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Anomalous mobility of a driven active particle in a steady laminar flow

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Abstract

We study, via extensive numerical simulations, the force–velocity curve of an active particle advected by a steady laminar flow, in the nonlinear response regime. Our model for an active particle relies on a colored noise term that mimics its persistent motion over a time scale τ_A. We find that the active particle dynamics shows non-trivial effects, such as negative differential and absolute mobility (NDM and ANM, respectively). We explore the space of the model parameters and compare the observed behaviors with those obtained for a passive particle ($\tau_A = 0$) advected by the same laminar flow. Our results show that the phenomena of NDM and ANM are quite robust with respect to the details of the considered noise: in particular for finite τ_A a more complex force–velocity relation can be observed.

Keywords: active matter, nonlinear response, negative mobility

(Some figures may appear in colour only in the online journal)

1. Introduction

The study of the motion of a tracer driven by an external force in a complex environment plays a central role in many research areas, ranging from transport phenomena at different scales [1–6], to the response theory in non-equilibrium systems [7–9]. Although some results have been obtained in the last decades in the framework of linear response, the behavior of the tracer for perturbations in the nonlinear regime is much less understood. It can show complex behaviors, featuring surprising phenomena such as negative differential mobility (NDM) and even absolute negative mobility (ANM). The former means a non-monotonic behavior of the force–velocity curve, while the latter indicates that, for certain values of the model parameters, the tracer can display a stationary velocity opposite to the direction of the applied external force. NDM has been recently studied in discrete lattice gas models, where also some analytical results are available [10–14], while ANM is observed in systems with continuous states as reported for instance in [15–19]. The general mechanisms responsible for these phenomena rely on some trapping effects occurring in the system due to the coupling of the tracer dynamics with the surrounding complex environment, and depend on the specific model.

In this paper we study a similar problem for the case of an active particle advected by a steady laminar flow. Active matter is generally characterized by self propulsion, namely an internal conversion of energy into unidirected motion, which results in a persistent direction, over an 'active' timescale τ_A. Instances of such systems range from biological organisms [20, 21] to man-made devices [22]. Several models have been proposed to study the dynamics of these non-equilibrium systems, that can show interesting phenomena, such as phase separation, clustering, symmetry breaking and so on [20, 23, 24]. The response of active particles moving in complex environments under the action of an external force, is an important issue in different contexts: on the one hand, from a theoretical perspective, this problem plays a central role in the theory of non-equilibrium (also in the non-linear regime) fluctuation-dissipation relations [25–29]; on the other hand, the study of the driven dynamics of active particles has important applications in active microrheology [30] as well as in the modeling of the dispersion of micro-organisms in fluids [31, 32]. Due to the non-equilibrium nature of these systems, non-trivial behaviors such as NDM are expected, as observed in recent molecular dynamics simulations of active matter particles moving through a random obstacle array [33], or in discrete models on a lattice [34, 35]. Many other interesting effects can be observed due to the coupling of the active (non-equilibrium) motion of the particles with the boundaries [36–39] or with the surrounding crowding environment [40–45]. In particular, driven motion along narrow channels or confined geometries can show subdiffusion and anomalous fluctuations [46–53].

Here we consider a different approach to describe active matter, where the persistent motion is introduced via a colored noise term, with a finite correlation time $\tau_{\rm A}$ [37, 54]. Inspired by this model, we study the nonlinear response to an external bias of an active particle advected by a divergenceless velocity field in the presence of colored noise. This model generalizes the system considered in [18, 19], where the dynamics of an inertial particle was considered. Indeed, in the limit of $\tau_{\rm A} \to 0$ one recovers the $\delta-$correlated 'passive' case, while for $\tau_{\rm A} \to \infty$ one obtains the deterministic, zero-noise dynamics. As shown in previous works [18, 19], the effective motion of the tracer in the passive case, for small noise, occurs along preferential 'channels', that can be aligned downstream or upstream with respect to the force, resulting in a non-trivial force–velocity relation. Here we show that phenomena such as NDM and ANM also take place for the active particle dynamics and therefore, in these models, they are rather robust with respect to the kind of considered noise. Moreover, we investigate some regions of the parameter space of the model, identifying the cases where NDM or ANM occur. In particular, we focus on the range of parameters where in the passive case with $\tau_{\rm A} = 0$ ANM occurs [19]: our results clarifies in what manner the behaviors for $\tau_{\rm A} = 0$ get modified for finite $\tau_{\rm A}$, and show that the effect of ANM can be amplified by taking larger values of $\tau_{\rm A}$. Indeed, both the range of forces where ANM is observed and the negative values of the stationary velocity, can be increased by increasing the persistence time of the particle.

