Activated Escape of a Self-Propelled Particle from a Metastable State

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We study the noise-driven escape of active Brownian particles (ABPs) and run-and-tumble particles (RTPs) from confining potentials. In the small noise limit, we provide an exact expression for the escape rate in terms of a variational problem in any dimension. For RTPs in one dimension, we obtain an explicit solution, including the first subleading correction. In two dimensions we solve the escape from a quadratic well for both RTPs and ABPs. In contrast to the equilibrium problem we find that the escape rate depends explicitly on the full shape of the potential barrier, and not only on its height. This leads to a host of unusual behaviors. For example, when a particle is trapped between two barriers it may preferentially escape over the higher one. Moreover, as the self-propulsion speed is varied, the escape route may discontinuously switch from one barrier to the other, leading to a dynamical phase transition.

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Activated escapes from metastable states play a major role in a host of physical phenomena, with applications in fields as diverse as biology, chemistry, and astrophysics [1,2]. They also play an important role in active matter, where they control nucleation in motility-induced phase separation [3], activated events in glassy self-propelled-particle systems [4,5], or escapes through narrow channels [6]. However, despite recent progress [7,8], little is known about the physics that controls the rare events leading to the escape of an active system from a metastable state.

In equilibrium, most of our intuition regarding such events is based on Kramers seminal work [9] on Brownian particles (see Ref. [10] for a review). When the thermal energy is much lower than the potential barriers, there is a timescale separation between rapid equilibration within metastable states and rare noise-induced transitions between them, a simple physical picture which is at the root of the modern view on metastability [11,12]. In this limit, the mean escape time over a potential barrier of height ΔV is given by $\langle\tau\rangle \sim \exp(\Delta V/k_B T)$. At the exponential level, the crossing time over a potential barrier only depends on its height.

To develop a corresponding intuition for activated processes in active matter, we follow Kramers and consider the dynamics of an active particle confined in a metastable well described by a potential V:

$$\dot{\mathbf{x}} = -\mu\nabla V + v\mathbf{u}(\theta) + \sqrt{2D}\boldsymbol{\xi}(t). \tag{1}$$

Here, $\mathbf{x}$ is the position of the particle, v its self-propulsion speed, and μ its mobility. The orientation of the particle $\mathbf{u}(\theta)$ evolves stochastically with a persistence time $1/\alpha$. Here, θ is a generalized angle parametrizing the $d-1$ dimensional unit sphere. Finally, $\boldsymbol{\xi}(t)$ is a Gaussian white noise which may stem from either thermal fluctuations, in which case $D = \mu k_B T$, or from fluctuations of the activity. As we show below, the escape of such an active particle from a metastable state is very different from the equilibrium case, leading to a host of interesting phenomena. For example, direct simulations of Eq. (1) show that active particles confined between two barriers may preferentially escape over the *higher* one, depending on the self-propulsion v (see Fig. 1).

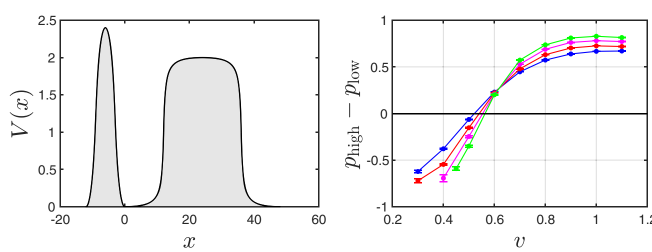

FIG. 1. Active escape from a metastable well confined by two barriers of different heights (left). We measured the fraction of particles escaping over the higher barrier, p_{high}, and over the lower one, p_{low}, depending on the value of v and with decreasing values of D, of Eq. (1). The right panel shows that, as v increases, the most likely escape route switches from the lower barrier to the higher one. The switch between preferred barriers is manifested as a dynamical phase transition in the small-noise limit. This can be seen as the transition becomes sharper when D is decreased (blue: $D = 0.08$, red: $D = 0.0675$, magenta: $D = 0.058$, green: $D = 0.051$, colors online). Details of the potential are given in Ref. [13].

