

Trapping instability of an active particle in steering potential fields

Guangle Du¹, Fangfu Ye^{1,2,3,4} and Rudolf Podgornik^{1,2,3,5,*}

¹*School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China*

²*Beijing National Laboratory for Condensed Matter Physics and Laboratory of Soft Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

³*Wenzhou Institute, University of Chinese Academy of Sciences, Wenzhou, Zhejiang 325001, China*

⁴*Oujiang Laboratory (Zhejiang Lab for Regenerative Medicine, Vision and Brain Health), Wenzhou, Zhejiang 325000, China*

⁵*Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China*



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A particle driven by active self-propulsion can be subject to inhomogeneous potential fields, steering its orientation and leading to confinement and eventual trapping. Analytical treatment of capture and/or release dynamics for general steering potentials presents a challenge due to its coupling between external potential fields and intrinsic active noise. By using the projection operator method, we obtain the coarse-grained Dynkin equations with orientation integrated out in the large fluctuation limit and derive explicit analytical solutions for the mean first passage time in radially symmetric point source trapping potentials. We analyze the ensuing trapping instabilities related to a critical value of the steering potential strength below which the particle either cannot be lured into the trap or above which it is unable to leave the trap after being lured into it.

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I. INTRODUCTION

Since his seminal work [1], the *Kramers problem* concerning the confinement and escape of a particle in potential fields with fluctuations has been generalized and elaborated for systems near equilibrium [2–5]. Its theoretical extension to self-propelled particles is mainly treated numerically or by simulations [6–8] but presents an analytical challenge due to the nonequilibrium nature of active systems [9–14]. While the analytical efforts until now have been focused on potentials affecting the positional dynamics, an effective scheme handling the presence of general orientational steering potentials in systems of self-propelled particles is lacking.

Confining and trapping self-propelled particles bear relevance in a wide range of active system scenarios such as animals foraging for food [15,16], chemotaxis of microorganisms and synthetic devices [17,18], as well as optimal control of smart particles [19,20]. In one scenario, a metameric active worm is attracted and steered by the presence of a food resource [21], a variant of the general confinement and trapping problem in active matter [22]. In this context, an important question would be: What is the critical strength of the steering

potential, such that the active particle can find and stay, i.e., be trapped in the vicinity of the food resource? Mean first passage time (MFPT) is often used to characterize the escape dynamics of confined particles, and the diverging MFPT at a critical potential strength defies simulations, requiring efficient and challenging rare event sampling algorithms [23]. On the other hand, the infinity of the domain in free space available in the search for food poses yet other, no lesser numerical obstacles. Therefore, analytical treatment is essential to address the entrapment dynamics in the regime of critical potential strengths.

Tackling the active Kramers problem analytically relies on effective approximation schemes suitable for specific systems. Relaxation and fluctuations are two competing ingredients in the active Kramers problem, and adiabatic elimination of the fast variable to separate relaxation and fluctuation regimes is widely used, e.g., in the local-equilibrium Maxwell-Boltzmann approximation, by comparing translational and rotational timescales [24], as well as in the unified colored-noise approximation [25,26] tailored for colored noise at small and large correlation timescales. These approximation varieties fall within the purview of the powerful projection operator formalism, applicable in a wide range of contexts [27,28].

In this Rapid Communication, we investigate the confinement and escape, i.e., the entrapment dynamics of an active particle as exemplified by a metameric worm in steering potential fields [21]. By using the projection operator method, we obtain the coarse-grained dynamical equations for general steering potentials in the limit of large orientational fluctuations. Analytical results for the MFPTs are obtained for radially symmetric potentials, allowing us to identify a finite critical steering potential strength for a trapping instability,

*To whom correspondence should be addressed: rudolfpodgornik@ucas.ac.cn; also affiliated with Department of Physics, Faculty of Mathematics and Physics, University of Ljubljana, 1000 Ljubljana, Slovenia.

