Escape problem for active particles confined to a disk

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(Received 5 July 2020; accepted 23 October 2020; published 4 December 2020)

We study the escape problem for interacting, self-propelled particles confined to a disk, where particles can exit through one open slot on the circumference. Within a minimal two-dimensional Vicsek model, we numerically study the statistics of escape events when the self-propelled particles can be in a flocking state. We show that while an exponential survival probability is characteristic for noninteracting self-propelled particles at all times, the interacting particles have an initial exponential phase crossing over to a subexponential late-time behavior. We use a phenomenological model based on nonstationary Poisson processes which includes the Allee effect to explain this subexponential trend and perform numerical simulations for various noise intensities.

DOI: 10.1103/PhysRevResearch.2.043314

I. INTRODUCTION

A common trait for many active matter systems, formed by the self-propelled (active) individuals, is their ability to self-organize into complex flowing states that arise due to many-body interactions and an energy input on the particle level [1,2]. A wide range of systems live under the umbrella of active matter, including biological microswimmers [3,4], Janus particles [5–7], and vibrated granular rods [8,9], and most of these systems are embedded into an environment or a spatial confinement which can alter the open-space particle dynamics [10]. Recently, experiments and simulations have shown that the interactions between the self-propelled particles or interactions with obstacles and boundaries give rise to interesting behaviors like particle migration towards walls [11,12], separation in systems with more than one type of active particles [13], as well as trapping [14]. The role of confinement of active particles is undoubtedly of central importance in realistic systems, especially for biological matter and biotechnology [15,16]. However, it is also one of the least understood and open topics in current active matter research.

Many living systems form ordered states where the underlying organizational principle is assumed to be local ferromagnetic-like alignment interactions. Just like in magnetic systems, such interactions can give rise to globally ordered states, in this case called flocks, as well as disordered states in the noise-dominated regime. In such systems, confinement will introduce a length scale which interacts with the many other length scales that are already present, possibly changing the emergent patterns in the ordered states. In the simple case of a confining disk, one can broadly distinguish between three phases, sketched in Fig. 1(a): a disordered gas-like phase at low densities or in the noise-dominated regime, and a flocking state with complete orbital order when interactions dominate. In between these phases there is what may be called a motile droplet phase where smaller flocks of varying sizes move as individual units with a renormalized interaction strength. In an open system, however, this picture may change. In the narrow escape problem, particles move inside a bounded two-dimensional (2D) domain with a small open window through which the particles may escape [see Fig. 1(b)]. In addition to geometric effects from the confining domain which may change the patterns of motion one can expect, the nonconservation of the particle number may also have a nontrivial effect on the order of the system.

Recently the narrow escape problem has gained renewed interest due to its relevance in biological processes, where the absorbing window may for example represent a small patch of a cellular membrane where receptors are located, and the diffusing particle represents an ion [17,18]. An exponential decay is also found in chaotic billiard systems, while deterministic billiards give rise to a $1/t$ decay in particle number [19]. Escape problems for active particles without alignment interactions have also been studied recently in the case of a wedge geometry and a disk geometry [20,21]. The survival probability in a 1D setting has also recently been studied in a run-and-tumble model of bacterial motion [22].

In this paper we study the narrow escape problem for interacting active particles, modeled with a Vicsek-like model, confined to a circular domain. The system is sketched in Fig. 1(b). In the high-noise, weak-interaction limit the problem is similar to that of the Brownian escape problem in the sense that interactions are negligible, while in the opposite regime we expect collective effects to alter the escape process, leaving the decay of particle number nonexponential. It is the low-noise regime that is of primary interest in this paper. We perform numerical simulations for both interacting and noninteracting self-propelled particles, and study both the rotational order and the escape statistics. The simulations reveal a subexponential decay at late times, which may be