In what follows, we provide a complete solution of the Kramers problem for active particles described by Eq. (1), in any dimension, using a path-integral formalism. In contrast to existing works on first-passage times [14–16], we focus on cases in which the potential is strictly confining at $D = 0$ and the barrier can only be crossed using fluctuations. We refer to such cases as *confining potentials*. We give an explicit expression for the mean escape time in terms of a variational problem for run-and-tumble particles (RTPs) [17,18] and active Brownian particles (ABPs) [19], the latter being studied only in $d \geq 2$ dimensions. In one dimension, RTPs had previously been studied in the limits $\alpha \to 0$ and $\alpha \to \infty$ [7]; Here, we provide the full solution of the activation time for RTPs for all α, including its subexponential prefactor. In cases with multiple competing reaction paths, our results provide the selection principle for the most likely escape route. In particular, we explain the dynamical phase transition observed in Fig. 1.

For confining potentials, it is natural to divide the barrier into separate regions depending on whether the force $|\nabla V|$ is larger or smaller than the propulsion force $f_p = v/\mu$. Consider, for instance, the escape in one dimension from a metastable well; see Fig. 2. We can identify four different regions separated by three points $\{C_1, C_2, C_3\}$ satisfying $|V'(C_i)| = f_p$. In regions (i) and (iii), when $x \leq C_1$ or $C_2 \leq x \leq C_3$, the particles feel a force $-V'$ smaller in magnitude than f_p. In the $D \to 0$ limit the contribution of the noise $\xi(t)$ to the dynamics can be neglected. In region (ii), where $C_1 \leq x \leq C_2$, the particles cannot climb the potential without the noise $\xi(t)$. Crossing this region is therefore a rare event which controls the escape from the metastable state. In region (iv), where $x > C_3$, the particles would need the noise to come back to region (i), were they to reverse direction. This is a rare event and the particle has thus effectively crossed the barrier once it has reached C_3. The generalization of these points to lines or surfaces in higher dimensions (denoted $\mathbf{C}_i$) is straightforward and an example is displayed in Fig. 2 [20]. Note that the problem is activated only if region (ii) exists. Otherwise, the problem, as considered, e.g., in one dimension in Ref. [21], is a first-passage problem with no instanton physics. The activated process only corresponds to moving across region (ii) so that the crossing probability is given, to leading order, by histories connecting points on $\mathbf{C}_1$ and $\mathbf{C}_2$. To obtain the escape time we then write the transition probability $P(\mathbf{x}_2, t|\mathbf{x}_1, 0)$ to be at $\mathbf{x}_2 \in \mathbf{C}_2$ at time t starting at $\mathbf{x}_1 \in \mathbf{C}_1$ as a path integral in its Onsager-Machlup form [22]

$$P(\mathbf{x}_2, t|\mathbf{x}_1, 0) = \int_{\mathbf{x}_1}^{\mathbf{x}_2} \mathcal{D}[\mathbf{x}(t), \theta(t)] e^{-(1/D)\mathcal{A}[\mathbf{x},\theta]} \mathcal{P}[\theta(t)]. \quad (2)$$

$\mathcal{P}[\theta(t)]$ is the probability of a history of the angle θ. For example, ABPs in two dimensions with rotational diffusivity α lead to $\mathcal{P}[\theta(t)] \propto e^{-\int_0^t \dot{\theta}^2/(4\alpha) dt'}$. In Eq. (2), the action $\mathcal{A}[\mathbf{x}, \theta]$ is given by

$$\mathcal{A}[\mathbf{x}, \theta] = \frac{1}{4} \int_0^t \|\dot{\mathbf{x}} + \mu \nabla V(\mathbf{x}) - v\mathbf{u}(\theta)\|^2 dt'. \quad (3)$$

We first integrate expression (2) over the paths $\theta(t)$ to obtain an effective action for the probability of a path $\mathbf{x}(t)$. In the limit $D \to 0$, we use a saddle-point approximation in Eq. (2) to get

$$\int \mathcal{D}[\theta(t)] e^{-(1/D)\mathcal{A}[\mathbf{x},\theta]} \mathcal{P}[\theta(t)] \underset{D\to 0}{\asymp} e^{-(1/D)\mathcal{A}[\mathbf{x},\tilde{\theta}]}, \quad (4)$$

where $\asymp$ stands for logarithmic equivalence and $\tilde{\theta}(t)$ is the path satisfying the variational problem

$$\mathcal{A}[\mathbf{x}, \tilde{\theta}] = \inf_{\theta} \left(\frac{1}{4} \int_0^t \|\dot{\mathbf{x}} + \mu \nabla V(\mathbf{x}) - v\mathbf{u}(\theta)\|^2 dt' \right). \quad (5)$$