2. Model

Consider a driven tracer particle, moving in two dimensions with position $\boldsymbol{x} = (x, y)$ and velocity $\boldsymbol{v} = (v_x, v_y)$, advected by a velocity field $\boldsymbol{U} = (U_x, U_y)$. The equations of motion are the following

$$\dot{x} = v_x, \qquad (1)$$

$$\dot{y} = v_y, \qquad (2)$$

$$\dot{v}_x = -\frac{1}{\tau_{\rm S}}(v_x - U_x) + F + w_x, \qquad (3)$$

$$\dot{v}_y = -\frac{1}{\tau_{\rm S}}(v_y - U_y) + w_y, \qquad (4)$$

where $\boldsymbol{U}$ is a divergenceless cellular flow defined by a streamfunction ψ as:

$$U_x = \frac{\partial \psi(x,y)}{\partial y}, \qquad U_y = -\frac{\partial \psi(x,y)}{\partial x}. \qquad (5)$$

In the above equations $\tau_{\rm S}$ is the Stokes time, F the external force in the $x-$direction, and

$$\psi(x,y) = \frac{U_0}{k}\sin(kx)\sin(ky), \qquad (6)$$

where $k = 2\pi/L$. w_x and w_y are stochastic terms described by an Ornstein–Uhlenbeck process

$$\dot{w}_x = -\frac{w_x}{\tau_{\rm A}} + \frac{\sqrt{2D_0}}{\tau_{\rm A}}\xi_x, \qquad (7)$$

$$\dot{w}_y = -\frac{w_y}{\tau_{\rm A}} + \frac{\sqrt{2D_0}}{\tau_{\rm A}}\xi_y, \qquad (8)$$

where ξ_x and ξ_y are uncorrelated white noises with zero mean and variance

$$\langle \xi_\alpha(t)\xi_\beta(t')\rangle = \delta(t-t')\delta_{\alpha\beta}. \qquad (9)$$

We set $U_0 = 1$ and $L = 1$, and the typical time scale of the flow becomes $\tau^* = L/U_0 = 1$. The parameter $\tau_{\rm A}$ represents the correlation time of the noise. The limit $\tau_{\rm A} \to 0$ recovers the case of uncorrelated noise, and the microscopic thermal noise with diffusivity D_0 can be expressed in terms of the temperature T of the environment by the relation $D_0 = T/\tau_{\rm S}$. In the opposite limit $\tau_{\rm A} \to \infty$, somehow the system approaches the deterministic (zero-noise) dynamics, because the stochastic terms w_x and w_y in equations (3) and (4) are negligible (order $\sqrt{D_0/\tau_{\rm A}}$). The overdamped version of this model (with no external force) has been introduced to study the transport of a fluid particle in the upper mesoscale ocean [55, 56] and has been analyzed using multiscale technique in [57].

3. Anomalous behaviors of the force–velocity curve

When a tracer particle is driven by a small external force in a simple (equilibrium) fluid, one expects that the asymptotic mean velocity selected by the tracer will increase with the applied force, in agreement with the linear response. However, when the system is out of equilibrium, due to the presence of currents, or when the applied force is beyond the linear regime, the behavior of the force–velocity curve can be highly non-trivial, showing surprising behaviors.

Considering models defined in continuous space, NDM and ANM can be observed when the dimensionality of the phase space is larger than two [58, 59]. For instance, ANM can be shown by: (i) a one-dimensional inertial Brownian particle subjected to a periodic time-dependent force [16]; (ii) an overdamped Brownian particle in two dimensions subjected to dichotomous noise [60]; (iii) an inertial particle in two dimensions advected by a velocity field [18]. In the first two cases a detailed analysis of the deterministic properties of the system identifies the subtle interplay between the stability of coexisting attractors, noise induced metastability, and transient chaos as the underlying physical mechanism [59]. In the latter case iii), corresponding to the limit $\tau_{\rm A} = 0$ of the model

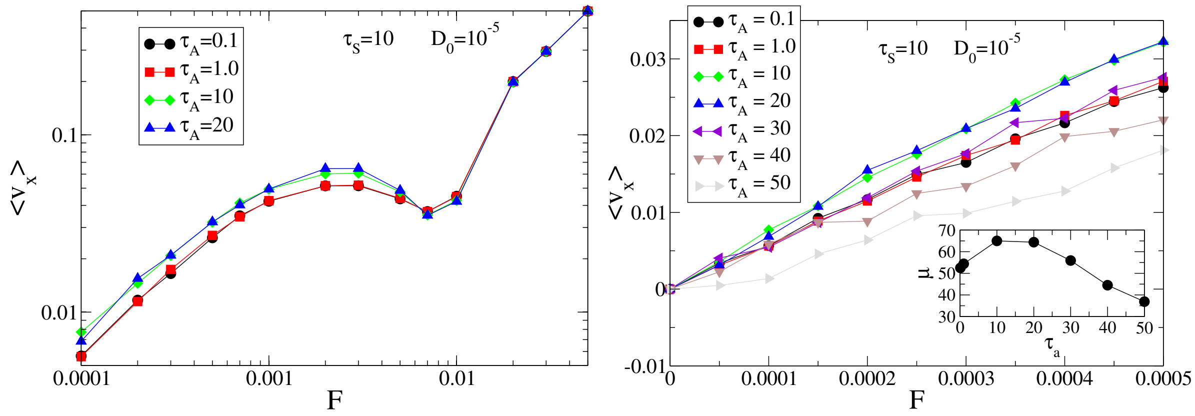

Figure 1. Force–velocity relation $\langle v_x \rangle(F)$ for $\tau_S = 10$, $D_0 = 10^{-5}$ and different values of τ_A. Data are obtained averaging over $\sim 10^4$ initial conditions and noise realizations. Left: note the non-monotonic behavior, corresponding to negative differential mobility. Right: zoom in the small force (linear) regime, from which the mobility μ is obtained (inset).

