


Current fluctuations of interacting active Brownian particles

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We derive the distribution of particle currents for a system of interacting active Brownian particles in the long-time limit using large deviation theory and a weighted many-body expansion. We find the distribution is non-Gaussian, except in the limit of passive particles. The non-Gaussian fluctuations can be understood from the effective potential the particles experience when conditioned on a given current. This potential suppresses fluctuations of the particles orientations and surrounding density, aligning particles and reducing their effective drag. From the distribution of currents, we compute the diffusion coefficient, which is in excellent agreement with molecular dynamics simulations over a range of self-propulsion velocities and densities. We show that mass transport is Fickian in that the diffusion constant determines the response of a small density gradient, and that nonlinear responses are similarly computable from the density dependence of the current distribution.

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Persistent currents are the hallmark of a system driven away from equilibrium. One of the simplest and most fundamental problems of nonequilibrium physics is to predict the structure of the fluctuations of currents around a nonequilibrium steady state and to decode the microscopic information contained in them. Nonequilibrium fluctuation-dissipation relations [1–7], fluctuation theorems [8–13], and thermodynamic uncertainty relations [14–16] are notable examples of successes toward this end. Much of this progress has been underpinned by the study of large deviation functions (LDFs), which supplies a general framework to compute and characterize fluctuations of extensive observables [17,18]. The LDFs of the current can be viewed as the analog of a free energy, making relationships between fluctuations and response to external perturbations transparent [19–21]. However, the evaluation of LDFs for interacting systems remains challenging. In this Rapid Communication, we characterize the fluctuations of currents in a system of interacting active Brownian particles (ABPs) and show how these fluctuations encode the response of the system.

ABPs are a simple model of active matter, a class of systems that convert energy from the environment into directed motion. ABPs evolve nonequilibrium steady states as they break detailed balance at the single-particle level due to a constant nonconservative driving force. More than just being non-Boltzmann, their steady states support unique phenomena such as motility-induced phase separation [22,23]. Laboratory realizations of active matter include cellular biopolymers [24–26], bacteria [27–33], and synthetic colloids [34–38], with the latter being a direct realization of ABPs [39–41]. Indeed, it has been demonstrated that the center-of-mass motion for bacteria and biopolymers can be well described by ABPs with an effective particle size when hydrodynamic

interactions and internal degrees can be neglected [41–48]. We derive the current LDFs for ABPs and validate it with molecular simulation. We find that small current fluctuations are Gaussian, and the associated linear response obeys Fick’s law, as has been shown for noninteracting ABPs [49]. Large current fluctuations are non-Gaussian and the associated nonlinear response results from a change in the particle’s orientational correlations, which we characterize with the effective potential that renders those fluctuations typical.

We consider a collection of N ABPs in two spatial dimensions, whose positions and orientations are denoted $\mathbf{r}^N = \{\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N\}$ and $\boldsymbol{\theta}^N = \{\theta_1, \theta_2, \dots, \theta_N\}$, respectively. These dynamical variables are coupled through their equations of motion, which for the position of the i th ABP is

$$\dot{\mathbf{r}}_i(t) = \mathbf{F}_i[\mathbf{r}^N(t)] + v_0 \mathbf{e}[\theta_i(t)] + \boldsymbol{\eta}_i(t), \quad (1)$$

and for its corresponding orientation is

$$\dot{\theta}_i(t) = \eta_r(t), \quad (2)$$

where the dot denotes time derivative, v_0 is the magnitude of the self-propulsion velocity, and $\mathbf{e}[\theta(t)] = \{\cos(\theta), \sin(\theta)\}$ is the unit vector on a circle. The Gaussian random variables, $\eta_{(t,r)}$, satisfy $\langle \eta_{(t,r)}(t) \rangle = 0$ and $\langle \eta_{(t,r)}(t) \eta_{(t,r)}(t') \rangle = 2D_{(t,r)} \delta(t - t')$, where $\langle \cdot \rangle$ denotes ensemble average. We use $D_t = 1$ and $D_r = 3$ in numerical simulations. The particles interact with a pairwise additive force, $\mathbf{F}_i[\mathbf{r}^N] = \sum_{j \neq i}^N F(r_{ij}) \hat{\mathbf{r}}_{ij}$, where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$, $F(r)$ is assumed to be short-ranged and repulsive, and $\hat{\mathbf{r}}$ denotes unit vector. In all the simulations, the system of ABPs interact through a Weeks-Chandler-Andersen potential [50] given by

$$U(r) = \begin{cases} 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right] + \epsilon, & r < 2^{1/6}\sigma \\ 0, & r \geq 2^{1/6}\sigma, \end{cases} \quad (3)$$

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where we set the energy scale, ϵ , and length scale, σ , to be 1. From this potential the force is given by $F(r) = -\nabla U(r)$. All simulation results are presented in reduced units with time in units of $\tau_{LJ} = \sigma^2/(D_t)$ and currents, J , in units of σ/τ_{LJ} . Our simulations are in two dimensions with a domain of $100\sigma \times 100\sigma$ and periodic boundary conditions. We used particle numbers of $N = 1000, 3000$, and 5000 , which corresponds to densities of $\rho = 0.1, 0.3$, and 0.5 . We used a second-order stochastic Runge-Kutta algorithm [51] with a time step of $\delta t = 10^{-5}\tau_{LJ}$. All data presented were computed with two to three independent simulations, with a total simulation time between 500 and $5000\tau_{LJ}$, including $200\tau_{LJ}$ of equilibration.