Note that $\mathcal{P}[\theta(t)]$ is a subdominant contribution and any cost to the action arising from it can be ignored to leading order [23]. Clearly, the optimum requires $\mathbf{u}(\theta)$ to be in the same direction as $\dot{\mathbf{x}} + \mu \nabla V(\mathbf{x})$ so that

$$\mathbf{u}(\tilde{\theta}) = \frac{\dot{\mathbf{x}} + \mu \nabla V(\mathbf{x})}{\|\dot{\mathbf{x}} + \mu \nabla V(\mathbf{x})\|}. \quad (6)$$

Using Eqs. (6) and (3), we find that the transition probability between $\mathbf{x}_1$ and $\mathbf{x}_2$ is dominated by paths that minimize the action

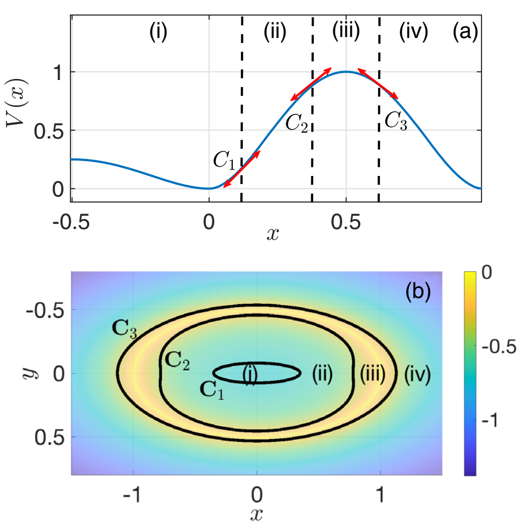

FIG. 2. Schematic representation of the active escape problem. Top: Escape in one dimension over a barrier, region (i) corresponds to the well whereas regions (ii)–(iv) make up the barrier. All are defined in the text. Bottom: The color code represents the height of the potential. The barrier is located around in the yellow region.

$$\mathcal{A}[\mathbf{x}] = \frac{1}{4}\int_{-\infty}^{\infty} (\|\dot{\mathbf{x}} + \mu\nabla V(\mathbf{x})\| - v)^2 dt', \tag{7}$$

where we have sent the limits of the integral to $\pm\infty$, using the fact that extremal trajectories start and end at stationary points (see, for instance, Refs. [24,25]). Finally, the escape time is given by

$$\begin{aligned} \langle\tau\rangle &\underset{D\to 0}{\asymp} e^{\frac{\phi}{D}}, \\ \phi &= \inf_{\{\mathbf{x}_1\in\mathbf{C}_1,\mathbf{x}_2\in\mathbf{C}_2\}} \inf_{\mathbf{x}(t)} \mathcal{A}[\mathbf{x}(t)]. \end{aligned} \tag{8}$$

The inner minimization corresponds to optimizing the action over different paths; it is realized by an instanton $\mathbf{x}(t)$ which connects $\mathbf{x}_1$ and $\mathbf{x}_2$. The outer minimization corresponds to optimizing over all possible initial and final positions of the instanton. Equation (8) provides a full solution to the escape problem for both ABPs and RTPs as a variational problem. It generalizes the Kramers law and we discuss the physics of the quasipotential barrier ϕ below. Note that when $v = 0$ the minimizers of the action are $\dot{\mathbf{x}} = \mu\nabla V(\mathbf{x})$ and we recover the usual Kramers law with $\phi = \mu\Delta V$, where ΔV is the minimal potential difference across the barrier. We now turn to apply our results to a general one-dimensional potential barrier and to an elliptic well in two dimensions.

RTPs in one dimension.—Here, $\mathbf{u}(\theta)$ is replaced by a binary variable $u = \pm 1$ which flips with rate $\alpha/2$. As in Fig. 2, the barrier is located on the right of the metastable well. $\mathbf{x}_{1,2}$ are then given by $C_{1,2}$. Clearly, the minimal action is obtained by particles with $u = 1$: particles that reverse their motion in the middle of the instanton are exponentially less likely to cross the barrier. The action then reduces to

$$\mathcal{A}[x] = \frac{1}{4}\int_{-\infty}^{\infty} [\dot{x} + \mu V'(x) - v]^2 dt'. \tag{9}$$

It is thus equivalent to an equilibrium problem in an effective titled potential $\varphi(x)/\mu$; the instanton solution obeys

$$\dot{x} = \partial_x\{\mu[V(x) - V(C_1)] - v(x - C_1)\} \equiv \partial_x\varphi(x), \tag{10}$$

which gives, for the quasipotential barrier introduced in Eq. (8),

$$\phi = \mu[V(C_2) - V(C_1)] - v(C_2 - C_1). \tag{11}$$

Our predictions (8) and (11) are verified in Fig. 3 using direct simulation of Eq. (1) with a single barrier.

