

Thermally Driven Escape with Fluctuating Potentials: A New Type of Resonant Activation

Peter Reimann

Limburgs Universitair Centrum, 3590 Diepenbeek, Belgium

(Received 13 December 1994)

The mean escape time \bar{T} for thermal diffusion in a fluctuating metastable potential is investigated. A new type of "resonant activation" (minimum of \bar{T} as a function of the correlation time τ of the potential fluctuations) is predicted analytically, explained in simple terms, and confirmed numerically. In its pure form it generically occurs for potentials without fluctuations near the barrier and the well. The effect is dominated by a minimum in the exponentially leading Arrhenius factor at a correlation time τ that stays finite for asymptotically small thermal and potential fluctuations.

PACS numbers: 05.40.+j, 02.50.-r, 82.20.Mj

The thermally driven escape over potential barriers plays an important role in chemical kinetics, the theory of diffusion in solids, homogeneous nucleation, electrical transport theory, etc. [1]. In many cases the potential itself shows *random* fluctuations on a characteristic time scale τ that may vary over a large range [2,3]. Examples are molecular dissociation in strongly coupled chemical systems [4], oxygen binding to hemoglobin [5], selective pumps for biological macromolecules, chromosomes, or viruses [6], and recently introduced ratchet models for the action of molecular motors [6]. In a seminal paper [7] Doering and Gadoua detected that the mean escape time \bar{T} may show a nonmonotonic dependence on τ with a resonancelike absolute minimum at a finite τ value. They coined the term "resonant activation" for this "astonishing phenomenon" [4] in contrast to the effect of "stochastic resonance" that may occur when the potential is subject to *deterministic* oscillations [8]. Stimulated by this first observation of "resonant activation" [7] the escape with fluctuating potentials has recently attracted much attention [9–17]. In this Letter we unify and extend previous findings by means of simple arguments and we predict a new type of resonant activation with nicer features than the usually considered type.

We investigate the standard one-dimensional model [2,3,7,9–15] of an overdamped particle

$$\dot{x}(t) = -U'(x(t)) - y(t)W'(x(t)) + \sqrt{2D}\xi(t), \quad (1)$$

where $\xi(t)$ is δ -correlated Gaussian noise (thermal fluctuations) and $U(x)$ a smooth metastable potential with a well at $x = 0$ and a barrier at $x = 1$, for instance, $U(x) = x^2/2 - x^3/3$. The potential fluctuations are driven by a *stationary Markovian* random process $y(t)$ with a symmetric invariant density $\rho(y) = \rho(-y)$ that decays faster than exponentially for $y \gg \sigma$, where $\sigma^2 := \int_{-\infty}^{\infty} y^2 \rho(y) dy$. We assume [7,9–14] that the time scale $\tau := \int_{-\infty}^{\infty} C(t) dt / 2\sigma^2$ characterizing the decay of the correlations $C(t) := \langle y(t)y(0) \rangle$ can vary between 0 and ∞ *without changing* $\rho(y)$. An example is dichotomic noise $y(t)$ that flips between $\pm\sigma$ at a rate $1/2\tau$, implying $\rho(y) = \delta(|y| - \sigma)/2$ and $C(t) = \sigma^2 e^{-|t|/\tau}$. Another

example is Ornstein-Uhlenbeck noise

$$\dot{y}(t) = -y(t)/\tau + \sqrt{2\sigma^2/\tau}\eta(t), \quad (2)$$

where $\eta(t)$ is δ -correlated Gaussian noise, giving rise to $\rho(y) = \sqrt{2\pi\sigma^2} e^{-y^2/2\sigma^2}$ and $C(t) = \sigma^2 e^{-|t|/\tau}$. We mainly have in mind these two examples in the following but we expect that our arguments are actually valid for more general random processes $y(t)$. For simplicity only, we finally assume that the fluctuating part of the potential $W(x)$ is smooth and that $x = 0$ and $x = 1$ are still the absolute minimum and maximum of $U_y(x) := U(x) + yW(x)$ in the regions $x \leq 1$ and $x \geq 0$, respectively, for any y value with non-negligible probability $\rho(y)$. Obviously, for dichotomic noise the latter condition must just be satisfied for $U_{\pm\sigma}(x)$. For Ornstein-Uhlenbeck noise we will come back to this condition in the last paragraph.