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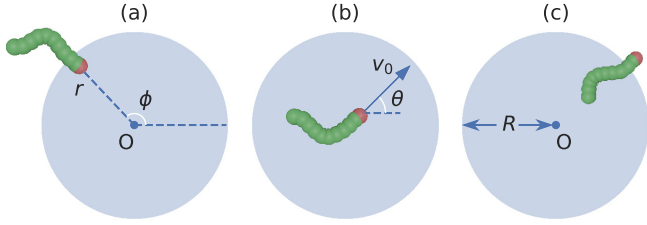


FIG. 1. (a) and (b) Schematics of the entrapment and (c) escape of an active worm (an active head and a passive trailing body) in an attractive steering potential field generated by a food resource (blue region). Note that the dimensions of the worm are assumed to be far smaller than the food source radius in text but have been exaggerated for visual clarity in the figure.

akin to the counterion condensation phenomenon in the polyelectrolytes theory. We further verify the analytical results by numerically solving the exact Dynkin equations fulfilled by the MFPTs and show that they effectively coincide with the analytical results. Our study underpins a quantitative understanding of the behaviors of active particles, subject to steering potentials, by identifying a critical potential strength governing their long-time entrapment behaviors.

II. MODEL

To model the confinement of an active particle in a steering potential field, we take a persistent turning walker (PTW) model [29,30] as exemplified by a metameric worm in two-dimensional free space [21], whose motion is steered by a *point source trapping potential* generated by a disk-shaped food source of radius R , as illustrated in Fig. 1. We assume the dimensions of the worm to be far smaller than the radius of the food resource, and hence, the worm will be subsequently deemed pointlike. The position of the worm relative to the center of the food resource is given in polar coordinates (r, ϕ) , where r and ϕ are, respectively, the radial distance and the polar angle. The velocity is of a constant norm v_0 and directed tangentially to its trajectory with orientational angle θ . The curvature dynamics is governed by a steered Ornstein-Uhlenbeck process [21]. When the curvature time-decay constant is large, the curvature is a fast variable and can be adiabatically eliminated [31] (see Supplemental Material [32]). Thus, the dynamics of the worm can be described by the following Langevin equations:

$$\frac{d\mathbf{r}(t)}{dt} = v_0 \mathbf{p}, \quad (1)$$

$$\frac{d\mathbf{p}(t)}{dt} = -v_0 \mathbf{n} \cdot \nabla U(\mathbf{r}; \gamma) \mathbf{n} + \sqrt{2D} \xi \mathbf{n}, \quad (2)$$

where $\mathbf{r} = r(\cos \phi, \sin \phi)$, $\mathbf{p} = (\cos \theta, \sin \theta)$, and $\mathbf{n} = (-\sin \theta, \cos \theta)$ are, respectively, the positional, orientational, and normal vectors, $U(\mathbf{r}; \gamma)$ is the steering potential dependent on position $\mathbf{r}$, with γ being a parameter representing the potential strength, D is a constant orientational diffusivity, and ξ describes a white noise, i.e., $\langle \xi(t) \rangle = 0$, $\langle \xi(t) \xi(t') \rangle = \delta(t - t')$. The term with $-\mathbf{n} \cdot \nabla U$ enables the orientational alignment down the gradient of the steering potential [17,18].

Note that confinement dynamics with similar equations was studied in Ref. [22], where the focus was placed on the particle trapping and capture in the limit of vanishing or small fluctuations. While analytical scaling results were given in the deterministic limit, results in the small fluctuation limit were given only numerically. In contrast, here, we study the confinement dynamics in the large fluctuation limit and obtain full analytical results for general radially symmetric potentials.

A. Dynkin equation

To investigate the entrapment properties, i.e., the stability of confinement generated by the steering potential, we define the two following criteria: (1) the worm should enter the food resource from outside in a finite time; (2) the worm should stick around infinitely long in the vicinity of the food resource after its entrance. The confinement is deemed as stable and the worm as trapped only when both criteria are fulfilled. In what follows, MFPT is used to quantitatively characterize the entrapment dynamics and calculating the MFPTs for the worm to go across the boundary of the food resource from the outside [Fig. 1(a)] and from the inside [Fig. 1(c)], the two situations are referred to as the *inward* and *outward problems*, respectively.