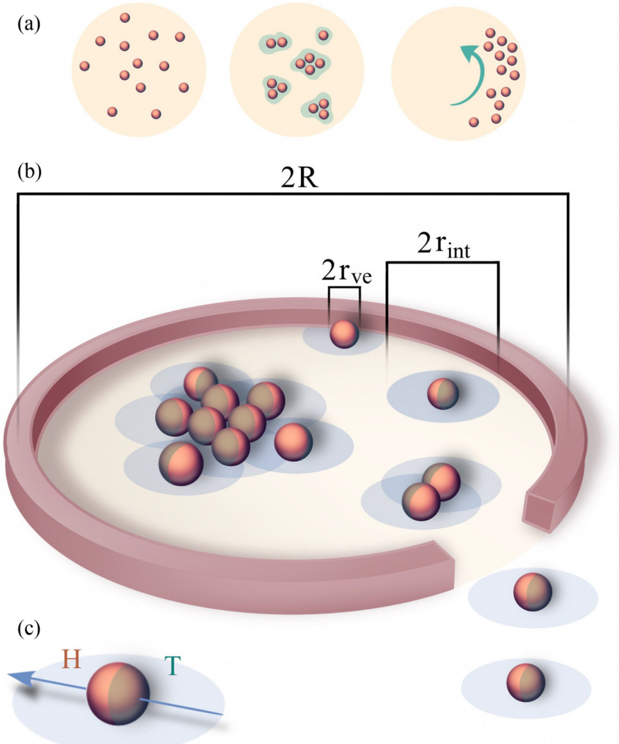

FIG. 1. A sketch of the system considered in this paper. The polar particles [head and tail particles as in (c)] have a small volume exclusion radius $r_{\rm ve} = 1$ in units of the particle step length. The particles interact through a Vicsek-type alignment interaction with range $r_{\rm int} = 5$, enabling collective escape events. The angular opening of the escape window is fixed to $2\pi/18$.

captured by a phenomenological model with an escape rate that is density dependent.

The paper is organized as follows. Section II discusses the rotational order in the system, and consequently which phases of the Vicsek model to be expected when the system is open and particles can escape. Section III discusses the connection to Poisson processes as well as the role of memory in the escape process, and proposes a phenomenological model to capture the escape statistics. Section IV discusses the results of escape simulations of both interacting and noninteracting particles, before concluding remarks are given in Sec. V.

II. ROTATIONAL ORDER IN OPEN SYSTEMS

The Vicsek model is undoubtedly the archetypal numerical model for collective swarming and flocking effects [23,24]. The particles are self-propelled with velocity $\dot{\vec{x}}_i = v_0 \hat{P}_i(\theta)$ where the polarization vector $\hat{P}_i(\theta)$ for particle i is updated according to the standard Vicsek rule [25]

$$\hat{P}_i(t+1) = D_\eta\left(\frac{\overline{v}_i}{||\overline{v}_i||}\right), \quad (1)$$

$$\overline{v}_i = \sum_{k:||\vec{x}_i - \vec{x}_k|| \leqslant r_{\rm int}} \vec{v}_k, \quad (2)$$

where D_η is a rotation matrix rotating a vector by a random uniformly chosen angle in $(-\eta\pi, \eta\pi)$. The parameter $\eta \in (0, 1)$ determines the noise in the system. The velocity $\overline{v}_i$ in Eq. (2) is the average velocity of the neighboring particles of particle i, representing the velocity with which particle i tries to align. The alignment interaction has a range $r_{\rm int}$. Note that the velocity of particle i itself is included in the sum leading to $\overline{v}_i$, so that in the noninteracting limit $r_{\rm int} \to 0$, the particle moves according to a very simple stochastic model governed only by the parameter η and the self-propulsion speed v_0, which we here set to unity without loss of generality.

Equations (1) and (2) must be supplemented with additional information when boundaries or obstacles are present. In the current case, the reflecting boundary of the disk can be simply dealt with by letting the director $\hat{P}_i$ be reflected about the tangent to the circle at the point of impact. When interactions are present and clusters of particles are formed, we include a small volume exclusion interaction with range $r_{\rm ve}$ to avoid clusters being compressed by the bounding walls. This is numerically included simply by moving particles a step length apart in the direction separating them should they come to close to each other. Figure 2 shows an example of the dynamics produced by this model.