Using asymptotic techniques [13,26], we also obtain the leading subexponential amplitude of the transition time (8). For simplicity we consider a boundary condition in which the potential is flat on the left of the barrier and the density

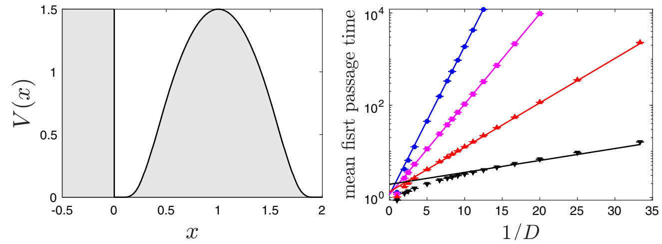

FIG. 3. We compute the mean-first passage time $\langle\tau\rangle$ over a confining barrier. Details of the potential shown in the left panel are given in Ref. [13]. The right panel shows the validity of our generalized Kramers law for several values of $v = 1.0$, 1.5, 2.0, and 2.5.

of particles in that region is ρ_0; other boundary conditions are discussed in Ref. [13]. The mean time between particles crossing the barrier is then given by $\langle\tau\rangle \underset{D\to 0}{\sim} Ae^{(\phi/D)}$, where

$$A = \frac{2\pi e^{-(\alpha/2)\mathcal{T}_{\text{inst}}}}{\rho_0 v^2 \Gamma(1-\frac{\alpha}{2k_2})\Gamma(\frac{\alpha}{2k_1})} \frac{[\frac{D}{v^2}k_1]^{[(k_1-\alpha)/2k_1]}}{[\frac{D}{v^2}|k_2|]^{[(k_2-\alpha)/2k_2]}} \times \frac{\int_{C_2}^{C_3}[\alpha - \mu V''(y)] e^{\alpha\mathfrak{F}\int_{C_2}^{y}\{\mu V'(z)/[v^2-(\mu V'(z))^2]\}dz} dy}{e^{-\alpha\mathfrak{F}\int_{-\infty}^{C_1}\{\mu V'(y)/[v^2-(\mu V'(y))^2]\}\mathrm{d}y}}. \tag{12}$$

Here, $\mathcal{T}_{\text{inst}} = \mathfrak{F}\int_{C_1}^{C_2}(dy/\partial_y\varphi)$ is the duration of the instanton, $k_i = \mu V''(C_i)$, $\Gamma(x)$ is the Euler Gamma function, and $\mathfrak{F}$ denotes the finite part of the integral, defined by removing the logarithmic divergences occurring at C_1 and C_2, e.g.,

$$\begin{aligned} &\mathfrak{F}\int_{-\infty}^{C_1} \frac{\mu V'(y)}{v^2 - [\mu V'(y)]^2} dy \\ &\quad = \lim_{x\to C_1}\left\{\int_{-\infty}^{x} \frac{\mu V'(y)}{v^2 - [\mu V'(y)]^2} dy \right. \\ &\qquad \left. + \frac{1}{2k_1}\log\left(\frac{k_1(C_1 - x)}{v}\right)\right\}. \end{aligned} \tag{13}$$

The term $e^{-(\alpha/2)\mathcal{T}_{\text{inst}}}$ has a simple interpretation: it is the probability that the particle does not flip along the instanton. Note that the $v = 0$ limit is singular: all histories of $u(t)$ are then equally likely, a degeneracy which otherwise does not exist.

Equations (11) and (13) provide an explicit solution to the Kramers problem in one dimension. Note that the effect of the activity cannot be cast into a simple description with an effective temperature. Both ϕ and the prefactor indeed depend on the full functional form of the potential V.