The time-integrated current for particle i is defined as

$$\mathbf{J}_i = \frac{1}{t} \int_0^t dt' \dot{\mathbf{r}}_i(t') = \frac{\mathbf{r}_i(t) - \mathbf{r}_i(0)}{t}, \quad (4)$$

where the observation time, t , is assumed to be large. The total current for all N particles in the system is $\mathbf{J}^N = \{\mathbf{J}_1, \dots, \mathbf{J}_N\}$. To characterize the statistics of \mathbf{J}^N in the long-time limit, we aim to compute its LDFs. We define a generating function,

$$\hat{P}(\boldsymbol{\lambda}, \mathbf{r}^N, \boldsymbol{\theta}^N, t) = \int d\mathbf{J}^N P(\mathbf{r}^N, \boldsymbol{\theta}^N, \mathbf{J}^N, t) e^{t\boldsymbol{\lambda} \cdot \mathbf{J}^N} \quad (5)$$

with $P(\mathbf{r}^N, \boldsymbol{\theta}^N, \mathbf{J}^N, t)$ being the joint distribution of observing all of the particles in a particular position, orientation, and total integrated current, at time t . The vector $\boldsymbol{\lambda}$ is conjugate to the current vector and exponentially reweights $P(\mathbf{r}^N, \boldsymbol{\theta}^N, \mathbf{J}^N, t)$.

The time evolution of the generating function is given by

$$\frac{\partial \hat{P}(\boldsymbol{\lambda}, \mathbf{r}^N, \boldsymbol{\theta}^N, t)}{\partial t} = L_\lambda^N \hat{P}(\boldsymbol{\lambda}, \mathbf{r}^N, \boldsymbol{\theta}^N, t) \quad (6)$$

that defines the Lebowitz-Spohn operator [18,52,53]. This operator has two pieces, $L_\lambda^N = L_0^N + \Delta L_\lambda^N$, where

$$L_0^N = \sum_{i=1}^N (\mathbf{F}_i[\mathbf{r}^N(t)] + v_0 \mathbf{e}[\theta_i(t)] + D_t \nabla_i \cdot \nabla_i + D_t \partial_{\theta_i}^2) \quad (7)$$

is conservative and whose adjoint gives the Fokker-Planck operator, and the piece dependent on $\boldsymbol{\lambda}$

$$\Delta L_\lambda^N = \sum_{i=1}^N (\mathbf{F}_i[\mathbf{r}^N(t)] + v_0 \mathbf{e}[\theta_i(t)] + 2D_t \nabla_i + D_t \boldsymbol{\lambda} \cdot \boldsymbol{\lambda}) \quad (8)$$

does not conserve probability. The spectrum of L_λ^N is generally complex, but its largest eigenvalue is guaranteed to be real, and whose dependence on $\boldsymbol{\lambda}$ yields the cumulant generating function (CGF) for the current.

Within this framework we can naturally describe two limiting cases. First, we can consider the statistics of the total system current defined as the sum over the individual particle currents, by setting $\boldsymbol{\lambda} = \lambda \cdot \mathbb{1}$ where λ is a scalar parameter and $\mathbb{1}$ the identity. However, this case is trivial because the sum of the interparticle force in Eq. (8) vanishes, decoupling the equation into a sum of N independent equations. In this case, the total current CGF is equivalent

to N times the CGF for a single ABP. Alternatively, we can consider the current statistics of a single tagged ABP, subject to the interactions of the surrounding particles. This is done by setting $\boldsymbol{\lambda}$ to be a vector with a single nonzero element, $\boldsymbol{\lambda} = \{0, 0, 0, \dots, \lambda, \dots, 0, 0, 0\}$. This second case contains the first in the limit of low density, and provides additional information on the dependence of current fluctuations on interactions. In the following we will consider the second definition.

In order to calculate the CGF for a tagged particle, we first introduce a weighted many-body expansion that follows from a Bogoliubov-Born-Green-Kirkwood-Yvon-like hierarchy [54]. Specifically, we define an n -particle reduced generating function

$$\hat{P}^{(n)}(\boldsymbol{\lambda}, \mathbf{r}^n, \boldsymbol{\theta}^n, t) = \frac{N!}{(N-n)!} \int \int d\mathbf{r}^{(N-n)} d\boldsymbol{\theta}^{(N-n)} \times \hat{P}(\boldsymbol{\lambda}, \mathbf{r}^N, \boldsymbol{\theta}^N, t), \quad (9)$$

which, when introduced into Eqs. (6)–(8), results in a set of coupled evolution equations for different $\hat{P}^{(n)}$'s. We close the single-particle equation with the two-particle generating function, decomposed as

$$g_\lambda(\mathbf{r}, \theta, \mathbf{r}', \theta', t) = \frac{\hat{P}^{(2)}(\boldsymbol{\lambda}, \mathbf{r}, \theta, \mathbf{r}', \theta', t)}{\hat{P}^{(1)}(\boldsymbol{\lambda}, \mathbf{r}, \theta, t) \hat{P}^{(1)}(\boldsymbol{\lambda}, \mathbf{r}', \theta', t)}, \quad (10)$$

where $g_\lambda(\mathbf{r}, \theta, \mathbf{r}', \theta', t)$ is the pair distribution function conditioned on a given current through λ [55,56]. This function can be simplified when the system is in a homogeneous steady state and assuming that it does not depend on the difference in orientations between particles. In this limit, $g_\lambda(\mathbf{r}, \theta, \mathbf{r}', \theta', t) \approx g_\lambda(r, \phi)$, where ϕ is the angle of the displacement vector of two particles relative to the orientation of the particle at the origin. This closure to the many-body hierarchy was introduced previously for the case of $\lambda = 0$ [57–60].

