Target search of active agents crossing high energy barriers

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Abstract

Target search by active agents in rugged energy landscapes has remained a challenge because standard enhanced sampling methods do not apply to irreversible dynamics. We overcome this non-equilibrium rare-event problem by developing an algorithm generalizing transition-path sampling to active Brownian dynamics. This method is exemplified and benchmarked for a paradigmatic two-dimensional potential with a high barrier. We find that even in such a simple landscape the structure and kinetics of the ensemble of transition paths changes drastically in the presence of activity, in particular, counterintuitive search patterns shape the dynamics.

INTRODUCTION

Active matter and directed motion are receiving increasing attention because of their relevance in a wide range of research fields, including biology, biomedicine, robotics, and statistical physics [1, 2]. Active propulsion allows bacteria and animals to explore their local environment and forage nutrients [1, 3] and is key to the development of new nanoparticles that may act as drug delivery agents [4–7]. Furthermore, phagocytes of the immune system perform chemotactic motion during injury or infection [8, 9] and also sperm cells navigate against chemical gradients to find the egg [10]. The central question in all these examples is how active agents find their target. In spite of its relevance in many fields, to date this problem has been addressed by relatively few theoretical studies. In particular, only the special case of run-and-tumble motion [11] was investigated within the framework of intermittent search patterns [12–16].

Target search crucially depends on the environment [11], and in many realistic scenarios it involves exploring a complex energy landscape, characterized by the presence of several local minima, separated by energy barriers. Unfortunately, the computational cost of simulating the dynamics by directly integrating the equations of motions grows exponentially with the ruggedness of the landscape and the height of the barriers.

In the case of passive systems, similar problems have been solved by the development of enhanced sampling methods [17–27] but much less attention has been devoted to enhanced
sampling applications on active particles, with the notable exceptions of a case study of alignment interactions in a modified Vicsek model [28] and of systems displaying motility-induced phase separation [29, 30]. Among the various enhanced sampling algorithms, transition path sampling (TPS) [20–22] has the advantage to provide a completely rigorous sampling of the reactive trajectories between a basin of initial states and a target basin. This algorithm is essentially a Metropolis Monte Carlo performed in the space of reactive trajectories. Trial moves are generated by choosing a random state on a known reactive path and integrating the equations of motion (shooting) forward and backward in time to obtain a new transition path. The trial moves are then accepted or rejected according to some probability, which can be explicitly calculated from the equations of motion. The main problem encountered when applying TPS to active target search concerns the calculation of the acceptance rule for trial moves. Indeed, to obtain the acceptance probability one needs to evaluate the contribution from the backward dynamics. In passive systems, this calculation is simple, because it is directly related to the standard (i.e. forward) dynamics due to microscopic reversibility. The dynamics of a self-propelled particle, however, is microscopically irreversible, therefore the calculation of the backward dynamics term is non-trivial. To overcome this problem, other methods such as forward flux sampling [26, 27] and, more recently, a modified version of TPS [28] have been specifically developed to account also for non-equilibrium systems. Nevertheless, these methods suffer other limitations, such as an efficiency drop due to the impossibility to shoot backward in time and/or the need to know a priori a proper reaction coordinate, which could be not always possible on complex energy landscapes.

In this work, we show that in the case of an active Brownian particle (ABP) the lack of microscopic reversibility can be circumvented. The result is a generalized version of the original TPS algorithm, in which the acceptance probability contains a new term depending explicitly on the particle’s activity. We then apply our new scheme to study how the activity affects target search in a two-dimensional landscape, characterized by the presence of a large energy barrier.

**MODEL**

We first consider an ensemble of microswimmers initially confined to some reactant region $R$, searching for some target region $T$. A single microswimmer is modeled as an ABP in
two dimensions, i.e. the equations of motion consist of a set of Langevin equations in which the activity is provided by a stochastic drive proportional to a velocity term of modulus \( v \) and subject to a rotational diffusion process. If the ABP diffuses in a conservative energy landscape \( U(x, y) \), the equations of motion discretized according to the Itô rule are

\[
\begin{align*}
\mathbf{r}_{i+1} &= \mathbf{r}_i + v u_i \Delta t - \mu \nabla U(\mathbf{r}_i) \Delta t + \sqrt{2D \Delta t} \xi_i, \\
\vartheta_{i+1} &= \vartheta_i + \sqrt{2D_\vartheta \Delta t} \eta_i,
\end{align*}
\]