Dynamical phase transition.—We now show how the analysis of the quasipotential accounts for the nontrivial choice of escape routes when the particle is trapped between two potential barriers. In the small D limit, the escape time is controlled by the quasipotential (11) of each barrier, which we can study separately. For the right barrier, the explicit dependence of ϕ on v reads

$$\phi(v) = \mu\{V[C_2(v)] - V[C_1(v)]\} - v[C_2(v) - C_1(v)]. \tag{14}$$

When $v = 0$, we recover the standard Kramers result $\phi(0) = \mu[V(C_2) - V(C_1)]$. Using $\mu V'(C_1) = \mu V'(C_2) = v$, one has $\phi'(v) = -(C_2 - C_1)$, which implies that ϕ is a decreasing function of v. When $v > v_{\mathrm{cr}} \equiv \max_x\{\mu|V'(x)|\}$, the particle can cross the barrier without thermal activation so that $\phi(v_{\mathrm{cr}}) = 0$. $\phi(v)$ thus decreases from the equilibrium $v = 0$ value to zero. The initial decrease of the escape time is given by $\phi'(0) = -[C_2(0) - C_1(0)] \equiv -\ell$, which is nothing but the distance between the maxima and the minima of the potential V, i.e., the width of the barrier. The same construction holds for the second barrier.

Next, consider the two potential barriers $V_{R,L}(x)$ of equal height described in Fig. 4. The right barrier is wider, $\ell_R > \ell_L$, but has a larger maximal slope than the left barrier so that $v_{\mathrm{cr}}^R > v_{\mathrm{cr}}^L$. To leading order, the escape rates over the two barriers for $v = 0$, $\phi_L(0)$ and $\phi_R(0)$, are equal. Following the above discussion, $\phi_R(v)$ decreases faster than $\phi_L(v)$ near $v = 0$ because the right barrier is wider than the left one: for small v, the particle is more likely to escape over the right barrier. $\phi_R(v)$, however, vanishes at a value v_{cr}^R larger than v_{cr}^L due to the existence of a steeper portion in the right barrier. For large v, the escape is thus more likely through the left barrier. Hence, there exists a critical self-propulsion speed at which the most likely escape route changes discontinuously. The physics presented in Fig. 1 can be understood from the above discussion, the sole difference being that the escape rates are different at $v = 0$ due to the different barrier heights.

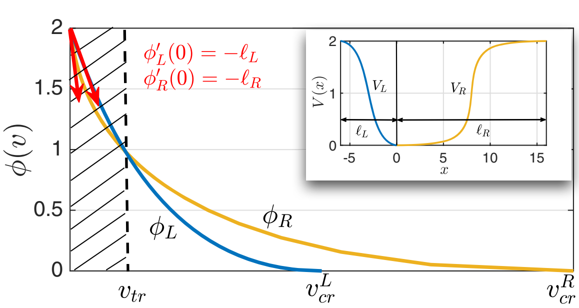

FIG. 4. The first panel displays the trap with two asymmetric escape walls V_L and V_R. The second panel displays the two quasipotentials $\phi_L(v)$ and $\phi_R(v)$ as functions of v (further explanations in the text). This illustrates the dynamical phase transition where v is the control parameter. For $v = 0$, particles have the same probability of escape (at the exponential level) through both sides. For $0 < v < v_{\mathrm{tr}}$ (hatched area), particles escape to the right, and for $v_{\mathrm{tr}} < v$ they escape to the left.

In the $D \to 0$ limit, the sigmoid function presented in Fig. 1 hence converges to a discontinuous step function. In fact, it is straightforward to see that one could also observe not one but two successive dynamical phase transitions if the larger and steeper barrier were also higher. Interestingly, the dependence of the escape time on v can be used to sort active particles depending on their velocities (See Supplemental Material [13], Movie).

Escape from two-dimensional elliptic potentials.—We now consider the escape of active particles from a two-dimensional potential well of the form

$$V(x, y) = \lambda_m \frac{x^2}{2} + \lambda_M \frac{y^2}{2}, \tag{15}$$

with $\lambda_M > \lambda_m$ (for an analysis of the steady-state distribution for the case $\lambda_m = \lambda_M$, see Ref. [27]). We assume that particles escape when they reach a given height $V(x, y) = V_0$. This level line $\mathbf{C}$ replaces $\mathbf{C}_2$ of the general discussion, see Fig. 5.