The equation of motion for the single-particle generating function will depend on the average interparticle force. We can decompose this force into components in the parallel and perpendicular direction of the self-propulsion; however, this will result in an average force that depends on both the relative angle between the interparticle displacement vector and the tagged particle's orientation. Following Speck *et al.* [57], if we approximate the component perpendicular to the orientation as that parallel to the surface of the particle, this will uncouple these two terms allowing for the expansion to be closed. This approximation to the perpendicular force is exact in the limit of passive particles, where there are no orientational correlations, and is numerically accurate when the parallel component is much larger than the perpendicular component, as occurs for $v_0 > 1$.

As we consider only homogeneous systems, for notational simplicity and without loss of generality we restrict our attention to currents in just the x direction. Under these assumptions, we obtain the evolution operator for the single-particle generating function for currents,

$$L_\lambda = V_\lambda(\rho) \cos(\theta) (\partial_x + \lambda) + D_t(\rho) (\partial_x + \lambda)^2 + D_t \partial_\theta^2, \quad (11)$$

that has the same drift-diffusion form as an independent ABP, but with renormalized effective propulsion speed, $V_\lambda(\rho)$, and translational diffusion constant, $D_t(\rho)$, where ρ is the local density, which in the homogeneous assumption is taken as the bulk density. The adjoint of the operator in Eq. (11) evaluated at $\lambda = 0$ yields the propagator for the single-particle density.

Both $V_\lambda(\rho)$ and $D_t(\rho)$ in principle depend on ρ , v_o , and λ , through the state-dependent pair-correlation function. Within this force decomposition, $D_t(\rho)$ is the diffusion coefficient for a system of interacting passive Brownian particles and we have found that for the conditions we study, $D_t(\rho)$ can be approximated by the mean-field form, $D_t(\rho) \approx D_t(1 - \rho)$ [59]. The effective propulsion speed takes the form $V_\lambda(\rho) = v_o - \rho \zeta_\lambda(\rho)$ where $\rho \zeta_\lambda(\rho)$ is an effective drag. This drag is given by an integral over the interparticle force

$$\zeta_\lambda(\rho) = \int_0^\infty dr \int_0^{2\pi} d\phi r \cos(\phi) g_\lambda(r, \phi) F(r) \quad (12)$$

weighted by the pair distribution function. This coefficient describes the decrease in the effective velocity of a tagged particle due to the increased density of impenetrable particles in the direction of self-propulsion [57]. In the following, we take $\rho \zeta_\lambda(\rho)$ as input for our evaluation of the CGF, though simple approximations to $\zeta_\lambda(\rho)$ exist in specific limits [61].

Using these definitions, we are able to solve for the CGF for this effective single-particle description of the system by the largest eigenvalue of the equation $L_\lambda v_\lambda = \psi(\lambda) v_\lambda$, with $\psi(\lambda)$ being the CGF and v_λ its corresponding right eigenvector. The solution is given by the zeroth characteristic function of Mathieu's equation [62], with a representation for small λ given by the expansion,

$$\psi(\lambda) = D_t(\rho) \lambda^2 + D_r \left[\frac{z_\lambda^2(\rho)}{2} - \frac{7z_\lambda^4(\rho)}{32} + \frac{29z_\lambda^6(\rho)}{144} \right] + \mathcal{O}(\lambda^8) \quad (13)$$

with $z_\lambda(\rho) = V_\lambda(\rho) \lambda / D_r$. The CGF is symmetric about $\lambda = 0$ as a consequence of spatial inversion symmetry and retains all even powers, alternating in sign. The terms up to second order in λ represent the Gaussian contribution. All higher order terms in λ give the non-Gaussian behavior. Specifically, the excess kurtosis, which is a common metric for Gaussian

deviations, is given by the term that is quartic in λ . For passive particles $z_\lambda(\rho) = 0$, and $\psi(\lambda)$ reduces to that for Brownian motion with an effective diffusion constant, $D_t(\rho)$. In the limit that the particles are noninteracting, or $\rho \rightarrow 0$, our results reduce to those obtained previously [63].

Given the CGF, the rate function for current fluctuations can be computed from the Legendre-Fenchel transform, $I(J) = \max_\lambda [\lambda J - \psi(\lambda)]$, where $I(J)$ is minus the logarithm of the probability of J divided by the observation time. Figure 1 shows the rate functions computed from the cloning algorithm [64,65] and predictions from $\psi(\lambda)$. For a variety of different ρ 's and v_o 's we find quantitative agreement between the analytical result and the simulations. Small fluctuations around $J = 0$ are Gaussian as expected, but larger fluctuations are markedly non-Gaussian, revealing fluctuations that are more rare than anticipated from the time-intensive variance, $t \langle J^2 \rangle$. The deviations from Gaussian behavior become more distinct with increasing v_o and decreasing ρ as highlighted in Fig. 1 by scaling the current by $\sqrt{t \langle J^2 \rangle}$.