The MFPTs can be obtained directly by solving the corresponding Dynkin equations. Denote by $T(r, \phi, \theta)$ the MFPT to cross the boundary of the food resource, which depends on the initial position (r, ϕ) and orientation θ . By rescaling with the characteristic size R and time R/v_0 , we have the following dimensionless quantities: $\tilde{r} = r/R$, $\tilde{T} = T v_0/R$, $\tilde{D} = DR/v_0$, and $\tilde{U}(\tilde{r}, \phi) = U(\tilde{r}R, \phi)$. For brevity, we will omit the tilde symbol subsequently, as long as this introduces no ambiguity. Transforming the angular coordinates $(\phi, \theta) \rightarrow (\phi', \psi)$ with $\phi' = \phi$ and $\psi = \theta - \phi$ then implies $\partial_\phi = \partial_{\phi'} - \partial_\psi$ and $\partial_\theta = \partial_\psi$. Denote furthermore $h(r, \phi, \psi) \equiv (\partial_r U - 1/r) \sin \psi - [(\partial_\phi U - \partial_\psi U)/r] \cos \psi$, so that the Dynkin equation can be written in dimensionless form as (see Supplemental Material [32])

$$\left(\cos \psi \partial_r + \frac{\sin \psi}{r} \partial_\phi + h \partial_\psi + D \partial_\psi^2 \right) T(r, \phi, \psi) = -1, \quad (3)$$

with a Dirichlet boundary condition $T(r, \phi, \psi)|_{r=1} = 0$.

B. Projection operator method

To obtain the coarse-grained dynamics, we now apply the projection operator method to approximate the Dynkin equation Eq. (3). We focus on the large fluctuation limit, where analytical results can be obtained. In this limit, one can expect that the MFPT is independent of the initial orientation. As shown in Fig. 2, the trajectories in polar coordinates (r, ψ) with large orientational fluctuations exhibit a circular pattern, where the effects of the initial orientation are quickly blurred out before the particle can travel a notable distance toward the boundary ($1/\tilde{D} = v_0/DR \ll 1$ with dimensions temporarily restored here). Shown in Fig. 3 are numerical results of solving the exact Dynkin equation for potential $U(r) = \gamma \ln r$ with small and large fluctuations. When fluctuations are small $D = 2$ [Figs. 3(a) and 3(b)], the MFPTs in both outward [Fig. 3(a)]

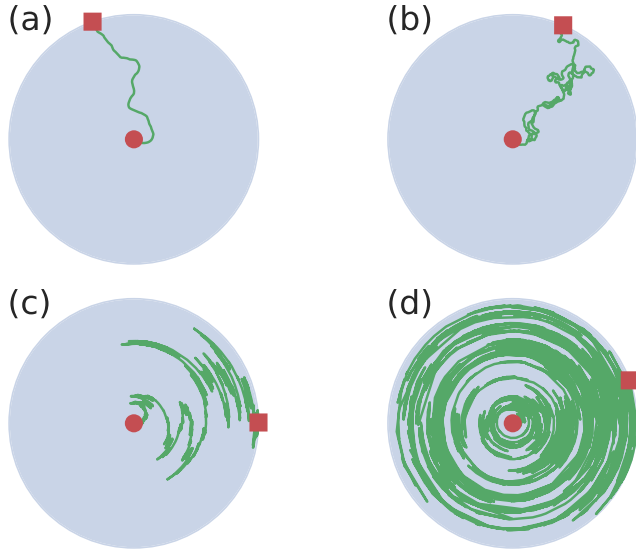


FIG. 2. Typical trajectories in (a) and (b) actual positional space coordinates (r, ϕ) and (c) and (d) polar coordinates (r, ψ) of an active worm in a steering potential $U(r) = \gamma \ln r$ ($\gamma = 1$) with different amplitudes of fluctuations quantified by orientational diffusivity D . The worm is initially at the center (circle), with $\phi = 0$ and $\psi = 0$ and finally passes across the boundary (square) of the food resource. In (a) and (c), $D = 2$; in (b) and (d), $D = 20$.

and inward [Fig. 3(b)] problems clearly depend on the initial value of ψ . In contrast, when fluctuations are large $D = 10^3$ [Figs. 3(c) and 3(d)], the MFPTs in both outward [Fig. 3(c)] and inward [Fig. 3(d)] problems are nearly independent of the initial ψ .