In unconfined space the Vicsek model is known to produce a wide range of phases, like the gaseous phase at high noise, a band phase, and a globally ordered phase. Confinement and complex environments typically interfere with these phases and result in new behaviors requiring new ways of characterization. For example, the band phase of the Vicsek model is a consequence of the toroidal topology of periodic boundary conditions [26]. Hence we do not expect that such phases are present in the confined case. Because of the symmetry of the circular domain it is natural to consider a rotational order parameter that distinguishes collective orbital motion where the particles are moving collectively clockwise or anticlockwise around the system boundary, and other types of dynamics of varying degree of correlation. Such an order parameter may be written as

$$\Phi_R(t) = \left|\frac{1}{n(t)}\sum_{i=1}^{n(t)}\left(\frac{\vec{x}_i}{||\vec{x}_i||} \times \hat{P}_i\right)\cdot\hat{z}\right|,$$

where we should note that when the system is open the particle number is no longer a conserved quantity so the range of the sum is time dependent. For a closed system, a gas phase ($\Phi_R \approx 0$) still exists at strong noise and/or weak interaction, and a motile droplet phase ($0 < \Phi_R < 1$), where smaller clusters of particles move as collective units, exists between the disordered $\Phi_R = 0$ and ordered $\Phi_R = 1$ phases.

In an open system the story is different. Here the order parameter does not stabilize at the would-be value in the closed case due to the inherent nonstationary nature of the problem. Instead, the order quickly increases at short times when the particles form flocks, while as time goes on the order decreases again due to the diminishing particle number. By construction the order parameter is an intensive quantity, so the diminishing nature of $\Phi_R(t)$ is a consequence of lack of order rather than an effect of the particle numbers. However, the rotational order does not immediately approach zero, but rather stabilizes at a lower value, indicating some remaining order. This is shown in Fig. 3. This may be interpreted as follows. At early times the particles form clusters in

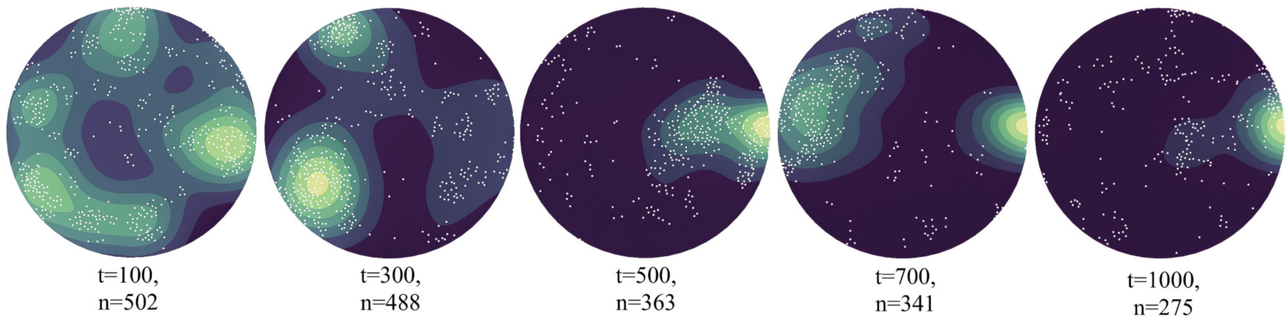

FIG. 2. Snapshots of a simulation based on Eqs. (1) and (2) with active particles confined to a disk with an absorbing window with opening angle $2\pi/18$ centered at $(R, 0)$. The background color map shows relative particle density for all the particles (absorbed and nonabsorbed), bright implying high density. We see that as time progresses the density at the absorbing window increases as particles accumulate. System parameters: $\eta = 0.2,\ r_{\rm ve} = 2,\ n(0) = 2^9$.

accordance with the given noise strength and interaction range. As time goes on, (collective) escape events take place, reducing the particle number. However, the rotational order does not immediately fall to zero, implying that the low-density states at late times still carry some correlations. Large flocks in the confined Vicsek model are well known to create edge currents that move along the system boundary, and such motion will eventually lead to large escape events as the cluster reaches the exit. At late times, it is therefore likely that smaller clusters, that may not move long the boundary, remain in the bulk for some time, with some remaining but decreased rotational order. Such flocks will move more or less ballistically, but since the flock size distribution is not likely to be sharply peaked around a constant value, one should not expect the $1/t$ scaling in particle number as in the case of ballistic billiards. Rather the size of the flocks depends on how many particles have already escaped, and hence depends on the history of the system. Such memory effects are discussed further in the next section.