We can gain insight into the shape of $I(J)$ by constructing an auxiliary process that generates the same ensemble of trajectories in the long-time limit as the original model conditioned on a given current [17]. The auxiliary process is a transformation of the Lebowitz-Spohn operator,

$$\begin{aligned} \mathcal{L}_\lambda &= v_\lambda(\theta)^{-1} L_\lambda v_\lambda(\theta) - \psi(\lambda) \\ &= L_0 + 2D_t(\rho) \lambda \partial_x + 2D_r \partial_\theta \ln v_\lambda(\theta) \partial_\theta, \end{aligned} \quad (14)$$

which leaves the diffusion terms unmodified, but adds additional drift terms that restore normalization. The auxiliary process for a tagged particle is

$$\dot{\mathbf{r}}(t) = \mathbf{F}[\mathbf{r}^N(t)] + v_o \mathbf{e}[\theta(t)] + 2D_t(\rho) \lambda \hat{\mathbf{x}} + \boldsymbol{\eta}_t(t), \quad (15)$$

where the added force is a constant proportional to λ in the x direction. The equation of motion for the orientation includes a force, $F_\lambda(\theta) = 2D_r \partial_\theta \ln v_\lambda(\theta)$, which for small λ is

$$\dot{\theta}_t(t) = -2V_\lambda(\rho) \lambda \sin(\theta) + \eta_t(t), \quad (16)$$

where the force has an amplitude that depends on λ directly and through the λ -dependent drag coefficient, $\zeta_\lambda(\rho)$. The exact form of $v_\lambda(\theta)$ can be evaluated by basis set expansion of Eq. (11) [63], and $\zeta_\lambda(\rho)$ can be evaluated self-consistently

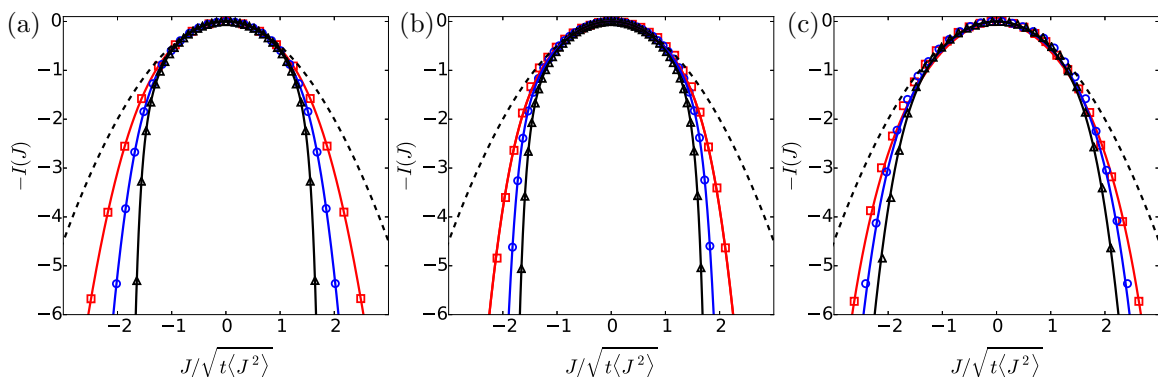


FIG. 1. Comparison between the analytical rate function and its numerical evaluation. (a) Rate functions for $\rho = 0$ and $v_o = 5$ (red squares), 10 (blue circles), and 60 (black triangles). (b) Rate functions for $\rho = 0.1$ and $v_o = 10$ (red squares), 30 (blue circles), and 60 (black triangles). (c) Rate functions for $v_o = 10$ with $\rho = 0.1$ (red squares), 0.3 (blue circles), and 0.5 (black triangles). Shown are the Legendre transforms of Eq. (13) (solid lines), numerical simulations (symbols), and reference Gaussian (dashed line).

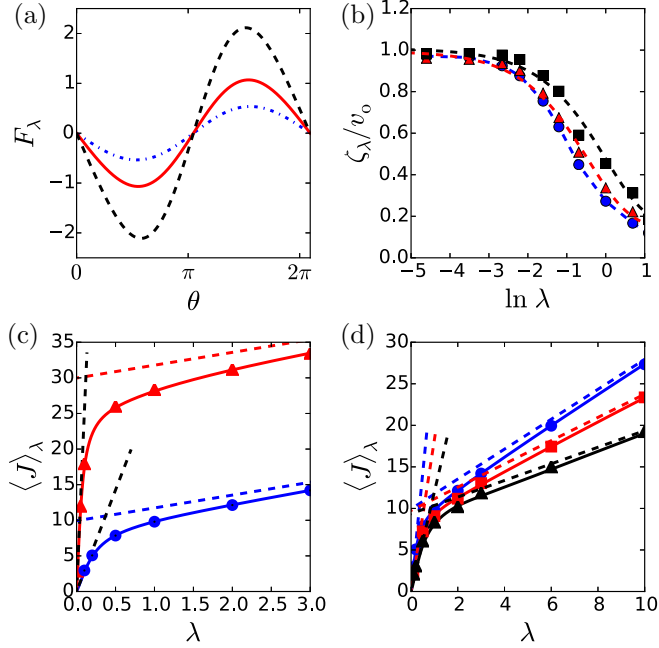


FIG. 2. Analysis of the auxiliary process. (a) The effective forces for $v_0 = 10$, $\rho = 0.1$ and $\lambda = 0.1$ (dashed dotted blue), 0.3 (solid red), and 0.5 (dashed black). (b) Damping coefficient, ζ_λ , as a function of λ for $v_0 = 10$ and $\rho = 0.1$ (blue circles), 0.3 (red triangles), and 0.5 (black squares). Dashed lines are a guide to the eye. (c),(d) The average current from the auxiliary process. (c) $\langle J \rangle_\lambda$ for $\rho = 0.1$ and $v_0 = 10$ (blue circles) and 30 (red triangles). (d) $\langle J \rangle_\lambda$ for $v_0 = 10$, and $\rho = 0.1$ (blue circles), 0.3 (red squares), and 0.5 (black triangles). The symbols are the results from simulations. The solid lines represent the derivative of the CGF and the dotted lines represent its limiting behavior.

using the generalized variational principle of Ref. [66], as direct evaluation of $g_\lambda(r, \phi)$ is exponentially difficult. From the result in Eq. (15), we could easily generalize to two-dimensional bias by adding one additional term of $2D_t(\rho)\lambda\hat{y}$.