where \( \Delta t \) is the integration step, \( \mathbf{r}_i = (x_i, y_i) \) is the position at time \( i\Delta t \) and \( u_i = (\cos \vartheta_i, \sin \vartheta_i) \) denotes the instantaneous orientation of the driving velocity. \( D \) and \( D_\vartheta \) are the translational and rotational diffusion coefficients, respectively, and \( \mu \) is an effective mobility. In the case of a passive particle, the mobility is related to the translational diffusion coefficient via the fluctuation-dissipation theorem \( D = \mu k_B T \). Here, since the system is out of equilibrium, this relation does not hold and \( T \) simply represents the temperature of the thermal bath in which the active particle is immersed. Finally, the components of the vector noise \( \xi_i = (\xi_{x,i}, \xi_{y,i}) \) and of the scalar noise \( \eta_i \) are independent random variables, distributed according to a Gaussian with zero average and unit variance. In the following we refer to the microstate of a single active particle as \( w = (\vartheta, \mathbf{r}) \).

results

Transition Path Sampling for Active Brownian Particles

To sample the reactive paths from R to T we reconsider the TPS algorithm \[21, 22\] and adapt it to the present case of ABPs. In the TPS algorithm, a Markov chain of reactive trajectories is generated starting from some arbitrary initial path. Trial moves (i.e. newly attempted transition paths \( \mathcal{W}^{\text{new}} \) generated starting from an old path \( \mathcal{W}^{\text{old}} \)) are proposed according to a three-step procedure: First, a microstate \( w_i^{\text{old}} \) is randomly picked from the frames in \( \mathcal{W}^{\text{old}} \). Next, the microstate may be modified by means of some random perturbation: \( w_i^{\text{old}} \to w_j^{\text{new}} \). Finally, a new trial trajectory \( \mathcal{W}^{\text{new}} \) is obtained by solving the system’s equations of motion forward and backward in time, starting from \( w_j^{\text{new}} \). The resulting new trajectory \( \mathcal{W}^{\text{new}} \) is then accepted with a probability \( \mathcal{P}_{\text{acc}} \), which is calculated from the underlying microscopic dynamics by imposing the detailed balance condition in the functional
space of reactive trajectories. This results in a standard Metropolis rule

\[ P_{\text{acc}} [W^{\text{old}} \rightarrow W^{\text{new}}] = h [W^{\text{new}}] \times \min \left\{ 1, \frac{P[W^{\text{new}}] P_{\text{gen}} [W^{\text{new}} \rightarrow W^{\text{old}}]}{P[W^{\text{old}}] P_{\text{gen}} [W^{\text{old}} \rightarrow W^{\text{new}}]} \right\}, \tag{3} \]

where \( h [W^{\text{new}}] \) is a characteristic function equal to one only if the new path is reactive and zero otherwise. In this equation, \( P[W] \) is the functional path probability density which reads

\[ P[W] \propto \rho(w_0) N^{-1} \prod_{i=0}^{N-1} p(w_i \rightarrow w_{i+1}), \tag{4} \]

where \( N \) is the number of frames of the reactive path \( W \), and \( \rho(w_0) \) is the quasi-stationary non-equilibrium distribution of initial conditions in the reactant. Further

\[ p(w_i \rightarrow w_{i+1}) \propto \exp \left\{ -\frac{(\vartheta_{i+1} - \vartheta_i)^2}{4D_\vartheta \Delta t} \right\} \times \exp \left\{ -\frac{(r_{i+1} - r_i - \nu u_i \Delta t + \mu \nabla U(r_i) \Delta t)^2}{4D \Delta t} \right\}, \tag{5} \]

is the conditional probability for performing a transition from \( w_i \) to \( w_{i+1} \) in the infinitesimal time interval \( \Delta t \) as is readily derived from the stochastic equation of motion, Eq. (1) (see Appendix A ). \( P_{\text{gen}} [W] \) in Eq. (3) is the probability of generating a trial path, according to the shooting procedure outlined above. Explicitly, we find

