Critical Asymmetry for Giant Diffusion of Active Brownian Particles

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We study the effect of an asymmetry on the transport properties of an active Brownian particle. We demonstrate the existence of a critical force or, more generally, of a critical asymmetry that separates parameter regimes of giant diffusion from those with reliable directed transport. We derive a condition for the critical asymmetry by means of an exact expression for the diffusion coefficient and by a simplified discrete picture. A critical asymmetry, as predicted by the simple model, is also found in a detailed model of coupled molecular motors displaying bidirectional motion.

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Self-propelled motion is one of the key features of life appearing on levels ranging from flocks of animals to single cell motility and intracellular transport by molecular motors [1]. One class of phenomenological motility models comprises active Brownian particles (ABP) that can describe non-Maxwellian velocity distributions [2], swarming behavior [3], and other phenomena [4].

Already the active Brownian motion in one dimension has remarkable stochastic features and is relevant for the dynamics of coupled molecular motors that walk on filaments like microtubuli carrying out various tasks in the cell. One striking collective effect arising in assemblies of coupled motors is the bidirectionality of motion [5] that can be qualitatively captured by ABP models [6] (bidirectionality can also arise from the interaction of several types of motors, e.g. [7,8]). Mean drift and effective diffusion around this drift are the most important characteristics of such motor assemblies and determine their respective function in the cell. As we show in this Letter, important conclusions about the diffusive behavior of coupled molecular motors can be drawn from the much simpler ABP dynamics.

An ABP obeys the nonlinear Langevin equation

$$\dot{x} = v, \qquad \dot{v} = f(v) + g(v)\xi(t), \tag{1}$$

where $\xi(t)$ is Gaussian white noise with $\langle \xi(t)\xi(t')\rangle = 2Q\delta(t-t')$ (Q sets the overall noise intensity). Essential for an ABP is an anomalous force-velocity relation with a region of negative friction at small speed $|v|$ ($f(v)/v > 0$). Generally, an active particle obeying Eq. (1) possesses a mean velocity $\langle v\rangle = \lim_{t\to\infty}\langle x(t) - x(0)\rangle/t$ and undergoes a diffusive spread around this mean motion which is characterized by an effective diffusion coefficient $D_{\mathrm{eff}} = \lim_{t\to\infty}[\langle x^2(t)\rangle - \langle x(t)\rangle^2]/(2t)$. In previous studies [4,9,10] the diffusive dynamics of ABPs has been mainly considered for symmetric functions $f_{\mathrm{odd}}(v)$, $g_{\mathrm{even}}(v)$ under which the ABP performs pure diffusion with $\langle v\rangle = 0$. Under the above conditions, the velocity dynamics then formally corresponds to an overdamped Brownian motion $v(t)$ subject to a potential force $-dU_{\mathrm{even}}(v)/dv = f_{\mathrm{odd}}(v)/g^2_{\mathrm{even}}(v)$ where the potential is bistable and symmetric as illustrated in Fig. 1(a) (dotted line). This symmetric bistability implies a bidirectional motion [see, e.g., dotted line in Fig. 1(b)] at weak noise and a divergence of the ABP's diffusion coefficient in the limit of vanishing noise [9,10].

In this letter, we study the effect of an asymmetry on the ABP's diffusion in one spatial dimension. For the case of a bias force breaking the symmetry, we show that the divergence of the diffusion coefficient for vanishing noise is removed if the bias F is beyond a critical value $|F| > |F_{\mathrm{crit}}|$. This value separates asymmetry parameters which yield giant diffusion from those which yield a reliable transport of ABPs. A criterion for F_{crit} can be found in terms of the effective velocity potential or in terms of the local extrema of the steady-state velocity histogram. We furthermore demonstrate by extensive simulations that the very same effect predicted by our theory occurs also in a detailed model of coupled molecular motors.