Within the auxiliary process, rare large currents result from the effective force that confines the orientation of the active particle to a given direction. This is shown in Fig. 2(a), where the force has stable points at $\theta = 0$ and π , depending on the sign of λ , with an amplitude that grows with increasing λ [63]. Additionally, the effective drag from the surrounding particles is reduced with increasing magnitude of λ . Shown in Fig. 2(b) is $\zeta_\lambda(\rho)$ computed from the molecular simulations for a variety of densities. From inversion symmetry, $\zeta_\lambda(\rho)$ is an even function about $\lambda = 0$, and we find for small values of $|\lambda|$, it decreases quadratically. In the large $|\lambda|$ limit, we find that $\zeta_\lambda(\rho)$ decreases exponentially to 0, resulting in effectively free particle evolution. This decrease reflects the reduced probability of particle collisions in the direction of the bias and the onset of hyperuniformity [67,68].

Derivatives of $\psi(\lambda)$ provide the cumulants of J , $d^n \psi(\lambda)/d\lambda^n = C_\lambda^n$, with the first, $C_\lambda^1 = \langle J \rangle_\lambda$, yielding the average current, and the second, $C_\lambda^2 = t \langle (J - \langle J \rangle_\lambda)^2 \rangle_\lambda$, its variance. When evaluated at $\lambda = 0$, these are cumulants of the original model, but for $\lambda \neq 0$, these report on rare fluctuations into the tails of $I(J)$. Shown in Figs. 2(c) and 2(d), are the average currents computed at finite λ , from the exact solution

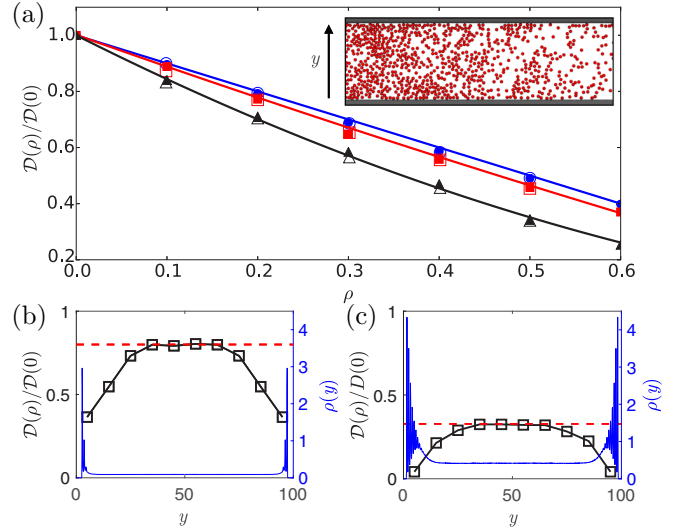


FIG. 3. (a) Density-dependent effective diffusion constant for $v_0 = 0$ (blue circles), 1 (red squares), and 60 (black triangles). The symbols are the results from simulations. The filled shapes are from the mean-squared displacement, open shapes are from an imposed density gradient, and the solid lines from Eq. (18). The inset shows a snapshot of the simulation with an imposed density gradient and bulk density of $\rho = 0.2$. The density and diffusion profiles along the width of the channel for (b) $v_0 = 60$ $\rho = 0.1$ and (c) $v_0 = 60$ $\rho = 0.5$. The dashed red lines are the predicted values.

of the eigenvalue equation and from evaluating Eq. (4) directly from simulations of the auxiliary process defined in Eqs. (15) and (16). For small λ , the current increases linearly from 0 with a slope set by variance at $\lambda = 0$, as is expected from linear response. For large λ , the system exhibits nonlinear response, manifesting the non-Gaussian current fluctuations. In this limit, the slope decreases dramatically. The asymptotic limit of this secondary response is given by an offset of v_0 and slope that depends only on the $D_t(\rho)$. The origin of this dependence is clear from the auxiliary process. For large $|\lambda|$, $V_\lambda(\rho) \rightarrow v_0$, and the force on the orientation suppresses angular fluctuations. An analysis of this limit provides an asymptotic form for $\psi(\lambda)$,

$$\psi(\lambda) = D_t(\rho)\lambda^2 \pm v_0\lambda, \quad \lambda \rightarrow \pm\infty, \quad (17)$$

which shows that the tails of the $I(J)$ are given by an effective Gaussian with mean, v_0 , a much smaller variance than at $\lambda = 0$. We note a simple effective temperature mapping between Brownian particles and ABPs would not explain the observed non-Gaussian fluctuations or concomitant secondary response [69–72]. Further, this qualitative behavior of two different effective diffusion constants for small and large fluctuations has been observed recently in active biopolymers [73,74].

We conclude with a discussion of the second cumulant,

$$C_0^2(\rho) = 2D_t(\rho) + \frac{V_0^2(\rho)}{D_r} \equiv 2\mathcal{D}(\rho), \quad (18)$$

that we define as twice a collective diffusion constant, $\mathcal{D}(\rho)$. In Fig. 3, numerical results obtained from simulations of the mean-squared displacement divided by a diffusive observation

time are plotted in excellent agreement with predictions from Eq. (18). This form of the diffusion coefficient has been shown to agree with simulations previously, and was derived by a moment expansion of the joint position and orientation distribution [22,75–77]. This density dependence of $\mathcal{D}(\rho)$ was shown by others [57,58,78] to correctly predict the spinodal instability signaling the onset of motility-induced phase separation [61].

