with $\ln \overline{W}$ being linear in $|F|/D$ [10]. One expects that the time modulation of $W(t)$ should *decrease* compared to (2) if t_r/τ_F is not small. Indeed, although the probability for the system to approach q_b still has one sharp peak per field period (see below), the system does not have time to leave the vicinity of q_b over the time τ_F, and there occurs averaging of the outgoing flow.

In what follows, we provide a general theory of escape rate for arbitrary t_r/τ_F and arbitrary F/D. Following Kramers [1], we characterize escape by the current $j(q,t)$ from the attraction basin of the metastable state where the system is located at $t = 0$. After a transient time $\sim t_r$ (but for $t \ll 1/\overline{W}$ where the population of the metastable state does not change), the current $j(q,t)$ is periodic in time. For small D, once the system has reached the area far enough behind the basin boundary $q_b^F(t)$ (see Fig. 1), it will move close to the noise-free trajectory $\dot{q} = -U'(q) + F(t)$. Therefore in the range $|U'(q)| \gg F$ the current scales with q as

$$j(q,t) = W[t - t_d(q)], \quad dt_d/dq = -1/U'(q). \quad (3)$$

Equation (3) essentially *defines* the instantaneous periodic escape rate $W(t) = W(t + \tau_F)$ by relating it to a directly measurable quantity $j(q,t)$. The time lag t_d is determined by the duration of drift to the point $q, t_d \sim t_r$.

We will calculate the current $j(q,t)$ from the distribution $\rho(q,t)$ inside the attraction basin close to the basin boundary. This distribution is periodic in time for $t \ll 1/\overline{W}$. We now explicitly find it, and then match to the exact distribution near the basin boundary found from the linearized Eq. (1).

For small D, the distribution $\rho(q,t)$ far from the attractor is given, to logarithmic accuracy, by the solution of the variational problem [7,11],

$$\rho(q,t) = C\exp[-S(q,t)/D], \qquad S(q,t) = \min S[q(t)],$$
$$S[q] = \frac{1}{4}\int_{-\infty}^{t} dt' \left[\frac{dq}{dt'} + U'(q) - F(t')\right]^2, \quad (4)$$

Here, the minimum is taken with respect to the paths $q(t)$ which arrive at a given point q at a given instant t and start for $t \to -\infty$ from the periodic attractor $q_a^F(t)$. For a dynamically weak field, $q_a^F(t)$ and the basin boundary $q_b^F(t)$ are given by linear equations,

$$\dot{q}_i^F = -U''(q_i)(q_i^F - q_i) + F(t),$$
$$q_i^F(t + \tau_F) = q_i^F(t), \quad (5)$$

where $i = a, b$ (see Fig. 1). Equation (4) can be easily obtained [12] by noting that the distribution of the noise trajectories $\xi(t)$ is given by $\exp[-\int dt\, \xi^2(t)/4D]$, and that the trajectories $q(t)$ and $\xi(t)$ are interrelated via Eq. (1) [13]. The probability of a large fluctuation is determined by the appropriate optimal realization of $\xi(t)$, and the corresponding $q(t)$ provides the minimum to $S[q]$. An example of an optimal path is shown in Fig. 1. For $F = 0$, the normalization constant in (4) $C = [U''(q_a)/2\pi D]^{1/2}$.

To find the distribution ρ in the limit of small noise intensity and dynamically weak driving, but for arbitrary F/D, it suffices to find S to the first order in F. This can be done by calculating $S[q]$ (4) along the optimal path $q^{(0)}(t)$ in the absence of driving [$\dot{q}^{(0)} = U'(q^{(0)})$, according to (4)], which gives

$$S(q,t) = U(q) - U(q_a) - \int_{-\infty}^{t} d\tau\, \dot{q}^{(0)}(\tau)F(\tau). \quad (6)$$

Here, the optimal path is chosen so that $q^{(0)}(t) = q$. The quantity $\chi(t) = -\dot{q}^{(0)}(t)$ determines the field-induced change of the *logarithm* of the fluctuation probability and may be called logarithmic susceptibility (LS) [10].