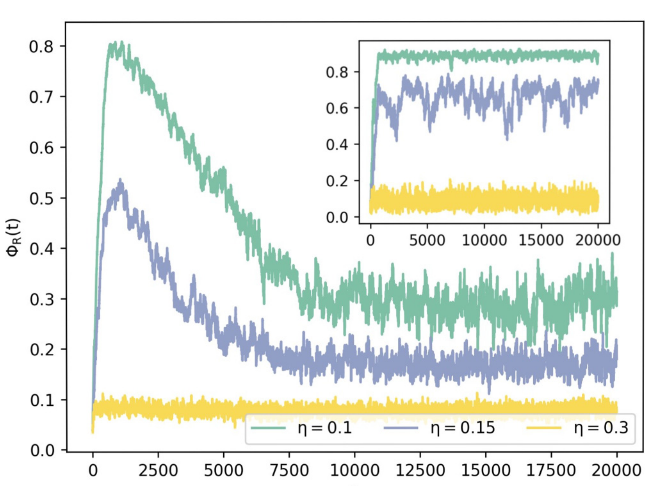

FIG. 3. Plot showing the rotational order parameter $\Phi_R(t)$ as a function of time for some select choices of the noise strength. The inset shows the corresponding order parameter for a system without an escape window. Timescale set by the ratio of particle size to self-propulsion speed, which for convenience is set to unity.

III. PHENOMENOLOGICAL MODEL FOR ESCAPE STATISTICS

In general terms, an escape process consists of particles moving in a 2D bounded domain Ω with boundary $\partial\Omega = \partial\Omega_r \cup \partial\Omega_a$, where the subscripts denote the reflective and absorbing parts of the boundary respectively. The particles have a density $\rho(\vec{x}, t)$, assumed to be normalized to unity at $t = 0$, which follows a continuity equation. From this probability density the survival probability is defined as

$$S(t) = \int_\Omega d\Omega\, \rho(\vec{x}, t). \tag{3}$$

The first hitting time (FHT), in this case also the escape time, is the time at which a particle escapes the domain. The distribution of first hitting times $H(t)$ is closely related to the survival probability, namely

$$S(t) = \int_t^\infty ds\, H(s),$$

which simply states that the probability of survival up to time t is equivalent to the FHT being larger than t. This implies for the FHT distribution that

$$H(t) = -\partial_t S(t). \tag{4}$$

We see that the distribution of escape times can be interpreted as the probability flux out of the system.

On the hydrodynamic scale, let us assume that the phase space density $\Psi(\vec{x}, \theta, t)$ of an active particle satisfies a Boltzmann-type mean field equation $\mathcal{D}_t\Psi = Q[\Psi]$, where the total time derivative includes the self-propulsion term and takes the form $\mathcal{D}_t = \partial_t + v_0\hat{P}(\theta)\cdot\nabla_x$. This must of course be supplemented with appropriate boundary conditions for the reflective and absorbing parts of the boundary. The operator $Q[\Psi]$ contains a part resulting from the noise in the direction of motion and a nonlinear part that originates in alignment interactions [27]. The particle density and velocity fields are simply the zeroth and first velocity moments of the field Ψ:

$$\rho(\vec{x}, t) = \int d\theta\, \Psi(\vec{x}, \theta, t), \tag{5}$$

$$\rho\vec{V} = \int d\theta\, \vec{v}(\theta)\Psi. \tag{6}$$

By integrating the Boltzmann equation over the angles one obtains the mass conservation equation

$$\partial_t \rho(\vec{x}, t) + \nabla_x \cdot (\rho(\vec{x}, t)\vec{V}(\vec{x}, t)) = 0. \quad (7)$$

Since the collision operator is in general nonlinear, we do not expect a full solution to be available for Ψ through the method of separation of variables. However, it is instructive to make the somewhat weaker assumption that the density is separable after integration of the angles, namely $\rho = X(\vec{x})S(t)$. Integrating Eq. (7) over the domain and using the divergence theorem then immediately gives

$$\dot{S}(t) = -\lambda(t)S(t), \quad (8)$$

$$\lambda(t) = \int_{\partial\Omega_a} d\ell(\hat{n}\cdot\vec{V})X(\vec{x}) \geqslant 0, \quad (9)$$

where $\hat{n}$ is the outward normal vector for the domain. This shows that rather generally we expect the escaping Vicsek particles to behave like a nonstationary Poisson process, allowing us to make phenomenological connections to other growth or decay processes like those in population ecology.