The current fluctuations encoded by $\mathcal{D}(\rho)$ provide the response of a hydrodynamic current, J_ρ , generated from a slowly varying spatial density, $\rho(x)$. From the Kramers Moyal expansion [79], J_ρ can be generally expressed as a gradient expansion

$$J_\rho = - \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \partial_x^{n-1} M^n[\rho(x)] \rho(x), \quad (19)$$

where $M^n[\rho(x)]$ is the local density-dependent n th moment of the current, $\langle (J - \langle J \rangle)^n \rangle$. To first order, the mass current is linear in the density gradient and is given by Fick's law, $J_\rho \approx -\mathcal{D}(\rho)(\partial\rho/\partial x)$, where $\mathcal{D}(\rho)$ is the proportionality constant relating the current to the gradient resulting from identifying the second moment with the second cumulant. For small average currents we have $\langle J \rangle_\lambda \approx 2\mathcal{D}(\rho)\lambda$, which shows that at linear response, λ can be related to an affinity for this nonequilibrium system. We have computed $\mathcal{D}(\rho)$ from $-J_\rho/(\partial\rho/\partial x)$ by simulating an open channel in contact with two reservoirs. As shown in Fig. 3(a), we find good agreement with $\mathcal{D}(\rho)$ computed in this way and from $\psi(\lambda)$.

The presence of the walls results in a nonuniform density distribution in the direction orthogonal from the walls, with decay lengths that increase with ρ and v_0 as found previously [41,49,80–84]. We simulate channels that are wide enough to be bulklike in the center of the channel. A boundary layer that results from the particle accumulation at the wall has a reduced local diffusion constant parallel to the walls. This is due to the increased density and the correlation of the self-propulsion vector and the normal force of the wall. Figures 3(b) and 3(c) show two representative diffusivity and density profiles at large v_0 and small and large ρ . The range over which the diffusion constant reaches its bulk plateau

value determines the effective width of the channel for computing the response due to the density gradient. Additional simulation details and discussion of the density layering near the walls can be found in the Supplemental Material [61].

From $\psi(\lambda)$, we have access to all moments of J , and together with its ρ dependence this framework allows us to quantify higher order responses [61] that are not naturally considered in standard field-theoretic treatments of ABPs [57–59,70,75]. While our focus has been on ABPs, the framework we have presented is general and allows for the quantification of current fluctuations, and the calculation of transport coefficients for continuous interacting systems. For ABPs, we found that large current fluctuations near the mean are not representative of rarer fluctuations which are restricted as a result of coherent active movement. These specific results are consistent with deviations from Gaussian behavior that have been reported in recent experimental studies of active colloids [85,86]. Furthermore, our results may explain the center-of-mass motion of cellular biopolymers that exhibit two types of transport characterized by two different diffusion constants for small and large fluctuations [73,74].

While other types of active matter such as active rods, biopolymers, and bacteria behave like ABPs in specific limits, each also adds complexities not accounted for in our present treatment. These include additional interactions like those due to preferential alignment or hydrodynamics, and internal degrees of freedom [40,80–86]. Developing many-body closures appropriate for these contexts can take inspiration from previous work on molecular fluids like the reference interaction site model [87] and polymer reference interaction site model equations [88], and is an interesting direction for further study. Finally, while we have focused on current fluctuations, our development of the weighted many-body expansion provides a way to calculate the LDFs of other relevant quantities for nonequilibrium systems such as activity [56,68,89–92], entropy production [93–96], and density [76,97] that are currently difficult to estimate.

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- [1] T. Speck and U. Seifert, *Europhys. Lett.* **74**, 391 (2006).
 [2] J. Prost, J.-F. Joanny, and J. M. Parrondo, *Phys. Rev. Lett.* **103**, 090601 (2009).
 [3] M. Baiesi, C. Maes, and B. Wynants, *Phys. Rev. Lett.* **103**, 010602 (2009).
 [4] U. Seifert and T. Speck, *Europhys. Lett.* **89**, 10007 (2010).
 [5] R. Chetrite and S. Gupta, *J. Stat. Phys.* **143**, 543 (2011).
 [6] M. Baiesi and C. Maes, *New J. Phys.* **15**, 013004 (2013).
 [7] C. Maes, *J. Stat. Phys.* **154**, 705 (2014).
 [8] D. J. Evans and D. J. Searles, *Phys. Rev. E* **50**, 1645 (1994).
 [9] J. Kurchan, *J. Phys. A: Math. General* **31**, 3719 (1998).
 [10] G. E. Crooks, *Phys. Rev. E* **60**, 2721 (1999).
 [11] U. Seifert, *Phys. Rev. Lett.* **95**, 040602 (2005).
 [12] C. Jarzynski, *Phys. Rev. Lett.* **78**, 2690 (1997).
 [13] G. Gallavotti and E. G. D. Cohen, *Phys. Rev. Lett.* **74**, 2694 (1995).
 [14] A. C. Barato and U. Seifert, *Phys. Rev. Lett.* **114**, 158101 (2015).
 [15] T. R. Gingrich, J. M. Horowitz, N. Perunov, and J. L. England, *Phys. Rev. Lett.* **116**, 120601 (2016).
 [16] M. Polettoni, A. Lazarescu, and M. Esposito, *Phys. Rev. E* **94**, 052104 (2016).
 [17] R. Chetrite and H. Touchette, *Ann. Henri Poincaré* **16**, 2005 (2015).
 [18] J. L. Lebowitz and H. Spohn, *J. Stat. Phys.* **95**, 333 (1999).