\[ P_{\text{gen}} [W^{\alpha} \rightarrow W^{\beta}] = P_{\text{sel}}(w_j^{\alpha} | W^{\alpha}) P_{\text{pert}}(w_j^{\alpha} \rightarrow w_i^{\beta}) \times \prod_{k=i}^{N^{\beta}-1} p(w_k^{\beta} \rightarrow w_{k+1}^{\beta}) \prod_{k=0}^{i-1} \bar{p}(w_{k+1}^{\beta} \rightarrow w_k^{\beta}), \tag{6} \]

where \( P_{\text{sel}}(w_j^{\alpha} | W^{\alpha}) = 1/N^\alpha \) is the probability of selecting as shooting point the state \( w_j^{\alpha} \) belonging to the reactive path \( W^{\alpha} \) of length \( N^\alpha \). \( P_{\text{pert}}(w_j^{\alpha} \rightarrow w_i^{\beta}) \) is the probability of perturbing \( w_j^{\alpha} \) to obtain the microstate \( w_i^{\beta} \) of the path \( W^{\beta} \) of length \( N^{\beta} \) [31]. Due to the stochastic nature of its dynamics, for an ABP the perturbation of the shooting point is not necessary. Hence, we set \( w_i^{\beta} = w_j^{\alpha} \) with probability equal to one. The first and second product of probabilities in the second line of Eq. (6) represent the probability of generating the two branches of the trial trajectory \( W^{\beta} \) connecting the microstate \( w_i^{\beta} \) to the target and reactant state, respectively. In particular, \( \bar{p}(w_{i+1} \rightarrow w_i) \) is the probability to observe a transition from the microstate \( w_{i+1} \) to the microstate \( w_i \) in a dynamics evolving backwards in time. For passive Brownian dynamics, this backward probability is directly related to
the forward one by microscopic reversibility. However, the dynamics of ABPs is intrinsically irreversible \[32\], so in this case the calculation of \(\bar{p}(w_{i+1} \rightarrow w_i)\) is non-trivial. In principle, one could use any sort of backward dynamics, and consistently derive the corresponding correction factor in the acceptance probability within the TPS approach by following the procedure explained below. However, the challenge is to find moves that are efficient in sampling the reactive paths, which is possible if the trial moves have a significant overlap with the “real dynamics”. Here we suggest for the backwards shooting the simple rule:

\[
\begin{align*}
\mathbf{r}_i &= \mathbf{r}_{i+1} - v \mathbf{u}_{i+1} \Delta t - \mu \nabla U(\mathbf{r}_{i+1}) \Delta t + \sqrt{2D \Delta t} \xi_{i+1}, \\
\vartheta_i &= \vartheta_{i+1} + \sqrt{2D \vartheta \Delta t} \eta_{i+1} .
\end{align*}
\]

Note that Eq. (7) is formally equivalent to Eq. (1) but with a flipped sign of the driving velocity. From this equation, it is possible to obtain an analytic expression of \(\bar{p}(w_{i+1} \rightarrow w_i)\), in complete analogy to the calculation of the forward transition probability \(p(w_i \rightarrow w_{i+1})\) starting from Eq. (1). The result is (see Appendix A)

\[
\bar{p}(w_{i+1} \rightarrow w_i) = p(w_i \rightarrow w_{i+1}) \frac{\pi(\mathbf{r}_i)}{\pi(\mathbf{r}_{i+1})} \times 
\exp\left\{ -\frac{v}{2D} \mathbf{u}_{i+1} \cdot (\mathbf{r}_i - \mathbf{r}_{i+1} + \mu \nabla U(\mathbf{r}_{i+1}) \Delta t) \right\} 
\exp\left\{ -\frac{v}{2D} \mathbf{u}_i \cdot (\mathbf{r}_i - \mathbf{r}_{i+1} - \mu \nabla U(\mathbf{r}_i) \Delta t) \right\},
\]

where \(\pi(\mathbf{r}) \propto e^{-\beta U(\mathbf{r})}\) is the Boltzmann distribution for a passive particle. We stress that the first line of Eq. (9) is the result for a passive Brownian particle, while the second line represents the correction term accounting for the microscopic irreversibility of active Brownian dynamics. Similar results expressing the ratio between the forward and backward probability may be obtained by a direct time-reversal transformation within the path integral formulation \[33\] or by means of Crooks-like relations for entropy production \[34\], in a similar fashion to what has been done in different contexts \[32, 35, 36\].