Numerical examples motivate us to make the operator decomposition $L = DL_1 + L_2$, where L is the backward Fokker-Planck operator on the left-hand side of Eq. (3), with $L_1 \equiv \partial_\psi^2$ and $L_2 \equiv \cos \psi \partial_r + 1/r \sin \psi \partial_\phi + h(r, \phi, \psi) \partial_\psi$. Next, define the projection operator $\mathcal{P}$ by $\mathcal{P}f(r, \phi, \psi) = 1/(2\pi) \int_0^{2\pi} f(r, \phi, \psi) d\psi$, $\forall f(r, \phi, \psi)$. By direct calculations, one can show that $\mathcal{P}$ satisfies $\mathcal{P}^2 = \mathcal{P}$, $\mathcal{P}L_1 = L_1\mathcal{P} = 0$, and $\mathcal{P}L_2\mathcal{P} = 0$. Denote $\rho(r, \phi) = \mathcal{P}T(r, \phi, \psi)$ and $w(r, \phi, \psi) = (1 - \mathcal{P})T(r, \phi, \psi)$. Application of $\mathcal{P}$ and $1 - \mathcal{P}$ on both sides of Eq. (3) then yields

$$-1 = \mathcal{P}L_2w, \quad 0 = DL_1w + (1 - \mathcal{P})L_2w + L_2\rho. \quad (4)$$

Subsequent elimination of w gives a closed equation for ρ , $\mathcal{P}L_2[DL_1 + (1 - \mathcal{P})L_2]^{-1}L_2\rho = 1$, which in the large D limit implies $D^{-1}\mathcal{P}L_2L_1^{-1}L_2\rho = 1$. Writing this explicitly, we remain with

$$\partial_r^2 \rho + \frac{1}{r^2} \partial_\phi^2 \rho - A(r, \phi) \partial_r \rho + B(r, \phi) \partial_\phi \rho = -2D, \quad (5)$$

where $A(r, \phi) = 1/\pi \int_0^{2\pi} h(r, \phi, \psi) \sin \psi d\psi$ and $B(r, \phi) = 1/(\pi r) \int_0^{2\pi} h(r, \phi, \psi) \cos \psi d\psi$. One can clearly see by rescaling and restoring dimensions that $\rho \propto Dv_0^{-2}$, which is consistent with previous results for total diffusivity [9]. Thus, by using the projection operator method, we have obtained the coarse-grained Dynkin equation with orientation integrated out in the large fluctuation limit.