A complete description of the system (1) is provided by the time-dependent probability distribution $\rho(x, y, t)$ of the particle x and the potential fluctuations y . Its evolution is governed by a master equation $\dot{\rho}(x, y, t) = \Gamma \rho(x, y, t)$, where the master operator $\Gamma = \Gamma_x + \Gamma_y$ consists of the Fokker-Planck operator $\Gamma_x = \partial_x[U_y'(x) + D\partial_x]$ corresponding to the Langevin equation (1) and the evolution operator Γ_y of the Markovian random process $y(t)$, e.g., $\Gamma_y = \partial_y[y + \sigma^2\partial_y]/\tau$ for Ornstein-Uhlenbeck noise (2). The initial condition, say at time $t = 0$, is of the form $\rho(x, y, 0) = \rho_0(x)\rho(y)$, where $\rho_0(x)$ is an initial distribution of particles mainly concentrated about the potential well $x = 0$. The quantity of central interest is the mean escape time $\bar{T} = \int_{-\infty}^b dx \int_{-\infty}^{\infty} dy \int_0^{\infty} dt \rho(x, y, t)$ from the region $x \leq b$ (note that the integrand ρ is equivalent to $-t\dot{\rho}$). The boundary b is required to be sufficiently far beyond the barrier $x = 1$ that particles, once they have left the region $x \leq b$, are very unlikely to return into the domain $x \leq 1$. We will mainly restrict ourselves to the most interesting case [1] that this typical escape time \bar{T} is much larger than the time scales of the deterministic dynamics $\dot{x} = -U_y'(x)$ for any y with non-negligible probability $\rho(y)$. In other words, the strengths D and σ^2 of the thermal and potential fluctuations must be small in comparison with the barrier height $\Delta U := U(1) - U(0)$. As a

consequence, \bar{T} becomes independent of the exact choice of $\rho_0(x)$ and b [1]. As a further consequence, a particle (1) typically spends most of its time near the well $x = 0$ before it escapes. The sojourn close to $x = 0$ is interrupted by unsuccessful escape attempts and is terminated by a successful escape attempt. It can be shown that the time scale T_a of the escape attempts increases like $\ln D^{-1}$ but is still much smaller than \bar{T} for sufficiently small D and σ^2 [18]. We therefore have the *three relevant time scales* τ , T_a , and \bar{T} , where $T_a \ll \bar{T}$ and $0 \leq \tau \leq \infty$.

Within the separation of time scales $\tau \ll \bar{T}$ the *rate concept* applies [1], i.e., $\rho(x, y, t)$ approaches an exponential decay $e^{-\bar{k}t} \rho(x, y)$ in the region $x \leq b$ on a time scale that is negligible in comparison with \bar{T} . It readily follows that the decay rate \bar{k} is equal to \bar{T}^{-1} , the quasi-invariant density $\rho(x, y)$ is governed by $\Gamma\rho(x, y) = -\bar{k}\rho(x, y)$, and $\int_{-\infty}^b \rho(x, y) dx = \rho(y)$. On the other hand, for $\tau \gg T_a$ the *kinetic models* studied in Refs. [10,16,17] provide a very accurate description of the problem since a particle (1) approximately sees a static potential $U_y(x)$ during any escape attempt and is thus successful at the well-known Smoluchowski rate [1]

$$k(y) = \frac{|U_y''(0)U_y''(1)|^{1/2}}{2\pi} \exp\left\{-\frac{\Delta U + y\Delta W}{D}\right\}, \quad (3)$$