Theory.—The first nontrivial feature of an asymmetric system is a finite mean velocity [this drift can be seen in Fig. 1(b), solid line] which can be calculated by standard methods. Interpreting here and in the following Eq. (1) in the sense of Ito, one can calculate from the corresponding Fokker-Planck equation the steady-state density and from the latter the stationary mean value

$$P_0(v) = \frac{e^{-U(v)/Q}/g^2(v)}{\int_{-\infty}^{\infty} d\tilde{v}\, e^{-U(\tilde{v})/Q}/g^2(\tilde{v})}, \qquad \langle v\rangle = \int_{-\infty}^{\infty} dv P(v) v. \tag{2}$$

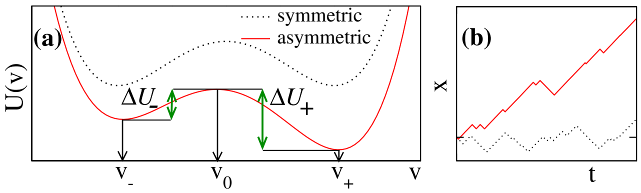

FIG. 1 (color online). The velocity potential (a) and sample trajectories (b) of an ABP in the symmetric (dotted) and in the asymmetric case (solid, $F = 0.085$), respectively. In (b): simulations of Eq. (5) with $Q = 0.05$, $F = 0$ (dotted) and $F = 0.02$ (solid).

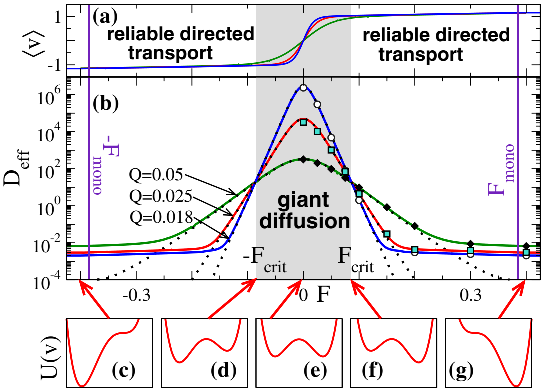

FIG. 2 (color online). Transport properties of active Brownian particles with an asymmetry. Mean velocity (a) and diffusion coefficient (b) vs bias for different noise levels Q. Exact result Eq. (4) compared to numerical simulations of Eq. (5) (symbols) and to the two-state theory Eq. (6) (dotted lines). Forces within the shaded region ($F \in (-F_{\mathrm{crit}}, F_{\mathrm{crit}})$ with $F_{\mathrm{crit}} \approx 0.0852$) lead to giant diffusion in the weak noise limit; outside this window, reliable transport is observed. Panels (c)–(g) show the velocity potentials at the forces as indicated.

The diffusion coefficient can be found from the integral of the velocity autocorrelation function

$$D_{\mathrm{eff}} = \int_0^\infty d\tau \langle v(t) v(t+\tau)\rangle = \langle \Delta v^2 \rangle \tau_{\mathrm{corr}}, \tag{3}$$

which can be written as the product of the velocity's variance $\langle \Delta v^2 \rangle$ and its correlation time τ_{corr}. The latter can be calculated in terms of quadratures [11], yielding the following exact expression for the diffusion coefficient:

$$D_{\mathrm{eff}} = \frac{\int_{-\infty}^{\infty} dx e^{U(x)/Q} [\int_{-\infty}^{x} dy \frac{y - \langle v \rangle}{g^2(y)} e^{-U(y)/Q}]^2}{Q \int_{-\infty}^{\infty} dv e^{-U(v)/Q} / g^2(v)}. \tag{4}$$

For a symmetric setup this reduces to the result in [10].

Diffusion of an active Brownian particle.—In the following we are particularly interested in the behavior at small-noise intensity Q. It is instructive to discuss the main physics of the asymmetric system for a simple example with additive noise ($g(v) \equiv 1$) and a cubic function $f(v) = v - v^3 + F$ where the asymmetry is introduced by a bias F. This can be written as

$$\dot{x} = v, \qquad \dot{v} = -dU(v)/dv + \xi(t) \tag{5}$$

in terms of a biased velocity potential $U(v) = v^4/4 - v^2/2 - Fv$ shown in Fig. 1(a) (solid line). This bistable potential displays two force-dependent minima at v_- and v_+ separated by a maximum at v_0 with associated barriers $\Delta U_\pm = U(v_0) - U(v_\pm)$. Note that the system is symmetric under inversion of x, v, and F from which we conclude that $\langle v(F) \rangle = -\langle v(-F) \rangle$ and $D_{\mathrm{eff}}(F) = D_{\mathrm{eff}}(-F)$.