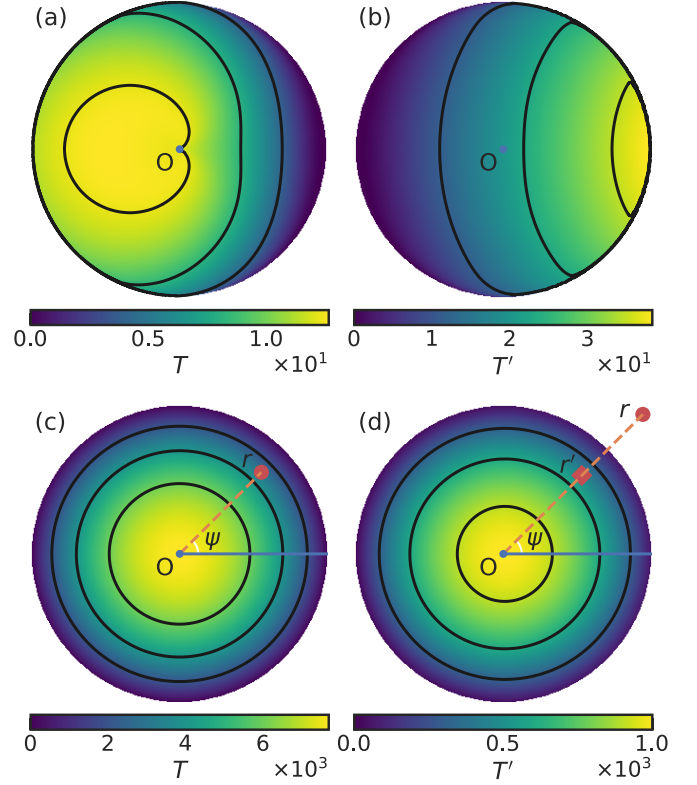


FIG. 3. Density plots of the mean first passage times (MFPTs) in potential $U(r) = \gamma \ln r$ with (a) and (b) small ($D = 2$) and (c) and (d) large ($D = 10^3$) fluctuations, obtained numerically from the exact Dynkin equations. (a) and (c) show the MFPTs $T(r, \psi)$ in the outward problem with $\gamma = 1.9$, and (b) and (d) show the MFPTs $T'(r', \psi)$ after the divergence separation $T' = T/r^2$ and conformal mapping $r' = 1/r$, $\psi' = \psi$ in the inward problem with $\gamma = 2.1$. MFPTs are nearly independent of the initial ψ when fluctuations are large.

C. Radially symmetric potentials

To obtain explicit analytical solutions of the Dynkin equations, we consider radially symmetric steering potentials $U(r)$. The exact MFPT $T(r, \phi, \psi)$ in this case should be independent of ϕ (see Supplemental Material [32]). Then the coarse-grained Dynkin equation Eq. (5) reduces to

$$\partial_r^2 \rho + \left[\frac{1}{r} - \partial_r U(r) \right] \partial_r \rho = -2D, \quad (6)$$

with a Dirichlet boundary condition $\rho(r)|_{r=1} = 0$. Conservation of probability in the whole space dictates two reflecting boundary conditions at origin and infinity, i.e., $\partial_r \rho(r)|_{r=0} = 0$ for the outward problem and $\partial_r \rho(r)|_{r \rightarrow \infty} = 0$ for the inward problem. The solutions of the coarse-grained Dynkin equations in the outward and inward problems are then, respectively,

$$\rho^{\text{out, in}}(r) = 2D \int_r^1 dr_1 r_1^{-1} \exp[U(r_1)] \times \int_{0, \infty}^{r_1} dr_2 r_2 \exp[-U(r_2)]. \quad (7)$$

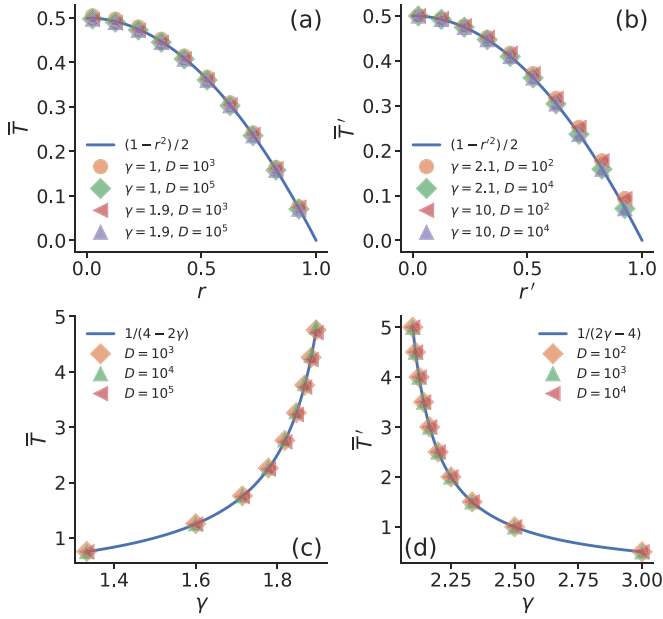


FIG. 4. Mean first passage times (MFPTs) in potential $U(r) = \gamma \ln r$ in the (a) and (c) outward and (b) and (d) inward problems, obtained analytically (solid lines) from the coarse-grained Dynkin equations and numerically (discrete data) from the exact Dynkin equations. In the inward problem, the MFPTs T are first transformed by $T' = T/r^2$ to remove the divergence at infinity and then—together with the domain of definition—transformed by the conformal mapping $r \rightarrow r' = 1/r$. All the MFPTs are reduced by $2D$, i.e., $\bar{T} = T/(2D)$ and $\bar{T}' = T'/(2D)$. In (a) and (b), the numerical MFPTs are along $\psi = 0$. In (c) and (d), the numerical MFPTs are at $r = 0$ and $r' = 0$, respectively.