After combining all terms, the final expression for the acceptance probability can be obtained. This formula is rather lengthy and can be found in Appendix B. Here we limit ourselves to noting that in the limit of vanishing activity (i.e. for \(v \rightarrow 0\)) we recover the standard TPS formula for passive Brownian dynamics: 

\[
P_{\text{acc}}[\mathcal{W}^\text{old} \rightarrow \mathcal{W}^\text{new}] = h |\mathcal{W}^\text{new}| \min\left\{1, \frac{N_{\text{old}}}{N^\text{new}}\right\}.
\]

We also stress that the acceptance probability involves the steady-state distribution of microstates in the reactant basin \(\rho(w)\), which is in general not known analytically. We numerically estimated this distribution from a frequency histogram.
FIG. 1. Distribution of Transition path times (TPTs) at different Péclet numbers. Each distribution is obtained from $10^6$ different TPTs.

FIG. 2. (a-b) A fast and a slow reactive path ($t_{\text{TPT}}/\tau_\theta = 0.65$ and 2.37 respectively) of a passive Brownian particle (Pe = 0). The red contour lines are the borders of the R and T basins. (c-d) A fast and a slow reactive path ($t_{\text{TPT}}/\tau_\theta = 0.53$ and 8.36 respectively) of an ABP (Pe = 10).

of the microstates in the reactant basin visited by active Brownian trajectories generated by solving numerically Eq. (1) (see also Fig.5 in Appendix D).
Target Search of Active Brownian Particle in a double well energy landscape

We use our TPS algorithm to characterize transition pathways of an ABP reaching a target region crossing the energy barrier in the two-dimensional energy surface

\[ U(x, y) = k_x \left(x^2 - x_0^2\right)^2 + \frac{k_y}{2} y^2, \]  

which provides the paradigmatic example of a double well problem. We set \( x_0 = 1 \), \( k_x = 6 \) and \( k_y = 20 \) and measure energy in units of the effective thermal energy \( k_B T \). We define a reactive trajectory as one leaving the reactive region (defined as the set of points with \( U(x, y) \leq 2k_B T \) and \( x < 0 \)) and reaching the target region (defined by \( U(x, y) \leq 2k_B T \) and \( x > 0 \)), before returning to the reactant. Here we study the ABP behavior for three different values of the Péclet number, \( \text{Pe} := v \sqrt{3/4D D_{v}} \), a dimensionless measure of the activity: \( \text{Pe} = 0 \) (\( v = 0 \)), \( \text{Pe} = 5 \) (\( v = 1.83 \)) and \( \text{Pe} = 10 \) (\( v = 3.65 \)) while keeping fixed \( D = 0.1 \), \( D_{v} = 1 \) and \( k_B T = 1 \). Important insight on the ABPs behavior in a potential well has already been achieved, for example the escape rates do not follow Kramers theory [37, 38]. Here we first consider the distribution of transition path times (TPTs), i.e. the time durations of reactive trajectories. This observable has received considerable attention in the context of passive dynamics, both from experimentalists [39–42] and theorists [43–52], because it carries information about the reactive dynamics. Yet, it appears that TPTs in the presence of activity have been studied only in the case of a one-dimensional particle crossing a parabolic barrier [53].
The TPT distribution using our TPS algorithm reproduces well the one obtained by direct integration of the stochastic equations of motion (see Fig. 1) for the different values of the Péclet number. Here, the TPTs are reported in units of the rotational diffusion time, $\tau_\theta = 1/D_\theta$. The computational advantage of sampling by TPS relative to brute force simulations is very high at low activities but drops significantly at very large activities. In the present landscape, the ratio between the time needed to obtain $10^6$ reactive paths with TPS and brute force simulations is $\sim 0.001$, $\sim 0.12$ and $\sim 0.27$ for $Pe = 0$, $Pe = 5$ and $Pe = 10$, respectively. This decrease in efficiency is because very active particles can easily explore high energy regions of the landscape, thus the crossing rate is relatively less affected by energy barriers. We expect that the computational advantage of TPS for very active particles increases for larger barriers. Our results show that the average TPT grows with the Péclet number, while the distribution becomes broader and broader. On the other hand, the most likely value of the TPT distribution remains nearly unchanged.