- [19] T. Speck, *Phys. Rev. E* **94**, 022131 (2016).
- [20] C. Y. Gao and D. T. Limmer, *Entropy* **19**, 571 (2017).
- [21] P. Gaspard and R. Kapral, *J. Chem. Phys.* **147**, 211101 (2017).
- [22] M. E. Cates and J. Tailleur, *Ann. Rev. Condens. Matter Phys.* **6**, 219 (2015).
- [23] G. S. Redner, M. F. Hagan, and A. Baskaran, *Phys. Rev. Lett.* **110**, 055701 (2013).
- [24] V. Schaller, C. Weber, C. Semmrich, E. Frey, and A. R. Bausch, *Nature (London)* **467**, 73 (2010).
- [25] Y. Sumino, K. H. Nagai, Y. Shitaka, D. Tanaka, K. Yoshikawa, H. Chaté, and K. Oiwa, *Nature (London)* **483**, 448 (2012).
- [26] V. Schaller, C. A. Weber, B. Hammerich, E. Frey, and A. R. Bausch, *Proc. Natl. Acad. Sci. USA* **108**, 19183 (2011).
- [27] H. C. Berg and D. A. Brown, *Nature (London)* **239**, 500 (1972).
- [28] J. A. Shapiro, *BioEssays* **17**, 597 (1995).
- [29] C. Dombrowski, L. Cisneros, S. Chatkaew, R. E. Goldstein, and J. O. Kessler, *Phys. Rev. Lett.* **93**, 098103 (2004).
- [30] J. Hill, O. Kalkanci, J. L. McMurry, and H. Koser, *Phys. Rev. Lett.* **98**, 068101 (2007).
- [31] E. Lauga, W. R. DiLuzio, G. M. Whitesides, and H. A. Stone, *Biophys. J.* **90**, 400 (2006).
- [32] X. Fu, L. H. Tang, C. Liu, J. D. Huang, T. Hwa, and P. Lenz, *Phys. Rev. Lett.* **108**, 198102 (2012).
- [33] M. R. Parsek and E. P. Greenberg, *Trends Microbiol.* **13**, 27 (2005).
- [34] J. Palacci, S. Sacanna, A. P. Steinberg, D. J. Pine, and P. M. Chaikin, *Science* **339**, 936 (2013).
- [35] V. Narayan, N. Menon, and S. Ramaswamy, *J. Stat. Mech.* (2006) P01005.
- [36] J. R. Howse, R. A. Jones, A. J. Ryan, T. Gough, R. Vafabakhsh, and R. Golestanian, *Phys. Rev. Lett.* **99**, 048102 (2007).
- [37] A. Walther and A. H. E. Müller, *Soft Matter* **4**, 663 (2008).
- [38] A. Bricard, J. B. Caussin, N. Desreumaux, O. Dauchot, and D. Bartolo, *Nature (London)* **503**, 95 (2013).
- [39] C. Bechinger, R. Di Leonardo, H. Löwen, C. Reichhardt, G. Volpe, and G. Volpe, *Rev. Mod. Phys.* **88**, 045006 (2016).
- [40] I. Buttinoni, J. Bialké, F. Kümmel, H. Löwen, C. Bechinger, and T. Speck, *Phys. Rev. Lett.* **110**, 238301 (2013).
- [41] J. Elgeti, R. G. Winkler, and G. Gompper, *Rep. Prog. Phys.* **78**, 056601 (2015).
- [42] Y. Yang, V. Marceau, and G. Gompper, *Phys. Rev. E* **82**, 031904 (2010).
- [43] F. Peruani, *Eur. Phys. J. Special Topics* **225**, 2301 (2016).
- [44] F. Ginelli, F. Peruani, M. Bär, and H. Chaté, *Phys. Rev. Lett.* **104**, 184502 (2010).
- [45] M. Abkenar, K. Marx, T. Auth, and G. Gompper, *Phys. Rev. E* **88**, 062314 (2013).
- [46] F. Peruani, J. Staruß, V. Jakovljevic, L. Søgaard-Andersen, A. Deutsch, and M. Bär, *Phys. Rev. Lett.* **108**, 098102 (2012).
- [47] C. W. Harvey, M. Alber, L. S. Tsimring, and I. S. Aranson, *New J. Phys.* **15**, 035029 (2013).
- [48] R. Chelakkot, A. Gopinath, L. Mahadevan, and M. F. Hagan, *J. R. Soc. Interface* **11**, 20130884 (2014).
- [49] C. G. Wagner, M. F. Hagan, and A. Baskaran, *J. Stat. Mech.* (2017) 43203.
- [50] J. D. Weeks, D. Chandler, and H. C. Andersen, *J. Chem. Phys.* **54**, 5237 (1971).
- [51] A. C. Brañka and D. M. Heyes, *Phys. Rev. E* **60**, 2381 (1999).
- [52] R. Chetrite and H. Touchette, *Phys. Rev. Lett.* **111**, 120601 (2013).
- [53] J. P. Garrahan and I. Lesanovsky, *Phys. Rev. Lett.* **104**, 160601 (2010).
- [54] J. P. Hansen and I. R. McDonald, *Theory of Simple Liquids* (Elsevier, New York, 1977).
- [55] C. Appert-Rolland, B. Derrida, V. Lecomte, and F. Van Wijland, *Phys. Rev. E* **78**, 021122 (2008).
- [56] L. O. Hedges, R. L. Jack, J. P. Garrahan, and D. Chandler, *Science* **323**, 1309 (2009).
- [57] T. Speck, A. M. Menzel, J. Bialké, and H. Löwen, *J. Chem. Phys.* **142**, 224109 (2015).
- [58] J. Bialké, H. Löwen, and T. Speck, *EuroPhys. Lett.* **103**, 30008 (2013).
- [59] B. Hancock and A. Baskaran, *J. Stat. Mech.* (2017) 033205.
- [60] R. Wittkowski, J. Stenhammar, and M. E. Cates, *New J. Phys.* **19**, 105003 (2017).
- [61] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevE.98.060601> for details of the simulations.
- [62] M. Abramowitz, I. A. Stegun, and D. Miller, *J. Appl. Mech.* **32**, 239 (1965).
- [63] P. Pietzonka, K. Kleinbeck, and U. Seifert, *New J. Phys.* **18**, 052001 (2016).
- [64] V. Lecomte and J. Tailleur, *J. Stat. Mech.* (2007) P03004.
- [65] C. Giardinà, J. Kurchan, and L. Peliti, *Phys. Rev. Lett.* **96**, 120603 (2006).
- [66] U. Ray, G. K. Chan, and D. T. Limmer, *Phys. Rev. Lett.* **120**, 210602 (2018).
- [67] S. Torquato and F. H. Stillinger, *Phys. Rev. E* **68**, 041113 (2003).
- [68] R. L. Jack, I. R. Thompson, and P. Sollich, *Phys. Rev. Lett.* **114**, 060601 (2015).
- [69] S. Steffenoni, G. Falasco, and K. Kroy, *Phys. Rev. E* **95**, 052142 (2017).
- [70] A. P. Solon, J. Stenhammar, R. Wittkowski, M. Kardar, Y. Kafri, M. E. Cates, and J. Tailleur, *Phys. Rev. Lett.* **114**, 1 (2015).
- [71] S. C. Takatori and J. F. Brady, *Soft Matter* **11**, 7920 (2015).
- [72] J. Palacci, C. Cottin-Bizonne, C. Ybert, and L. Bocquet, *Phys. Rev. Lett.* **105**, 088304 (2010).
- [73] B. Wang, J. Kuo, S. C. Bae, and S. Granick, *Nat. Mater.* **11**, 481 (2012).
- [74] B. Stuhmann, M. Soares E Silva, M. Depken, F. C. MacKintosh, and G. H. Koenderink, *Phys. Rev. E* **86**, 020901(R) (2012).
- [75] J. Stenhammar, D. Marenduzzo, R. J. Allen, and M. E. Cates, *Soft Matter* **10**, 1489 (2014).
- [76] S. Chakraborti, S. Mishra, and P. Pradhan, *Phys. Rev. E* **93**, 052606 (2016).
- [77] Y. Fily and M. C. Marchetti, *Phys. Rev. Lett.* **108**, 235702 (2012).
- [78] A. P. Solon, M. E. Cates, and J. Tailleur, *Eur. Phys. J.* **224**, 1231 (2015).
- [79] H. Risken, *The Fokker-Planck Equation* (Springer, Berlin, Heidelberg, 1996), pp. 63–95.
- [80] G. Li and J. X. Tang, *Phys. Rev. Lett.* **103**, 078101 (2009).
- [81] J. Elgeti and G. Gompper, *Eur. Phys. Lett.* **101**, 48003 (2013).
- [82] Y. Fily, S. Henkes, and M. C. Marchetti, *Soft Matter* **10**, 2132 (2014).
- [83] X. Yang, M. L. Manning, and M. C. Marchetti, *Soft Matter* **10**, 6477 (2014).