Equations (4) and (6) can be simplified for small distances $Q = q - q_b^F(t)$ from the point q to the basin boundary $q_b^F(t)$, where $U(q)$ is quadratic in Q,

$$S(q,t) = \Delta U - \frac{1}{2}\lambda Q^2 + s[\phi(Q,t)], \tag{7}$$

where

$$\phi(Q,t) = \omega_F[t + \lambda^{-1}\ln(Q/Q_0)],$$
$$s(\phi) = \sum_n \tilde{\chi}(n\omega_F)F_n \exp(in\phi). \tag{8}$$

Here, F_n are Fourier components of the force $F(t)$, $\omega_F = 2\pi/\tau_F$ is the force frequency, $\lambda = -U''(q_b)$ is the curvature of the potential $U(q)$ at the local maximum q_b, ΔU is the barrier height for $F = 0$, and

$$\tilde{\chi}(\omega) = -\int_{-\infty}^{\infty} dt\, \dot{q}^{(0)}(t)e^{i\omega t}, \quad q^{(0)}(0) = q_b + Q_0. \tag{9}$$

In (7) we singled out the dependence of the field-induced correction s on $q \approx Q + q_b$ by calculating the LS $\tilde{\chi}$ along the trajectory that passes through the chosen point $q_b + Q_0$ at the instant $t = 0$ (we assume that $Q, Q_0 < 0$, cf. Fig. 1). The choice of Q_0 determines the phase of $\tilde{\chi}$, but $s[\phi(Q,t)]$ as a whole is independent of Q_0. We have also extended the range of integration over t in (6) to ∞ with account taken of smallness of the velocity $\dot{q}^{(0)} \approx -\lambda Q$ near the barrier top.

Clearly, the perturbation theory (7) diverges for $-Q \to 0$. This is related to nonintegrability of the variational problem (4) [7] for $F \neq 0$. Equation (7) applies if $\partial s/\partial Q$ is small compared to $\partial S(q,t)/\partial q$, i.e., for $-Q \gg |\omega_F \tilde{\chi} F|^{1/2}/\lambda$, which imposes a limitation on $-Q$ from below. An additional limitation follows from the neglect of the current away from the metastable state. This current becomes substantial at the distance from the basin boundary of the order of the diffusion length, $-Q \sim (D/\lambda)^{1/2}$. However, in the whole vicinity of the basin boundary the distribution $\rho(q,t)$ can be obtained from the linearized in Q Fokker-Planck equation:

$$\partial\rho/\partial t = -\lambda\partial(Q\rho)/\partial Q + D\partial^2\rho/\partial Q^2.$$

This equation can be solved by reducing it to the first-order equation for a generating function $\tilde{\rho}(p,t)$, which can be found then by the method of characteristics,

$$\rho(Q,t) = \int_0^{\infty} dp\, \exp(-pQ/D)\tilde{\rho}(p,t),$$
$$\tilde{\rho}(p,t) = \exp(-p^2/2\lambda D) f\big(p\exp(\lambda t)\big). \tag{10}$$

Here, $f(x)$ is an arbitrary function. It can be obtained by matching Eq. (10) to Eqs. (4) and (7) in the range of comparatively large negative Q. The matching can be done by evaluating the integral over p in (10) by the steepest descent method, with the assumption that f is a smooth function of p near the maximum of the integrand. This gives

$$f\big(p\exp(\lambda t)\big) = (W_0/\lambda D)\exp\{-s[\phi(-p/\lambda,t)]/D\}, \tag{11}$$

where W_0 is the Kramers escape rate for $F = 0$ [1]. It is clear from Eq. (8) that $\phi(-p/\lambda,t)$ indeed has the right form of a function of $p\exp(\lambda t)$.