At low noise ($Q \ll \Delta U_\pm$), the mean velocity [Fig. 2(a)] corresponds roughly to the location of the deeper potential minimum determined by the bias F. Around zero force there is a jump in $\langle v \rangle$; at finite force, the velocity varies smoothly with F. The diffusion coefficient displays a more surprising dependence on the force. Our numerical evaluation of the quadrature result Eq. (4) as well as extensive simulations of Eq. (5) shown in Fig. 2(b) reveal a critical value of the force that separates values of F with different small-noise behavior. For $|F| < F_{\mathrm{crit}}$ (shaded region in Fig. 2), the diffusion coefficient diverges for $Q \to 0$; for F outside this range, the diffusion decreases to zero as $D_{\mathrm{eff}} \propto Q$. We may distinguish the two cases as those of incoherent (strongly diffusive) and coherent (reliable directed) transport. Note that for $F = F_{\mathrm{crit}}$, the diffusion coefficient attains a moderate value which does not change for $Q \to 0$.

A criterion for the critical asymmetry.—One might be tempted to think that the critical force F_{crit} equals F_{mono} [vertical lines in Fig. 2(b)] at which the potential becomes monostable. However, the value of the critical force is much smaller than this value, i.e. $F_{\mathrm{crit}} < F_{\mathrm{mono}}$.

The origin of the critical force becomes clear by considering separately the two factors $\langle \Delta v^2 \rangle$ and τ_{corr} in Eq. (3). For $Q \ll \Delta U_\pm$, we use a simple two-state theory in which the velocity performs transitions between two discrete states [12], specifically, from $v_\pm$ to $v_\mp$ with Kramers rates $r_\pm = \omega_\pm |\omega_0| / (2\pi) \exp[-\Delta U_\pm / Q]$ ($\omega_{\pm,0}^2$ is the curvature of the potential at $v_{\pm,0}$). The variance in this approximation is $\langle \Delta v^2 \rangle = (v_+ - v_-)^2 r_+ r_- / (r_+ + r_-)^2$ and approaches zero for $Q \to 0$ if $F \neq 0$. On the contrary, the correlation time $\tau_{\mathrm{corr}} = 1/(r_- + r_+)$ diverges in the same limit. In the regime of giant diffusion, the diverging correlation prevails whereas for $|F| > |F_{\mathrm{crit}}|$ the vanishing variance dominates. Right at the critical value F_{crit}, the two factors balance such that the product remains finite for $Q \to 0$. Specifically, we find

$$D_{\mathrm{eff}} \approx \frac{2\pi (v_+ - v_-) \omega_+ \omega_- / |\omega_0|}{[\omega_- e^{-(2\Delta U_- - \Delta U_+)/(3Q)} + \omega_+ e^{-(2\Delta U_+ - \Delta U_-)/(3Q)}]^3}, \tag{6}$$

which can be also achieved by a saddle point approximation of the exact result Eq. (4). The approximation agrees well with Eq. (4) for small to moderate forces [see dotted lines in Fig. 2(b)] and, in particular, at the critical force. Moreover, Eq. (6) provides us with a simple criterion for the critical force in terms of the two potential barriers $\Delta U_\pm$: the higher barrier is just twice the smaller barrier

$$\Delta U_+(F_{\mathrm{crit}}) = 2\Delta U_-(F_{\mathrm{crit}}). \tag{7}$$

This general condition does not change for a system with multiplicative noise and a more general kind of asymmetry as long as the effective potential is bistable and the asymmetry controls the height of the potential barriers.

The relation for the critical asymmetry has a remarkable consequence for the stationary probability density $P(v)$ of the velocity. For weak noise and $F > 0$, this density shows two maxima of different height ($P(v_+) > P(v_-)$) and a minimum $P(v_0)$ in between. If we consider the following ratio of these extrema

$$R_P(F, Q) = P(v_0)P(v_+)/P^2(v_-) \qquad (8)$$

and use the steady-state density in Eq. (2) and the condition Eq. (7), we find at the critical asymmetry $R_P(F_{\mathrm{crit}}, Q) = g^2(v_0)g^2(v_+)/g^4(v_-)$; i.e., the ratio is independent of the noise intensity Q.

Giant diffusion has been also reported for the passive Brownian motion in a spatially periodic potential biased with a threshold force [13]. Studies of this system revealed a maximum of D_{eff} vs bias force and discussed the dependence of the threshold force on damping and the scaling of the maximal diffusion with noise intensity. For the ABP dynamics studied here, the threshold force is simply at zero ($F = 0$) and the maximal diffusion scales exponentially with the inverse noise intensity [9,10]. Our main point here is not the presence of this maximum but the existence of a finite window of forces [determined by Eq. (7)] which lead to giant diffusion of ABPs. Whether a similar window exists for passive particles in a biased periodic potential is an interesting but open question.