In the absence of interactions when the nonlinear collision term is not present, one can attempt a solution in terms of a fully separated set of variables. Writing the phase-space density as $\Psi = X(\vec{x})\Theta(\theta)S(t)$, we easily see that the velocity field equation (6) reduces to

$$\vec{V} = \int d\theta\, \vec{v}(\theta)\Theta(\theta),$$

which is time independent. In this case Eq. (9) becomes a constant, and we expect a stationary Poisson process to be a valid description of the escape process. That the noninteracting system behaves like a stationary Poisson process can also understood from the memorylessness property [28]. This property states that if one waits some time t_1 and no escape events has taken place, the probability of having to wait a further time t_2 is simply the probability of having to wait a time t_2 in the first place. This type of lack of memory, regarding how much time has passed, can be written in terms of the survival probability simply as $S(t_1 + t_2) = S(t_1)S(t_2)$ which is only satisfied by an exponential function. We expect the correlations between the particles in the interacting case to break this memoryless property through the fact that the system now depends on its history: flocks of particles may form and escape the system collectively, and the potential size of the clusters is limited by how many particles have already left the system. We therefore expect the escape rate to be a function of the particle number $\lambda(t) = \lambda[n(t)]$.

Such processes where rates are dependent on density or number of particles are ubiquitous in nature. In epidemiology, for example, both death and infection rates may have nontrivial density or population size dependencies, which may be traced back to some sort of competition of resources or the simple fact that a higher-density population will have more contacts which act as possible disease transmission routes [29,30]. These ideas are found in several mathematical models in population ecology, and are sometimes associated with the Allee effect [31]. Roughly speaking, this is the effect where there is a correlation between the general well-being or chance of survival for an individual in a population and that population's size or density.

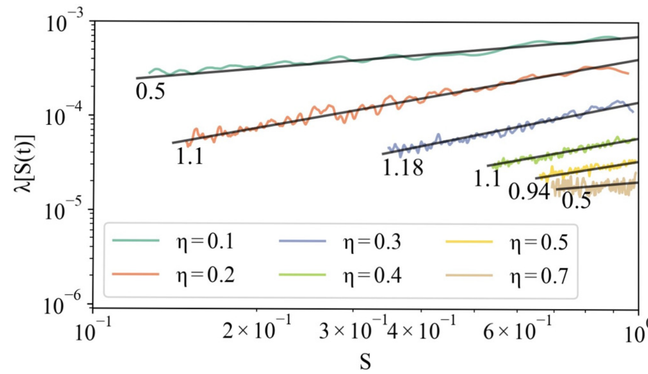

FIG. 4. Escape rates plotted as a function of $S(t) = n(t)/n(0)$ showing a power-law behavior. Although the range is insufficient for a highly reliable extraction of the power-law exponent (number attached to each solid black line), the numerical values can be used as initial guesses in a nonlinear regression to fit $S(t)$ as a function of time.

Trying to solve the full mean field equations for the Vicsek model with the appropriate boundary conditions is outside the scope of this paper as it is a numerical study, and we therefore proceed with an empirical model. While we do not make connections to the microscopic parameters that control the Vicsek particles, this approach allows us to quantify how far from exponential the decay process is. Generally the process $\partial_t S(t) = -\lambda[S(t)]S(t)$ has stationary states given either by $S = 0$ or by the roots of $\lambda[S]$. Since there is no reason to expect anything but a decaying particle number until no particles remain, the only zero of $\lambda[S]$ should be $S = 0$. It should also be a monotonically increasing function of the number of particles, since a large number of particles implies more, or larger, collective escapes. This already constrains the functional form of the rate somewhat, and, to numerically extract the density dependence from the simulation data, we consider Eq. (8) in the form $\lambda[S] = -\dot{S}/S$, where we used $S = n(t)/n(0)$ to write the rate in terms of the survival probability. Figure 4 shows these data, displaying a power-law behavior. This motivates the use of the simple ansatz $\lambda[n(t)] = \lambda_0 S^{\zeta}(t)$. This is easily shown to have the solution