where $\Delta W := W(1) - W(0)$. Therefore the probability $P(y, t) := \int_{-\infty}^b \rho(x, y, t) dx$ that a particle sees a potential $U_y(x)$ and has not yet escaped from the region $x \leq b$ evolves under the simultaneous action of the master operator Γ_y governing the potential fluctuations $y(t)$ and the loss rate $k(y)$ due to successful escapes, $P(y, t) = [\Gamma_y - k(y)]P(y, t)$, with initial condition $P(y, 0) = \rho(y)$. Formally the same follows [14] by adiabatic elimination of x in the master equation governing $\rho(x, y, t)$. Introducing $P(y) := \int_0^\infty P(y, t) dt$ one finally obtains

$$[\Gamma_y - k(y)]P(y) = -\rho(y) \quad (4)$$

and $\bar{T} = \int_{-\infty}^\infty P(y) dy$. "Kinetic equations" like (4) have been extensively studied in the context, e.g., of random walks with traps; see [19] and further references therein.

For very small τ the particle (1) does not feel in leading order approximation that the fluctuations $y(t)$ are actually correlated, and we can replace them by white Gaussian noise (in Stratonovich interpretation) of the same mean $\langle y(t) \rangle = 0$ and intensity $\int_{-\infty}^\infty C(t) dt = 2\tau\sigma^2$ [3,15]. The well-known escape rate \bar{k} of such a stochastic process [1] has the same form as $k(0)$ in (3) but with $\int_0^1 dx U'(x)/[D + \tau\sigma^2 W'(x)^2]$ instead of $\Delta U/D$. With $\bar{T} = \bar{k}^{-1}$ one thus obtains in leading order τ

$$\bar{T}(\tau) = k(0)^{-1} \exp\left\{-\frac{\tau\sigma^2}{D^2} \int_0^1 U'(x) W'(x)^2 dx\right\} \quad (5)$$

in agreement with all known rigorous results for dichotomic [9,10,14] and Ornstein-Uhlenbeck noise $y(t)$ [3,12,14,15]. Hence, for small τ the mean escape time $\bar{T}(\tau)$ decreases with increasing τ .

Regarding more general correlation times compatible with a rate description, $\tau \ll \bar{T}(\tau)$, we first address *potentials $W(x)$ of type I* by which we mean that $W'(x)$ does not change sign on the interval $[0, 1]$, for instance, $W(x) = U(x)$. Without loss of generality, we assume that $\Delta W > 0$ in the sequel. In this case a particle (1) typically escapes [7,20] while the potential $U_y(x)$ is in a "low" state, $y < 0$. Although the distribution $\rho(y)$ is always the same, with decreasing τ any realization $y(t)$ tends to fluctuate faster and faster, and favorable escape conditions $y(t) < 0$ during the entire typical time T_a of a successful escape attempt become less and less probable. We thus expect that $\bar{T}(\tau)$ is a decreasing function of τ in agreement with all exactly solvable models [7,9,10,12]. Next we address *potentials $W(x)$ of type II* defined by the property that $W(x)$ identically vanishes close to the well $x = 0$ and the barrier $x = 1$, for instance, $W(x) = \cos^2(2\pi x)$ for $1/4 \leq x \leq 3/4$ and $W(x) = 0$ else. In this case the basic escape mechanism is sketched in Fig. 1 [for convenience only, we focus on a single humped $W(x)$]: Typically, a successful escape attempt starts while the potential $U_y(x)$ is in a low state [Fig. 1(a)], then the particle is lifted by a large fluctuation of $y(t)$ [Fig. 1(b)], and finally it moves in a potential $U_y(x)$ in a "high" state across the saddle $x = 1$ [Fig. 1(c)]. Since this mechanism requires *one* large fluctuation of $y(t)$ during a successful escape attempt, the mean escape time $\bar{T}(\tau)$ will increase both when τ tends to very large and very small values. More precisely, we expect that $\bar{T}(\tau)$ exhibits a minimum resonant activation at a τ value comparable to the time that the particle needs to pass through the domain with $W(x) \neq 0$ during the successful escape attempt. Closer inspection shows [18,20] that this time is comparable to the one which the particle would need to pass deterministically through the same domain but in the opposite direction. Typically, this deterministic dynamics $\dot{x} = -U'(x)$ can be roughly approximated by $\dot{x} = -\Delta U$ in the domain with $W(x) \neq 0$. Under the further assumption that the length of this domain is comparable to the distance between the saddle and the well of $U(x)$, i.e., of the order 1, the minimal τ is thus of the order $1/\Delta U$. For both type I and type II potentials the escape mechanisms as well as the properties