- [84] J. Elgeti and G. Gompper, *Eur. Phys. Lett.* **109**, 58003 (2015).
- [85] X. Zheng, B. Ten Hagen, A. Kaiser, M. Wu, H. Cui, Z. Silber-Li, and H. Löwen, *Phys. Rev. E* **88**, 032304 (2013).
- [86] C.-W. Io, T.-Y. Chen, J.-W. Yeh, and S.-C. Cai, *Phys. Rev. E* **96**, 062601 (2017).
- [87] D. Chandler and H. C. Andersen, *J. Chem. Phys.* **57**, 1918 (1972).
- [88] J. G. Curro and K. S. Schweizer, *J. Chem. Phys.* **87**, 1842 (1987).
- [89] S. Whitlam, K. Klymko, and D. Mandal, *J. Chem. Phys.* **148**, 154902 (2018).
- [90] E. Pitard, V. Lecomte, and F. Van Wijland, *Eur. Phys. Lett.* **96**, 56002 (2011).
- [91] J. P. Garrahan, R. L. Jack, V. Lecomte, E. Pitard, K. Van Duijvendijk, and F. Van Wijland, *Phys. Rev. Lett.* **98**, 195702 (2007).
- [92] S. Katira, J. P. Garrahan, and K. K. Mandadapu, *Phys. Rev. Lett.* **120**, 260602 (2018).
- [93] D. Mandal, K. Klymko, and M. R. DeWeese, *Phys. Rev. Lett.* **119**, 258001 (2017).
- [94] E. Fodor, C. Nardini, M. E. Cates, J. Tailleur, P. Visco, and F. Van Wijland, *Phys. Rev. Lett.* **117**, 038103 (2016).
- [95] J. Mehl, T. Speck, and U. Seifert, *Phys. Rev. E* **78**, 011123 (2008).
- [96] T. Speck, A. Engel, and U. Seifert, *J. Stat. Mech.* (2012) P12001.
- [97] B. Derrida, J. L. Lebowitz, and E. R. Speer, *Phys. Rev. Lett.* **87**, 150601 (2001).