D. Trapping instability

To explicitly write the analytical MFPTs in Eq. (7), we specifically consider two kinds of radially symmetric steering potentials: logarithmic and power law. For a radially symmetric logarithmic potential $U(r) = \gamma \ln r$,

$$\rho^{\text{out},\text{in}}(r) = \frac{D}{2-\gamma} (1-r^2), \quad (8)$$

where $\gamma < 2$ in the outward problem and $\gamma > 2$ in the inward problem. As shown in Figs. 4(c) and 4(d) (solid lines), the MFPTs in the outward and inward problems diverge when the potential strength γ approaches $\gamma = 2$ from below and above, respectively. Combination of the results for the outward and inward problems then yields the critical trapping strength for the whole problem $\gamma_c = 2$. When $\gamma > \gamma_c$, the trapping is stable; when $\gamma < \gamma_c$, the trapping is destabilized. It is remarkable that the existence of a finite critical γ_c mathematically arising from the factors $\int_0^{r_1} dr_2 r_2 \exp[-U(r_2)]$ in Eq. (7) resembles the counterion condensation phenomenology in polyelectrolytes theory [33]. As shown in Figs. 4(a) and 4(b) (solid lines), the MFPTs, when finite, decrease and increase quadratically with increasing r in the outward and inward problems, respectively.

Moreover, consider radially symmetric power law potentials $U(r) = \gamma r^\alpha / \alpha$ with α being a nonzero real number. When $\alpha > 0$, both ρ^{out} and ρ^{in} are finite, indicating that

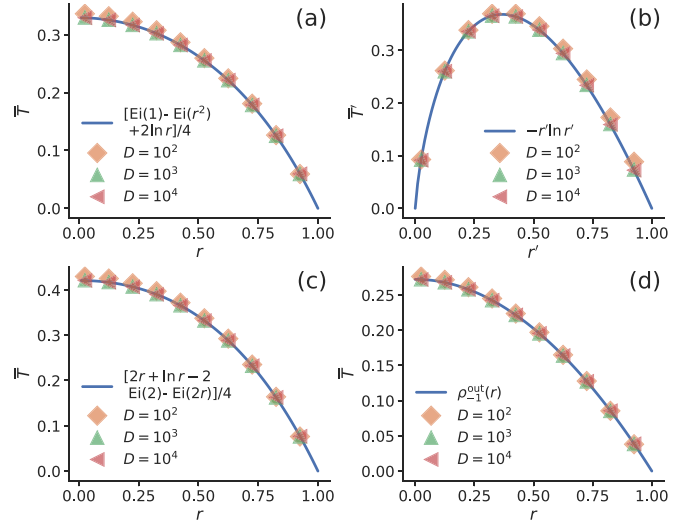


FIG. 5. Mean first passage times (MFPTs) in potentials $U(r) = \gamma r^\alpha / \alpha$, $\alpha = 2, 1, -1$ in the (a), (c), and (d) outward and (b) inward problems obtained analytically (solid lines) from the coarse-grained Dynkin equations and numerically (discrete data) from the exact Dynkin equations. All the MFPTs are reduced by $2D$, i.e., $\bar{T} = T/(2D)$ and $\bar{T}' = T'/(2D)$. The numerical MFPTs are along $\psi = 0$. (a) $\alpha = 2$ and $\gamma = 2$; (b) $\alpha = 2$, $\gamma = 1$, $T' = T/r^2$, and $r' = 1/r$; (c) $\alpha = 1$ and $\gamma = 2$; (d) regularized Coulomb-like potential $U(r) = -\gamma/(r+a)$ with $\gamma = 0.1$ and $a = 0.1$.