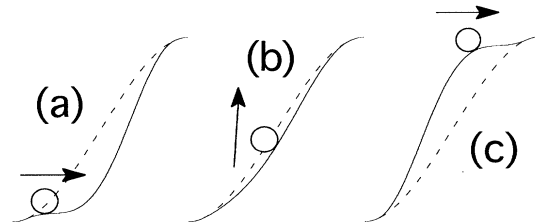


FIG. 1. Typical successful escape attempt for resonant activation of type II at three successive time instances. Solid lines: fluctuating potential $U_y(x) = U(x) + yW(x)$ for $0 \leq x \leq 1$; dashed lines: unperturbed potential $U(x)$; arrows: motion of the escaping particle.

of $\bar{T}(\tau)$ discussed in this paragraph are confirmed by rigorous calculations [20] for asymptotically weak thermal and Ornstein-Uhlenbeck-type potential fluctuations.

We finally discuss the regime $\tau \gg T_a$ which overlaps with the previous one $\tau \ll \bar{T}$. Since for type II potentials $W(x)$ the rates (3) are y independent, the solution of (4) is trivial, and we immediately find $\bar{T}(\tau) = \bar{T}(0)$. Together with the small- τ asymptotics (5) this proves the existence of resonant activation of type II independently of the heuristic arguments in the last paragraph (see Fig. 2). Equation (5) also shows that the effect is already present in the exponentially leading weak noise behavior (i.e., the Arrhenius factor) of $\bar{T}(\tau)$. Regarding non-type-II potentials $W(x)$ we first note that for $T_a \ll \tau \ll \bar{T}(\tau)$ both the rate concept and the kinetic model are valid. Since $T_a \ll \tau$, a particle (1) approximately sees a nonfluctuating potential $U_y(x)$ during any escape attempt and thus will escape at a rate (3). Since the rate concept applies, the probability that a particle which has not yet escaped sees a potential $U_y(x)$ is given by $\int_{-\infty}^b \rho(x, y) dx = \rho(y)$. Hence the average escape rate is $\bar{k} = \int_{-\infty}^{\infty} k(y) \rho(y) dy$ independent of τ . With $\bar{k} = \bar{T}^{-1}$ and ignoring the y dependence of the prefactor $|U_y''(0)U_y''(1)|^{1/2}$ in (3) we obtain

$$\bar{T}(\tau) = \bar{T}(0) \int_{-\infty}^{\infty} e^{-y \Delta W/D} \rho(y) dy =: T_- \quad (6)$$

for $T_a \ll \tau \ll T_-$. On the other hand, for extremely slow potential fluctuations $\tau \gg \bar{T}(\tau)$ each realization $y(t)$ does practically not change on any relevant time scale. Thus the evolution operator Γ_y of $y(t)$ in (4) is negligible and we obtain the τ -independent result

$$\bar{T}(\tau) = \bar{T}(0) \int_{-\infty}^{\infty} e^{y \Delta W/D} \rho(y) dy =: T_+ \quad (7)$$

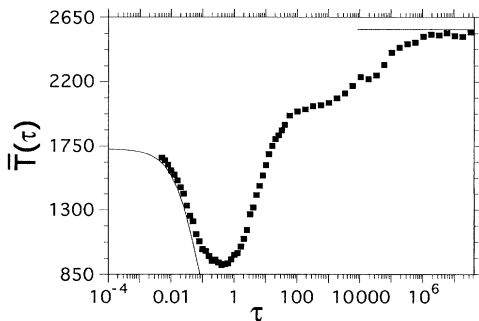


FIG. 2. Numerical simulations of the mean escape time $\bar{T}(\tau)$ out of the region $x \leq b = 3/2$ for the noisy dynamics (1) with stationary Ornstein-Uhlenbeck potential fluctuations (2), $U(x) = x^2/2 - x^3/3$, $W(x) = \cos^2(2\pi x)$ for $1/4 \leq x \leq 3/4$ and $W(x) = 0$ else, $D = 0.03$, $\sigma^2 = 0.0048$, and an initial distribution of particles $\rho_0(x) = \delta(x)$. The numerical uncertainty due to the time discretization and the finite number of realizations is a few percent. The typical features of type II resonant activation are clearly visible. The solid lines are the asymptotically exact results $\bar{T}(\tau) = T_\tau(0)$ from (8) and (9) for small and large τ .