In order to investigate the origin of this difference, it is instructive to analyze the structure of typical transition pathways as the Péclet number is increased. For a passive particle the slow and fast trajectories are quite similar, with the reactive paths narrowly focused around the minimum-energy path crossing the barrier (see Fig. 2 a-b). In contrast, for active particles the trajectories associated with fast and slow transitions are qualitatively very different. Namely, fast active transition pathways are similar to passive ones and travel close to the minimum free energy path (see Fig. 2c). In contrast, the main contribution to the right tail of the TPT distribution comes from trajectories which leave the reactant basin in the direction opposite to energy saddle point (see Fig. 2d). Clearly, it takes a time of the order of the rotational diffusion time before the particle points again in a favorable direction, thus leading to long TPTs.

This mechanism is confirmed by a systematic statistical analysis of the reactive processes, based on computing the transition path density, $m(r)$, and the transition current, $J(r)$ [54]. Here $m(r)$ measures the probability that a transition path visits a specific position $r$ in the reactive region, while $J(r)$ provides the information on the probability current. At vanishing $Pe$ the transition path density is highest in the saddle point region, while upon adding activity the transition path density becomes largest in the regions behind the basins, as shown in Fig. 3. This behavior is reflected in the reactive current (see Fig. 3) as well as in the marginalized reactive probability density $m(x) = \int m(x, y)dy$ and $m(y) = \int m(x, y)dx$. 
Altogether, our results demonstrate that, at high activity, transition paths are qualitatively different from those undergone by passive systems. In particular, thanks to the self-propulsion and the persistence of motion, the ABPs reach the target by exploring regions of the energy landscape that are effectively inaccessible for the passive particle. Moreover, in contrast to the passive case, the structure of the transition pathways of active particles qualitatively changes as a function of its TPT: while short trajectories travel along the minimum energy path (in qualitative analogy with the passive case), long-lasting trajectories reach the target in a counter-intuitive way, by climbing the energy surface in the direction opposite to the transition state and then “surfing” high energy regions in the potential energy landscape, before landing into the target. Interestingly, the average TPT increases with the activity of the particle while the opposite behavior is observed in one-dimensional systems [53]. Yet, there the reactive pathways reaching the target from the back cannot even occur, correspondingly the observed trend underlines the non-trivial interplay arising between the activity of the particle, the dimensionality of the system, and the environment topology.

**DISCUSSION**

In summary, we have addressed the problem of characterizing the structure and kinetics of rare transition pathways undergone by ABPs in search for a target. To this end, we have derived and validated an extension of TPS which can be used to efficiently and directly sample rare events undergone by ABPs. Due to the explicit breaking of microscopic reversibility, the acceptance probability for trial paths in our scheme contains a correction term which resembles Crooks’ entropy production formula. Using our TPS algorithm, we have compared the behavior of active and passive Brownian particles reaching a target in a two-dimensional energy landscape characterized by a high energy barrier.

Our results show that, far from equilibrium conditions, significant differences emerge between the reactive kinetics of active and passive particles, suggesting counter-intuitive target search patterns. We expect similar counter-intuitive results to be found in a wide range of physical systems of biological, chemical and technological relevance and the enhanced path sampling scheme developed in this work provides a powerful tool to investigate these
processes in a computationally efficient way. Furthermore, the mathematical scheme we adopted to derive the acceptance rule for ABPs may in principle be applied to a wider class of irreversible systems, as long as it is possible to identify an integration scheme analog to (7) generating backward trajectories with the correct statistical weight.

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Appendices

A. STOCHASTIC PATH INTEGRAL FOR ACTIVE PARTICLES

Here we provide the stochastic path integral derivation for the single step transition probability in the case of an active particle.

Considering that the succession of the states $w_i = (r_i, \vartheta_i)$ constitutes a Markov process, the probability of finding the system in a specific microstate $w_N$ at time $\tau = N \Delta t$ provided the initial condition $w_0$ at time $t = 0$ can be obtained from the following stochastic path integral:

$$P(w_N|w_0) = Z^{-1} \int D\vartheta \int Dr \exp \left(-\frac{1}{4D_\vartheta} S_{\text{rot}}[\vartheta]\right) \exp \left(-\frac{1}{4D} S_{\text{trans}}[r, \vartheta]\right), \quad (11)$$

where $Z$ is a normalization constant and $S_{\text{rot}}$ and $S_{\text{trans}}$ are functionals encoding the rotational and translational noise:

$$S_{\text{rot}}[\vartheta] = \int_0^\tau dt \left[\vartheta(t)\right]^2, \quad (12)$$

$$S_{\text{trans}}[r, u] = \int_0^\tau dt \left[\dot{r}(t) - v u(t) + \mu \nabla U(r(t))\right]^2. \quad (13)$$

Note that $S_{\text{trans}}$ is the active equivalent of the Onsager–Machlup functional of a passive particle [55, 56].