The most-probable escape routes can be computed by solving the Euler-Lagrange equations for the action given in Eq. (7), as detailed in the Supplemental Material [13]. Following the previous argument, we introduce

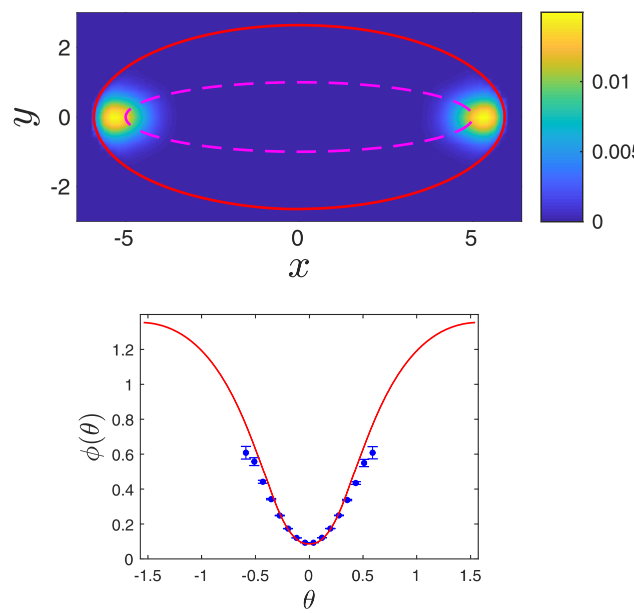

FIG. 5. Active escape from an elliptic trap (top). Activated escapes have to go from the curve C_1 (purple) up to the trap boundary C (red) defined by $V(\mathbf{x}) = V_0$. Color encodes the density of particles during the last $\delta t = 0.05$ before the escapes, highlighting the preferential route through the apices of the elliptic well. Bottom: numerical (dots) and analytical (curve) computation of the quasipotential φ along C (up to a trivial geometric Jacobian) parametrized by $\theta \equiv \arctan(y/x)$. As expected, the quasipotential reaches a minimum on the major axis (direction $\mathbf{e_x}$). For an equilibrium system, the quasipotential would be flat in the $D \to 0$ limit.

$$\varphi(\mathbf{x}_\mathrm{f}) \equiv \inf_{\mathbf{x}(\mathbf{t})}\{\mathcal{A}[\mathbf{x}(t)]|\mathbf{x}(-\infty) \in \mathbf{C}_1, \mathbf{x}(\infty) = \mathbf{x}_\mathrm{f}\}, \quad (16)$$

which yields, at the exponential level, the probability to reach any point $\mathbf{x}_f$ on the boundary. This log probability, which we compute in Ref. [13], is plotted in Fig. 5 as a function of the angular parametrization of $\mathbf{x}_f$, and compared with numerics. Interestingly, the quasipotential is not constant over the boundary: the particles have a much larger probability to escape in the direction of the major axis of the ellipse. This is the most striking difference with the equilibrium problem: For passive Brownian particles, the quasipotential is $\varphi(\mathbf{x}) = \mu V(\mathbf{x})$, so that particles have an equal probability (at the exponential level) to escape through any point along the boundary $\mathbf{C}$. Activity thus breaks the equilibrium quasipotential symmetry.

Furthermore, one can compute explicitly the full expression of ϕ given by the minimum of the function $\varphi(\mathbf{x}_\mathrm{f})$ along $\mathbf{C}$:

$$\phi = \mu V_0\left(1 - \sqrt{\frac{v^2}{2\mu^2\lambda_m V_0}}\right)^2. \quad (17)$$

The escape time from the elliptical well is then given by $\langle\tau\rangle \asymp \exp(\phi/D)$. It solely depends on the potential height, the particle speed, and the semi-axis corresponding to the most likely exit direction. As expected, we recover the standard equilibrium result $\phi = \mu V_0$ when $v = 0$.

By providing a full solution to the Kramers problem for both ABPs and RTPs in any dimensions, we have highlighted how the physics of these nonequilibrium systems is very different from that of the equilibrium problem. In particular, the activation barrier, encoded in the quasipotential, is not solely defined by the height of the potential well. Instead, it corresponds to the region where the self-propelling force fails to overcome the confining one, leading to activation paths and times that depend in a nontrivial way on both the self-propelling speed and the full shape of the potential, and to a wealth of unusual features. Our results also highlight why an effective equilibrium approach is inappropriate. Beyond the case addressed here of an external potential, escape problems play an important role in a host of collective phenomena, from nucleation to glassy physics. It will thus be very interesting to see how the phenomena uncovered in this Letter play a role in these more complicated systems.

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