for $\tau \gg T_+$. From our assumptions that $\rho(y)$ is symmetric and decays faster than exponentially for $y \gg \sigma$ we can infer that $T_-/\bar{T}(0) = \bar{T}(0)/T_+ \leq 1$ and $T_+ < \infty$. For instance, one recovers [9,10] $T_\pm \approx \bar{T}(0) e^{\pm \sigma \Delta W/D}$ for dichotomic and [14] $T_\pm = \bar{T}(0) e^{\pm \sigma^2 \Delta W^2/2D^2}$ for Ornstein-Uhlenbeck noise $y(t)$. In the first example the consistency condition $T_a \ll T_-$ requires that $\sigma < \Delta U/\Delta W$ and in the second that $\sigma^2 < 2D \Delta U/\Delta W^2$. If $T_a \ll T_-$ were not fulfilled and, in particular, if $\rho(y)$ did not decay faster than exponentially for large y , there would be a regime of τ values where neither the rate concept nor the kinetic model would apply. In this regime the particles would typically escape while the potential barrier is completely gone [7]. This shows that $T_a \ll T_-$ actually follows from our assumptions on $\rho(y)$ and $W(x)$ in the second paragraph. Regarding the crossover from (6) to (7) one expects that a particle typically will escape with a mean escape time $k(y)^{-1}$ if it experiences a potential $U_y(x)$ for which this mean escape time is smaller than τ . Otherwise it will wait during a time of the order τ until the fluctuations have changed the potential $U_y(x)$ such that $k(y)^{-1} < \tau$. The entire escape time of this kind of particle is thus of the order τ . Therefore, the mean escape time $\bar{T}(\tau)$ is approximately given by $\int_{-\infty}^{\infty} \rho(y) \min\{k(y)^{-1}, \tau\} dy$. It is not difficult to see that this expression increases with τ and matches (6) and (7). By closer inspection of Eq. (4) these properties of $\bar{T}(\tau)$ can be rigorously proven for *general* Markovian random processes $y(t)$ [19].

For the usually considered potentials $W(x)$ of type I the mean escape time $\bar{T}(\tau)$ is monotonically decreasing and increasing within the validity of the rate and the kinetic description, respectively. The minimum resonant activation τ_{RA} occurs in the rather extended regime $T_a \ll \tau \ll T_-$ where both descriptions are very good approximations and thus $\bar{T}(\tau)$ is almost constant. Since T_a diverges in the weak noise limit, the same follows for τ_{RA} . The breakdown of the rate concept is thus crucial [14] and resonant activation will not be seen within a rate [12] or kinetic [10,16,17] description alone. The essential quantitative properties of $\bar{T}(\tau)$ follow from (5)–(7). On the other hand, for the novel type II potentials $W(x)$ the minimum of $\bar{T}(\tau)$ occurs at $\tau_{RA} = O(1/\Delta U)$ and, in particular, stays finite in the weak noise limit. Within the validity of the rate formula (3), i.e., for sufficiently small thermal and potential fluctuations, we have $\bar{T}(\tau) \equiv \bar{T}(0)$ for $\tau \gg T_a$, and the rate concept actually never breaks down. Moreover, the assumption that the potential fluctuations $y(t)$ are stationary does not play a crucial role, in contrast to the type I case [17,19]. Although the minimum of $\bar{T}(\tau)$ is present already in the exponentially leading Arrhenius factor for both types according to (5)–(7), it is sharply peaked about $\tau = \tau_{RA}$ only in the type II case. For more general potentials $W(x)$ one finds [20] either qualitatively similar results for $\bar{T}(\tau)$ as in the type I and type II cases or a truly mixed type

of behavior with two minima. Apart from a missing quantitative approximation for $\bar{T}(\tau_{RA})$ in the type II case, our understanding of the escape problem (1) is thus rather complete for small thermal and potential fluctuations.