By discretizing this path integral, the probability for a transition between two microstates
is obtained as:

\[ p(w_i \rightarrow w_{i+1}) = N \exp\left\{ -\frac{(\vartheta_{i+1} - \vartheta_i)^2}{4D \Delta t} \right\} \exp\left\{ -\frac{(r_{i+1} - r_i - vu_i \Delta t + \mu \nabla U(r_i) \Delta t)^2}{4D \Delta t} \right\} \]  \hspace{1cm} (14)

where \( N \) is again a normalization constant.

**B. FINAL ACCEPTANCE PROBABILITY**

Here we present the final form of the acceptance probability implemented in our generalized TPS algorithm obtained by combining Eq. (3-6,9).

\[
P_{\text{acc}}[\mathcal{W}^{\text{old}} \rightarrow \mathcal{W}^{\text{new}}] = h[\mathcal{W}^{\text{new}}] \min\left\{ 1, \frac{N^{\text{old}}}{N^{\text{new}}} \frac{\rho(w^\text{new}_0)}{\rho(w^\text{old}_0)} \frac{\pi(r^\text{old}_0)}{\pi(r^\text{new}_0)} \right\} \times \prod_{k=0}^{i-1} \exp\left\{ -\frac{v}{2D} u^\text{old}_k \cdot (r^\text{old}_k - r^\text{old}_{k+1} + \mu \nabla U(r^\text{old}_{k+1}) \Delta t) \right\} \times \prod_{k=0}^{j-1} \exp\left\{ \frac{v}{2D} u^\text{old}_k \cdot (r^\text{old}_k - r^\text{old}_{k+1} - \mu \nabla U(r^\text{old}_{k+1}) \Delta t) \right\} \times \prod_{k=0}^{i-1} \exp\left\{ -\frac{v}{2D} u^\text{new}_k \cdot (r^\text{new}_k - r^\text{new}_{k+1} + \mu \nabla U(r^\text{new}_{k+1}) \Delta t) \right\} \times \prod_{k=0}^{j-1} \exp\left\{ -\frac{v}{2D} u^\text{new}_k \cdot (r^\text{new}_k - r^\text{new}_{k+1} - \mu \nabla U(r^\text{new}_{k+1}) \Delta t) \right\} \right\} \] \hspace{1cm} (15)

**C. DETAILED ANALYSIS FOR PE = 5**

Greater details on the reactive path ensemble can be collected by studying the behavior of the angle \( \vartheta \) in the states belonging to the transition paths. Here we discuss the case of medium activity Pe = 5. Due to symmetry with respect to the axis \( y = 0 \), the average angle as a function of \( x \) is zero. More interesting, the standard deviation of the angles as a function of \( x \) shows that the angles are more focused in forward direction (\( \vartheta = 0 \)) just at the right of the reactants basin (see blue lines Fig. 4b). In fact, the angular distributions of \( \vartheta \) conditioned to specific values of \( x \) are spread around \( \vartheta = 0 \) at \( x = 0 \), while they are bimodal in the proximity of the basins (see Fig. 4d). Along the \( y \) coordinate, instead, on average the angle points upward for positive \( y \) values and downward for negative \( y \) values while the standard deviation remains about constant (see Fig. 4c). This behavior is reflected in the angular distributions of \( \vartheta \) conditioned to specific values of \( y \), as reported in Fig. 4e.
Angular distributions conditioned to a specific position show that for points close to the reactant basin the most likely velocity angle points in the direction opposite to the basin itself. However, the angular distribution conditioned to a specific position just above the target basin displays again angles contained in the first quadrant (see Fig. 4 f-g). Altogether, the picture emerging from Fig. 4 is that there are few fast reactive paths similar to the one reported in Fig. 2(c) and many paths similar to the one in Fig. 2(d) that surf along the energy walls before falling in the T basin (see also Fig. S5).