$$S(t) = [1 + \lambda_0\zeta t]^{-1/\zeta}. \quad (10)$$

Here the parameter λ_0 is an escape rate, while the shape parameter ζ deforms the decaying function $S(t)$ away from the exponential behavior, which is regained in the limit $\zeta = 0$. For short times we have an exponential-type behavior $S(t) = 1 - \lambda_0 t + \cdots$ which is independent of the shape parameter. For $\zeta > 0$, the solution in Eq. (10) represents a subexponential growth at intermediate and late times, while for negative shape parameters the decay reaches zero at some finite time.

IV. RESULTS

We are interested in the effect of collective order in a low-density system where we are far away from the jamming or glassy transitions at high densities. We consider two cases, with $n(0) = 2^9$ and $n(0) = 2000$ particles, with volume filling

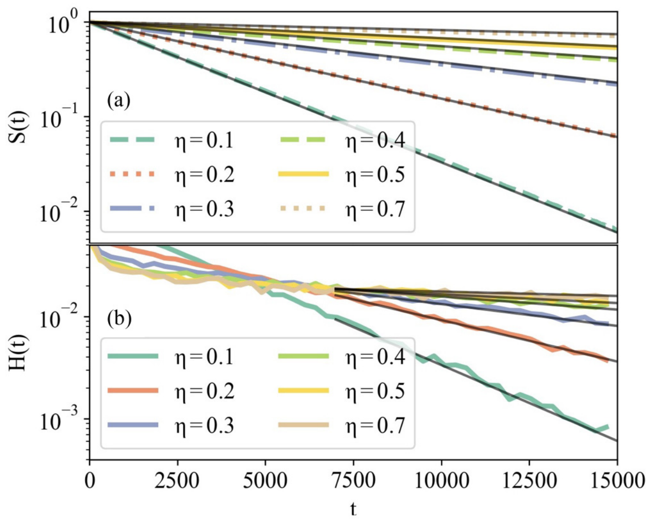

FIG. 5. Behavior of the survival probability for self-propelled noninteracting particles. Simulations use $n(0) = 2^9$ particles in a system with volume fraction 5%. (a) Survival probability in semilog plot for some different values of noise strength showing exponential behavior. (b) FHT distribution also consistent with exponential decay.

fractions of around 5% and 10% respectively. This is well within the range of filling fractions where ordered collective states have been previously observed but also far from the jamming or glassy states [32].

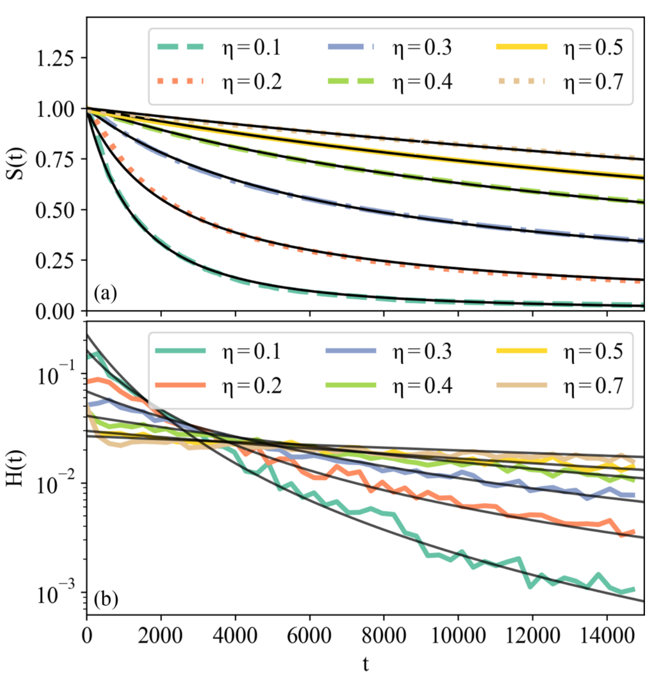

FIG. 6. Behavior of the survival probability for self-propelled interacting particles. Simulations use $n(0) = 2^9$ particles in a system with volume fraction 5%. (a) Survival probability for some different values of noise strength showing nonexponential behavior together with best fit of Eq. (10) in solid black lines. The exponent ζ is taken from Fig. 4. (b) FHT distribution also consistent with the same parameters.