If the fluctuations are no longer small, the different types of resonant activation cannot be clearly distinguished anymore and both the rate and the kinetic descriptions break down. However, for small τ one still may approximate $y(t)$ in (1) by Gaussian white noise [3] similarly as in the derivation of (5). Then one readily finds [1,3] the mean first passage time $T_\tau(x)$ across b for a particle (1) with seed $x \leq b$

$$T_\tau(x) = \int_x^b dv \int_{-\infty}^v dw \frac{\exp\left\{\int_w^v \frac{U'(z)}{D_\tau(z)} dz\right\}}{\sqrt{D_\tau(v)D_\tau(w)}}, \quad (8)$$

where $D_\tau(x) := D + \tau \sigma^2 W'(x)^2$. Similarly, in the static limit $\tau \rightarrow \infty$ one immediately obtains [1] the rigorous expression

$$T_\infty(x) = \int_{-\infty}^{\infty} dy \rho(y) \int_x^b dv \int_{-\infty}^v dw \frac{\exp\left\{\frac{U_y(v) - U_y(w)}{D}\right\}}{D}. \quad (9)$$

Both (8) and (9) are valid for *arbitrary* D , σ , and $W(x)$, and the mean escape time follows by averaging over the seeds $\bar{T}(\tau) = \int_{-\infty}^b \rho_0(x) T_\tau(x) dx$ (see Fig. 2). For small D , one recovers Eqs. (5) and (7) as well as their finite noise corrections which are responsible for the deviations in Fig. 2 from the weak noise predictions $\bar{T}(0) \approx 1625$ according to (3) and (5), and $\bar{T}(\tau) = \bar{T}(0)$ for $\tau \rightarrow \infty$. Since $\rho(-y) = \rho(y)$ we can infer from (8) and (9) that $\bar{T}(0) \leq \bar{T}(\infty)$, and since $\rho(y)$ decreases faster than exponentially for large y we see that $\bar{T}(\infty)$ is finite. The property $\bar{T}(0) \leq \bar{T}(\infty)$ can be used to *prove the existence of resonant activation under very general conditions*. For instance, a sufficient condition is that (8) decreases with increasing τ which again is certainly true if D becomes small [14] [see Eq. (5)] or if $W'(x)$ vanishes whenever $U'(x) < 0$ and $x \leq b$.

For Ornstein-Uhlenbeck noise (2) the y integral in (9) can be performed explicitly, and the integrand then takes the form $\exp\{F(v, w)/D\}/D$, where $F(v, w)$ is given by $U(v) - U(w) + (\sigma^2/2D)[W(v) - W(w)]^2$. It follows that our previously derived weak noise results (7) and $\bar{T}(\tau) = \bar{T}(0)$ for potentials $W(x)$ of types I and II, respectively, are recovered from (9) only if the maximum of $F(v, w)$ (with the restriction $w \leq v \leq b$) is taken for $v = 1$, $w = 0$. Together with $\sigma^2 < 2D \Delta U/\Delta W^2$ [see

below Eq. (7)], this is the quantitative version of the condition introduced below Eq. (2) in the case of Ornstein-Uhlenbeck noise $y(t)$. In particular, it is satisfied by the example in Fig. 2. Further, it follows that σ must decrease at least proportional to \sqrt{D} in the weak noise limit. Note that the variations of $\bar{T}(\tau)/\bar{T}(0)$ as a function of τ still become exponentially large for small D as can be concluded from (5)–(7).

I would like to thank P. Hänggi, C. Van den Broeck, and P. Talkner for helpful discussions. Financial support by the Program on Inter-University Attraction Poles of the Belgian Government is gratefully acknowledged.

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