D. ADDITIONAL FIGURES

Figs. 5 to 8.
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FIG. 5. Steady state distributions within the reactant basin. (a) equilibrium distribution for a passive particle, with \( k_x = 6 \) and \( k_y = 20 \). The passive particle is Boltzmann-distributed within the reactant basin. (b) steady state distribution for an active particle with Pe = 5, \( k_x = 6 \) and \( k_y = 20 \), not Boltzmann-distributed. For each \((x, y)\) point, the distribution value is obtained as the cumulative distribution over all the possible angles \( \vartheta \) of the self-propulsion speed. (c-f) steady state distribution marginalized on the value of the angle \( \vartheta \). The four plot report distributions marginalized on the four quadrant: \(-\pi/4 < \vartheta \leq \pi/4\) (c), \(\pi/4 < \vartheta \leq 3\pi/4\) (d), \(3\pi/4 < \vartheta \leq 5\pi/4\) (e) and \(5\pi/4 < \vartheta \leq 7\pi/4\) (f). See also the blue portion in the pie plots.

The distribution (b) shows that when the ABP is inside the reactants basin, it is more likely to be on the left side of the basin. On the other hand, panels (c-f) report that the positional probability distribution of an ABP inside the basin strongly depends on the angle \( \vartheta \) determining the direction of its velocity. The results show that the ABP is more likely to have a velocity that points in the opposite direction with respect to the center of the basin. The observed overall behavior is due to the fact that the left side of the basin is characterized by a steeper potential wall. When the ABP has a velocity pointing towards positive \( x \) values, it can easily exit the reactant basin. In contrast, when the ABP has a velocity pointing towards the steeper potential wall (direction towards negative \( x \) values), it is more likely that the particle remains inside the basin, at least for a time of the order \( \tau_\theta \), which is the typical time necessary for the particle to change the velocity direction.
FIG. 6. (a-c) $m(r)$ and $J(r)$ in the reactive region for $Pe = 10$ at different potential stiffnesses $k_x$ with $k_y = 20$. The variation in the quartic part of the potential is not introducing substantial changes in the reactive probability densities and currents, rather they remain quite similar for all explored values of $k_x$. The most notable difference resides again in the region explored by the active particles, that is getting closer to the basins along the $x$ direction upon increasing the potential stiffness $k_x$. 

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FIG. 7. (a) Reactive probability density $m(x)$ for $Pe = 10, k_x = 6, k_y = 20$. (b-c) marginal reactive probability density $m(x) (m(y))$ (red line) and average angle $\bar{\vartheta}$ with its standard deviation $\sigma_{\vartheta}$ (thick blue line) as a function of $x$ ($y$) alone. (d-e) distribution of angle $\vartheta$ among the states having x-coordinate in the intervals $X_1 : [-1 - \Delta, -1 + \Delta], X_2 : [-\Delta, \Delta]$ and $X_3 : [1 - \Delta, 1 + \Delta]$ ($Y_1 : [-0.72 - \Delta, -0.72 + \Delta], Y_2 : [-\Delta, \Delta]$ and $Y_3 : [0.72 - \Delta, 0.72 + \Delta]$) respectively ($\Delta = 0.04$). (f-g) distribution of angle $\vartheta$ in the states $P_1, \ldots, P_4$ at the intersection of previously defined intervals. Each angular distribution is normalized.
FIG. 8. Frequency of different trajectory types for two values of the Péclet number, Pe = 5 and Pe = 10. A sketch of the trajectory type is given above the bars. Different transition pathway are sorted in the three categories by studying their behavior in the region $X : -1 < x < 1$, when going from the R basin to the T basin: Type I) paths whose positions contained in the region $X$ have only positive (or only negative) $y$ values; Type II) paths whose portion contained in the region $X$ has positive (negative) $y$ coordinates when close R and negative (positive) $y$ coordinates when close to T; Type III) other types of trajectories. For Pe = 5 most of the trajectories are of type I, a relevant part is of type II while almost no other types of trajectories are observed. For Pe = 10 instead the percentage of trajectories of the first kind increases as well as other possible types of trajectories, while the second type of trajectories decreases. The higher (lower) fraction of transition paths belonging to type I (II) for Pe = 10, in comparison to Pe = 5, is due to the fact that particles with higher activity are more likely to “surf” along the potential energy walls.