Equations (7)–(11) describe the probability distribution and provide a solution of the escape problem for a periodically driven system. As discussed above, the escape probability $W[t - t_d(q)]$ (3) is determined by $\rho(q,t)$ (10) for the "observation point" $q = Q + q_b^F(t)$ lying far behind the diffusion region near the basin boundary. Yet it can be chosen within the region where the potential $U(q)$ is parabolic, and then the outgoing current is $j(q,t) \approx \lambda Q\rho(q,t)$. The major contribution to $\rho(q,t)$ (10) comes from the range $p \lesssim D/Q \ll (\lambda D)^{1/2}$. By changing in (10) to integration over $x \propto \ln p$, we obtain

$$j(q,t) = W[t - t_d(q)] = W_0 \int_{-\infty}^{\infty} dx\, e^{G\{x-\lambda[t-t_D(q)]\}}$$
$$\times \exp[-s(\omega_F x/\lambda)/D], \qquad G(x) = x - e^x. \tag{12}$$

Here, $t_D(q) = \lambda^{-1}\ln(\lambda Q|Q_0|/D)$ [overall, Eq. (12) is independent of Q_0]. The time lag $t_d(q)$ differs from $t_D(q)$ by a q-independent constant which depends on the choice of the initial condition for t_d in Eq. (3).

Equation (12) provides an explicit general expression for the escape rate of a driven system. This is the major result of the paper. It applies for an arbitrary ratio of the field-induced change of the activation energy of escape $\sim|s|$ to the noise intensity D, but for small $|s|/\Delta U$.

The outgoing current (12) is determined by two processes: large fluctuations which form a time periodic distribution close to the barrier top on the intrawell side, and diffusion over the barrier top. The first process depends on the global motion inside the well. The effect of the field on this process is described by the logarithmic susceptibility $\tilde{\chi}(\omega)$ which determines the function s. The second process is spatially localized to the vicinity of the barrier top, but, since it involves diffusion, the resulting transmission is described by an integral over the scaled time x [14]. We note that the overbarrier diffusion is unaffected by the field.

It follows from Eq. (12) that the period averaged escape rate $\overline{W}$ is given by a simple expression:

$$\overline{W}/W_0 = (2\pi)^{-1}\int_0^{2\pi} d\phi\, \exp[-s(\phi)/D]. \tag{13}$$

Since $s(\phi)$ (7) is a zero-mean periodic function, $\overline{W}$ always exceeds the Kramers escape rate W_0. For small F/D, the correction to W_0 is quadratic in F/D (cf. [8]). In the opposite limit of large F/D, the escape rate is changed exponentially strongly,

$$\overline{W}/W_0 = [D/2\pi s''(\phi_m)]^{1/2} \exp[|s(\phi_m)|/D], \qquad (14)$$

where ϕ_m is the position of the maximum of $-s(\phi)$, $s'(\phi_m) = 0$. The exponent in (14) for the general case of nonadiabatic driving was obtained earlier [10]. We emphasize that it is *linear* in the field amplitude. In particular, for sinusoidal driving, $F(t) = 2F_1 \sin \omega_F t$, we have $s''(\phi_m) = |s(\phi_m)| = 2|\chi(\omega_F)F_1|$. We note that the prefactor in (14) is a smooth function of the noise intensity D, in contrast to what was obtained in [5] for escape over a limit cycle.

The amplitude and frequency dependence of the average escape rate are illustrated in Fig. 2 for a simple model potential $U(q) = \frac{1}{2}q^2 - \frac{1}{3}q^3$. From (9), the LS for this potential $\tilde{\chi}(\omega) = \pi\omega/\sinh(\pi\omega)$. It falls off exponentially at large ω, which is a generic consequence of the smoothness of the instantonlike optimal path $q^{(0)}(t)$ in (9) (the phase of the LS corresponds to the path $q^{(0)}(t)$ that passes through $q = 1/2$ at $t = 0$).

The general expression for the time-dependent current (12) takes a simple form in the case of sinusoidal driving, $F(t) = 2\,\mathrm{Re}\,F_1 \exp(i\omega_F t)$,

$$j(q,t) = W_0 \sum_{k=-\infty}^{\infty} I_k\left(\frac{2|\tilde{\chi}(\omega_F)F_1|}{D}\right)\Gamma\left(1 + ik\frac{\omega_F}{\lambda}\right) \times \exp\{ik\omega_F[t - t_D(q)] + ik\phi_F\}, \qquad (15)$$

where $I_k(x)$ and $\Gamma(x)$ are the Bessel and gamma functions, respectively, and $\phi_F = \arg[\tilde{\chi}(\omega_F)F_1]$. It follows from (15) that, for *arbitrary* $\tilde{\chi}F/D$, the average escape rate is simply $\overline{W} = W_0 I_0(2|\tilde{\chi}(\omega_F)F_1|/D)$. In particular, for relatively strong fields $\ln\overline{W} \propto F_1$, in agreement with (14).