the worm enters the food resource in a finite time, but it wanders away later. When $\alpha < 0$, both ρ^{out} and ρ^{in} are infinite, indicating that the worm cannot enter the food resource in a finite time but will linger infinitely long around the food source if put there. Specifically, for harmonic potential $\alpha = 2$, $\rho^{\text{out}}(r) = D[\text{Ei}(\gamma/2) - \text{Ei}(\gamma r^2/2) + 2 \ln r]/\gamma$ and $\rho^{\text{in}}(r) = 2D \ln r/\gamma$, where Ei is exponential integral function. For linear potential $\alpha = 1$, $\rho^{\text{out}}(r) = 2D[\text{Ei}(\gamma) - \text{Ei}(\gamma r) - \gamma + \gamma r + \ln r]/\gamma^2$ and $\rho^{\text{in}}(r) = 2D(-\gamma + \gamma r + \ln r)/\gamma^2$. To compare with numerical results, a regularized version of Coulomb-like potential $U(r) = -\gamma/(r+a)$ with a being a small positive number is considered instead.

These analytical results for the MFPTs are fully corroborated by numerically solving the corresponding exact Dynkin equations (see the discrete data in Figs. 4 and 5). It is noteworthy that the infinite domain and diverging MFPT at infinity arise as numerical difficulties in the inward problem but are solved by a method referred to as *Kelvin transformation* [34]. Specifically, the MFPT is rescaled by an upper bound of its diverging factor at infinity such that it has no singularity anymore at infinity or elsewhere (see Supplemental Material [32]), and the infinite domain is transformed by the conformal mapping $r \rightarrow r' = 1/r$ into a compact one [see Fig. 3(d)]. The exact Dynkin equations are transformed accordingly and then numerically solved (see Supplemental Material [32]). As one can see from Figs. 4 and 5, the reduced MFPTs obtained numerically with different large diffusivities and radially symmetric potentials all collapse onto the lines representing the analytical results, validating the analytical results obtained above.

III. DISCUSSION AND CONCLUSIONS

The trapping instability for logarithmic potential mathematically results from the integrals $\int_{0,\infty}^{r_1} r_2^{1-\gamma} dr_2$ with possible divergence from the interval near origin or infinity. The instability is, therefore, not limited to a logarithmic potential *per se* but can be extended to potentials with logarithmic asymptotics near origin or infinity, e.g., $\gamma \sum_{\alpha=0}^N r^\alpha/\alpha$ or $\gamma \sum_{\alpha=-N}^0 r^\alpha/\alpha$ with $N > 0$. Potentials without logarithmic asymptotics generally do not lead to the trapping instability. In this sense, the logarithmic potential, as is also the case in polyelectrolytes [33], vortex pairs [35], DNA bubbles [36], and optical lattices [37], is indeed special.

We assumed that the curvature in the PTW model is fast relaxing and obtained the overdamped Langevin equations and consequently the Dynkin equation by its adiabatic elimination. For slower curvature relaxation, the dynamics would depend on the competition between the facilitated orientational alignment dynamics down the potential gradient and enhanced orientational fluctuations [21]. A quantitative investigation would entail heavy numerical handling, which can be listed for future studies.

In the Langevin equations we investigated so far, the velocity has a constant norm and translational drift and/or fluctuations are therefore absent (for their inclusion, see Supplemental Material [32]), which is a reasonable model cor-

responding to a macroscopic PTW, applicable to metameric animals/robots [21] and fish [29]. By using the projection operator method, we obtain the analytical results for the corresponding MFPTs and find the trapping instability for logarithmic potential. We note that the same approach can be applied to analytic solutions of the forward/backward Fokker-Planck equations and the corresponding Dynkin equations in other active systems with fast variables.

Our findings elucidate the properties of an active, tangentially constrained, and orientationally fluctuating Kramers problem by analyzing the explicit analytical solutions and providing a switch mechanism to regulate the entrapment of such steered active particles. A possible experimental test setup may involve generating controlled steering electric fields in electrically conductive media or in electro-osmotic flows [38], with active particles susceptible to orientational steering.

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