Diffusion of coupled molecular motors.—An ABP model like Eq. (5) was suggested in [6] as a simplified description of more detailed models of coupled molecular motors in the limit of large but finite number of motors. For motor assemblies, the dominance of either diffusion or drift may determine their biological function in the cell. Hence, it is an important question whether the critical asymmetry observed above is also present in biophysically detailed models of coupled molecular motors. To answer this question, we consider in the following the model by Badoual *et al.* [6] which captures many features of experimental data from motility assays [5] (for other models of coupled Brownian motors see [14]).

In the model (see Fig. 3), N molecular motors are rigidly attached equidistantly with spacing q to a backbone. The overdamped dynamics of the backbone reads

$$\lambda \dot{x} = F - \sum_{i=1}^{N} (\sigma_i(t)/N) W'_{\sigma_i}(x_i) + \sqrt{k_B T \lambda / N}\,\eta(t), \qquad (9)$$

where λ and F are the friction coefficient and external force per motor. The backbone is subject to three forces:

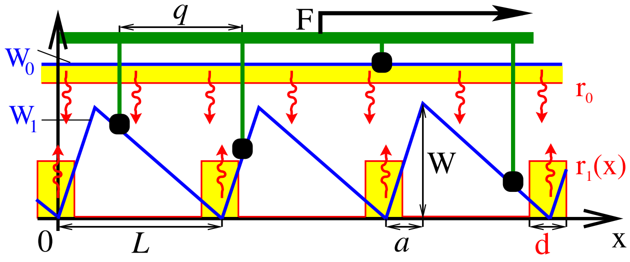

FIG. 3 (color online). Coupled molecular motors. Following Ref. [6] and working in nondimensional units, we use a rate $r_1(x)$ which is $r_1 = 500$ in a region of width $d = 0.2$ centered at the potential minima, otherwise $r_1(x) = 0$. The rate $r_0 = 40$ is spatially independent. Other parameters: $W = 1$, $L = 1$, $\lambda = 0.01$, simulation time step $\Delta t = 10^{-3}$; q is incommensurate with L.

(i) an external bias F; (ii) forces exerted by the filament onto the single motors; (iii) thermal fluctuations $\eta(t)$ (for simplicity, we set $T = 0$). Noise is introduced by independent switching of the motors between different conformational states in which the motor either interacts with the filament [for $\sigma_i(t) = 1$] or does not [for $\sigma_i(t) = 0$]. The interaction is given by a periodic and asymmetric (a so-called ratchet) potential with period L and asymmetry parameter a (the symmetric case corresponds to $a = L/2$). Switchings from $\sigma_i(t) = 1 \rightarrow 0$ occur with a space-dependent switching rate $r_1(x + iq)$ only close to the minima of the potential; the reverse rate r_0 is spatially homogeneous. For large N and the proper choice of a and F, the backbone displays bidirectional motion and, consequently, the velocity histogram becomes bimodal. The stochastic period for which the assembly keeps one direction depends exponentially on the number of motors. Most importantly in the following, the overall noise intensity introduced by the independent switchings of the motors scales like $Q \propto 1/N$ [6].

Velocity and diffusion coefficient of the backbone for a symmetric spatial potential $W_1(x)$ with $a = L/2$ are shown in Figs. 4(a) and 4(b), respectively. Both measures display the same features as observed for the ABP diffusion above:

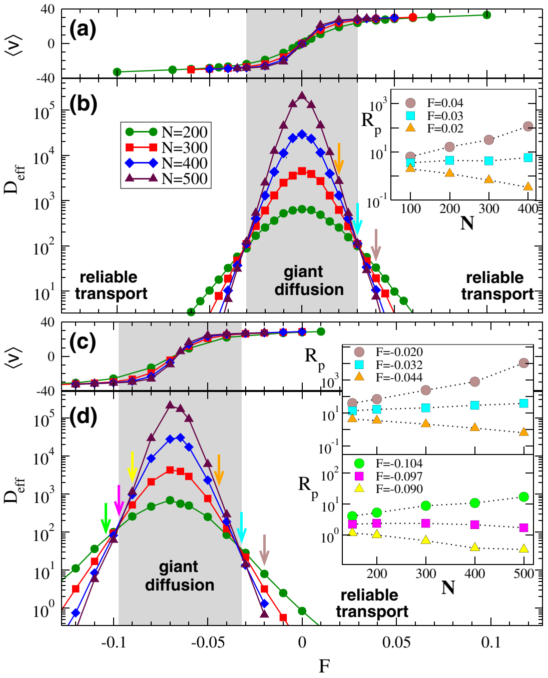

FIG. 4 (color online). Transport properties of an assembly of molecular motors. Mean velocity (a) and diffusion coefficient (b) for a symmetric spatial potential ($a = L/2$) vs external force for different numbers of motors as indicated. The inset shows the ratio R_P Eq. (8) vs the number of motors for three values of F indicated by arrows in (b). Panels (c) and (d) show the mean velocity and effective diffusion coefficient for an asymmetric potential ($a = 0.4L$); note that the range of forces has shifted to negative values. Insets in (d): ratios R_P measured at six values of the force close to the critical values.

between two critical values of the force $-F_{\rm crit} < F < F_{\rm crit}$ the diffusion increases by orders of magnitude upon an increase of the motor number N (corresponding to a decrease of the effective noise intensity $Q \propto 1/N$). Beyond this critical range, diffusion is reduced to small values. The critical force is not noticed in the curves for the velocity which varies smoothly with F. If the ratchet potential is asymmetric [$a = 0.4L$, see Figs. 4(c) and 4(d)], the backbone moves at zero external force reliably (with low diffusion) into its preferred direction (determined by the ratchet mechanism). Biasing the dynamics against this direction ($F < 0$) we observe, however, again a critical range at negative forces where the diffusion coefficient increases rapidly upon increase of the number of motors. Outside this range reliable transport is obtained as in the symmetric case at large bias force. Note that the critical values of the force as well as the diffusion coefficient at these two values now differ. This is also expected in general for an ABP with asymmetric functions $f(v)$ and $g(v)$.

We have further verified that the stochastic mechanism already seen in the ABP model underlies the critical values of the force or, more generally, the combined asymmetry resulting from the choices of a and F. Above, below, and close to the critical asymmetry we have numerically determined the velocity histograms for different values of N, extracted their local extrema, and computed the ratio R_P defined in Eq. (8). If our picture of the mechanism at work is correct, the ratio R_P should be flat as a function of N only if the system is poised at the critical asymmetry. Indeed, in agreement with this prediction, only under the latter condition the dependence of R_P on N is weak whereas for other values, the ratio depends strongly on N [insets of Figs. 4(b) and 4(d)]. Note that in the critical case, the ratio is not equal to one as it would be for a system with effective additive noise. This indicates that the system of coupled molecular motors is described by Eq. (1) with a multiplicative noise.

Discussion.—To summarize, we have shown that an active Brownian particle undergoes a qualitative change of its weak noise behavior upon increasing an asymmetry in its dynamics. We demonstrated for a simple example with a constant bias F the existence of a finite window of forces $|F| < F_{\rm crit}$ for which the ABP shows giant diffusion similar to its behavior in the symmetric case (this strong diffusion may in a finite system completely overshadow the effect of a finite mean velocity). For forces $|F| > F_{\rm crit}$, diffusion is (in particular, at weak noise) drastically reduced and the motion is dominated by the drift (reliable transport). The critical value $F_{\rm crit}$ can be understood as a compromise between a vanishing variance and a diverging correlation time. The product of these two factors is finite in the limit of vanishing noise if the effective velocity potential obeys a simple condition: the barrier for transitions from the more likely velocity should be twice as large as the barrier seen from the less likely velocity state. We also could formulate this condition in terms of extremal values of the velocity histogram. This condition could be also assessed in experimental systems in which the overall noise level can be controlled.

We also observed the critical range in the asymmetry in a model of coupled molecular motors, for which a correspondence to an active Brownian particle model had been previously suggested [6]. In accordance with our predictions, the critical force as well as its corresponding ratio $R_P(F_{\rm crit})$ do not depend on the number of motors which determines the effective noise level in this system. Our results also bear possibly relevance for the biophysics of coupled molecular motors. These molecular machines have diverse functions in the cell: force generation and generation of rhythmic behavior [15], directed transport of cargo [16], and active diffusive transport [8]. Regarding the latter two tasks, we have shown that changing the asymmetry by external forces or intrinsic interactions (parameter a of the ratchet model), the assembly of molecular motors can display either (i) reliable directed transport of cargo needed in a specific place of the cell or (ii) a huge diffusion which may serve to distribute products generated in one place but needed in many different places all over the cell.

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