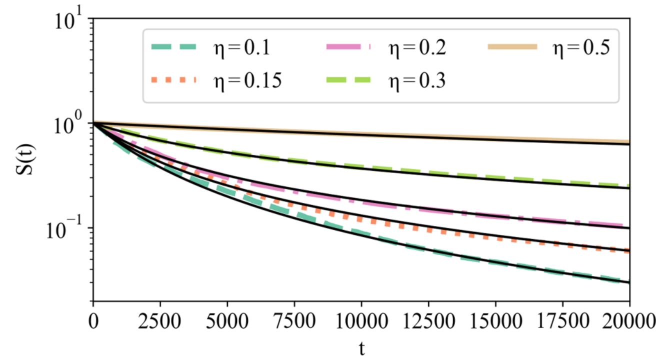

FIG. 7. Survival probability for $n(0) = 2000$ particles in a system with volume fraction of 10%, together with fits from the phenomenological model. Quantitatively, a larger system and a larger initial filling fraction do not alter the escape process.

Recall from our earlier discussions that the noninteracting case is expected to be described by a memoryless Poisson process, just like Brownian motion. The noninteracting limit is only formally equivalent to Brownian particles when the self-propulsion velocity is set to zero and the noise is maximal, or equivalently the timescale of rotational diffusion approaches zero. Simulation results from noninteracting active point particles are shown in Fig. 5, together with best fit exponential lines. We see that both the survival probability and the FHT distribution are exponential at late times as expected, with a rate that decays rapidly as a function of angular noise strength. Note that in the noninteracting case we use point particles without spatial extent, to probe only the effect of activity and noise.

Results from fully interacting simulations are shown in Fig. 6 for the 5% volume fraction case and in Fig. 7 for the 10% volume fraction case, both together with best fits from the phenomenological model showing good agreement. Figure 8 shows the interacting and noninteracting survival probability together for some chosen values of the noise for the 5% case. We clearly see that while the interacting particles are leaving the system more rapidly at short timescales, they are less efficient at emptying the system at late times. Note that the limit of high noise produces equivalent curves for

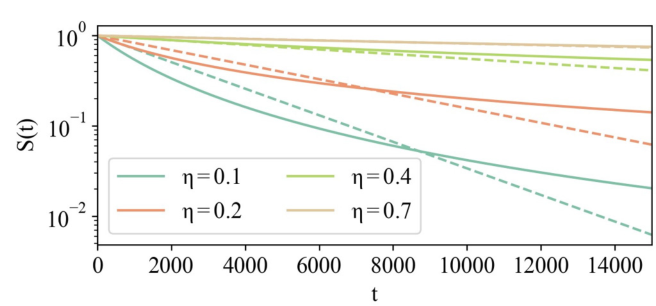

FIG. 8. Plot showing the interacting and noninteracting survival probabilities for the 5% volume fraction case as a function of time for the same system parameters. The interactions make the number of escapes be higher at early times, while the behavior is clearly subexponential at late times.

interacting and noninteracting particles, since in this limit we expect a disordered phase.

V. CONCLUSION

We have studied the effect of collective motion on the escape process for self-propelled active particles. In the interacting case, the numerical results agree well with a phenomenological model where the escape rate is a power-law in the population fraction, leading to an early time exponential behavior followed by a subexponential decay in time. In the flocking phase, the collective alignment effects make the escape process slower than the noninteracting case in the long run, and faster on short time scales. In the disordered phase, fluctuations will dominate over the alignment mechanism and the interacting and noninteracting cases are more or less identical and characterized by an exponential decay.

ACKNOWLEDGMENTS

The authors thank Gaute Linga, Bjarke Frost Nielsen and Vidar Skogvoll for insightful input and discussions during this work. This work was supported by the Research Council of Norway through the Center of Excellence funding scheme, Project No. 262644 (PoreLab). L.A. acknowledges support in part by the National Science Foundation under Grant No. NSF PHY-1748958 through the Kavli Institute for Theoretical Physics.

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