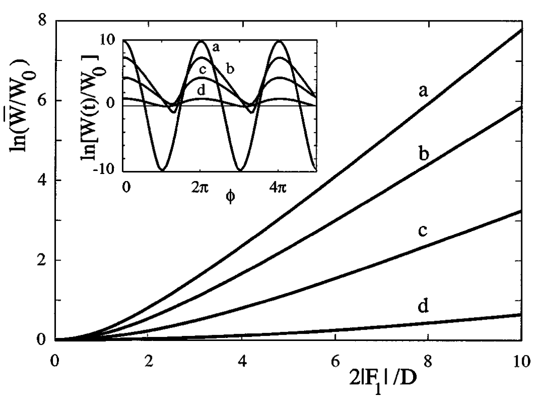

FIG. 2. The logarithm of the average escape rate as a function of the scaled field amplitude $2|F_1|/D$ for the potential $U(q) = q^2/2 - q^3/3$. The curves a to d refer to the dimensionless frequency $\omega_F = 0.1$, 0.4, 0.7, and 1.2. Inset: Time dependence of the *logarithm* of the instantaneous escape rate for the same frequencies and $2|F_1|/D = 10$ ($\phi = \omega_F t$), illustrating loss of synchronization of escape events with increasing ω_F.

An interesting feature of the time dependence of the outgoing current is *nonadiabatic rectification* with increasing field frequency. Since $|\Gamma(1 + ix)| = [\pi x/\sinh(\pi x)]^{1/2}$, the amplitudes of the harmonics of j (15) decay exponentially fast for large $k\omega_F/\lambda$.

The evolution of the temporal shape of the current is illustrated in the inset of Fig. 2. The *logarithm* of the escape rate is nearly sinusoidal for small ω_F, the transition rate is highly nonsinusoidal, and most transitions occur when the barrier is lowest. Modulation of $\ln W(t)$, and thus synchronization of escape events by the field, sharply decrease with increasing ω_F.

To explain this effect and the overall time dependence of the current, we note first that, irrespective of the field frequency, for $|\tilde{\chi}F|/D \gg 1$ the system is most likely to approach the vicinity of the basin boundary *once per period*, at the instants $n\tau_F + \phi_m/\omega_F$ ($n = 0, \pm 1, \ldots$), where ϕ_m is introduced in (14). The incoming probability pulses are nearly Gaussian in time far from the boundary. However, diffusion near the boundary effectively integrates them [cf. Eq. (12)], and as a result the outcoming current pulses become strongly asymmetric, and the current components with frequencies much higher than the relaxation rate λ are filtered out.

Equation (15) relates the escape rate to the logarithmic susceptibility. This makes it possible to *find* the logarithmic susceptibility experimentally, for an unknown potential. We note that time oscillations of the escape rate can be found from the mean first passage time-type measurements. For a system prepared in the metastable state for $t = 0$, the probability density per unit time of reaching a given point q is given by $W(t - t_d(q)) \exp(-\overline{W}t)$ (the last factor allows for the decay of the state population). Therefore the mean number density (per unit time) of the field periods before the system escapes and passes through q for a *given phase* of the field ϕ is $\langle n\rangle = W(t_\phi)/\overline{W}^2\tau_F^2$, where $t_\phi = (\phi/\omega_F) - t_d(q)$.

In this paper, we have analyzed the time-dependent and period-average rate of activated escape in driven systems, in a broad range of field frequencies and amplitudes. The field dependence of the escape rate changes from quadratic to exponential in the *amplitude* (not intensity) with increasing field. The effect of the field is determined by the logarithmic susceptibility, which may display strong frequency dependence and is accessible by experimental measurements. The amplitude of the time oscillations of the escape rate decreases with field frequency.

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