introduced above, the behavior of the force–velocity curve of the tracer has been analyzed as a function of the Stokes time τ_S and of the amplitude of microscopic white-noise D_0, obtaining a 'phase chart' of the regions of the parameters space where NDM and ANM occur [19]. For large values of the noise $D_0 \gg 1$, one observes a simple monotonic behavior, as expected, because in that case the effect of the underlying velocity field is negligible with respect to the noise; by decreasing D_0, instead, one finds NDM for small enough values of τ_S, with a narrow region of ANM for $0.6 \lesssim \tau_S \lesssim 1$ (and $D_0 \lesssim 5 \times 10^{-3}$): in particular, ANM is observed when the Stokes time of the particle and the characteristic time of the velocity field are comparable, namely for $\tau_S \sim \tau^* = 1$. All these peculiar phenomena can be traced back to the general expression for the average of equation (3)

$$\langle v_x \rangle = F\tau_S + \langle U_x(x, y) \rangle. \tag{10}$$

This shows that the external force has a twofold effect: it drives the tracer along its direction, but at the same time, it pushes the particle towards specific regions of the underlying velocity field. ANM and NDM, thus, emerge from the subtle competition between the terms $F\tau_S$ and $\langle U_x(x, y) \rangle$.

3.1. Negative differential mobility

In order to investigate the effect of colored noise, i.e. the role of the new parameter τ_A, we first study the case with Stokes time $\tau_S = 10$ and $D_0 = 10^{-5}$. The average velocity $\langle v_x \rangle$ is reported in figure 1 as a function of the applied force F. Here $\langle \cdots \rangle$ is computed over many different ($\sim 10^4$) initial conditions and on long trajectories. One observes first a linear increase of the velocity and then a non-monotonic behavior. Eventually, for larger values of the force, the linear behavior is recovered, as expected. The intermediate region shows that even in the case of finite τ_A, the phenomenon of NDM occurs, suggesting that it is quite robust with respect to the kind of noise considered in the model. In the right panel of figure 1 we focus on the small force, linear regime to study the mobility $\mu = \lim_{F\to 0} \langle v_x \rangle / F$, that turns out to be a non-monotonic, weakly dependent function of the correlation time τ_A (see inset).

3.2. Absolute negative mobility

A more interesting behavior is observed if the Stokes time and the characteristic time of the velocity field are of the same order, $\tau_S \sim \tau^*$. In this case, for the passive inertial tracer ($\tau_A = 0$) it has been shown [18, 19] that there exists a region of the parameters space (τ_S, D_0), where absolute negative mobility can be observed. Here we investigate the robustness of this phenomenon when a more general model, including colored noise, is considered, and show how the phase diagram gets modified.

We first focus on the case with Stokes time $\tau_S = 1$ (see figure 2). We investigate the behaviors of the force–velocity curve as a functions of the time τ_A and of the noise amplitude D_0. For $\tau_A = 1$ we find ANM for $D_0 = 10^{-5}$ and $D_0 = 10^{-3}$, but not for $D_0 = 10^{-4}$. Interestingly, in the case $D_0 = 10^{-3}$, we observe a negative *linear* response (green diamonds): this behavior does not violate any fundamental principle beacause the system is out of equilibrium even when the external force is zero, due to the non-gradient form of the velocity field $\boldsymbol{U}$. For $\tau_A = 10$ we find ANM for all explored values of D_0; for $\tau_A = 20$ we find ANM for $D_0 = 10^{-5}$, and $D_0 = 10^{-4}$, but not for $D_0 = 10^{-3}$. With respect to the passive case ($\tau_A = 0$) we find that the region of the parameter space where ANM is observed is enlarged for finite τ_A, see table 1.

In the bottom right panel of figure 2 we focus on the case $D_0 = 10^{-5}$ and zoom in the region of ANM: we observe that for finite τ_A an interesting two-minima behavior of the force velocity relation is observed. It is also worth noting that the negative minima of the velocity depend on τ_A and increase (in absolute value) with increasing τ_A. This suggests that the phenomenon of ANM can be amplified by considering a finite τ_A.

More specifically, this seems to be related to the underlying deterministic structure. Indeed, in the limit $\tau_A \to \infty$ the stochastic terms w_x and w_y appearing in equations (3) and (4) become small (order $\sqrt{D_0/\tau_A}$) constants, depending on the initial conditions. In figure 3 we show the force–velocity relation for $\tau_S = 1$ and zero noise, namely $w_x = w_y = 0$. In this deterministic case we find two deep negative minima (note the scale of ordinates), suggesting that the underlying

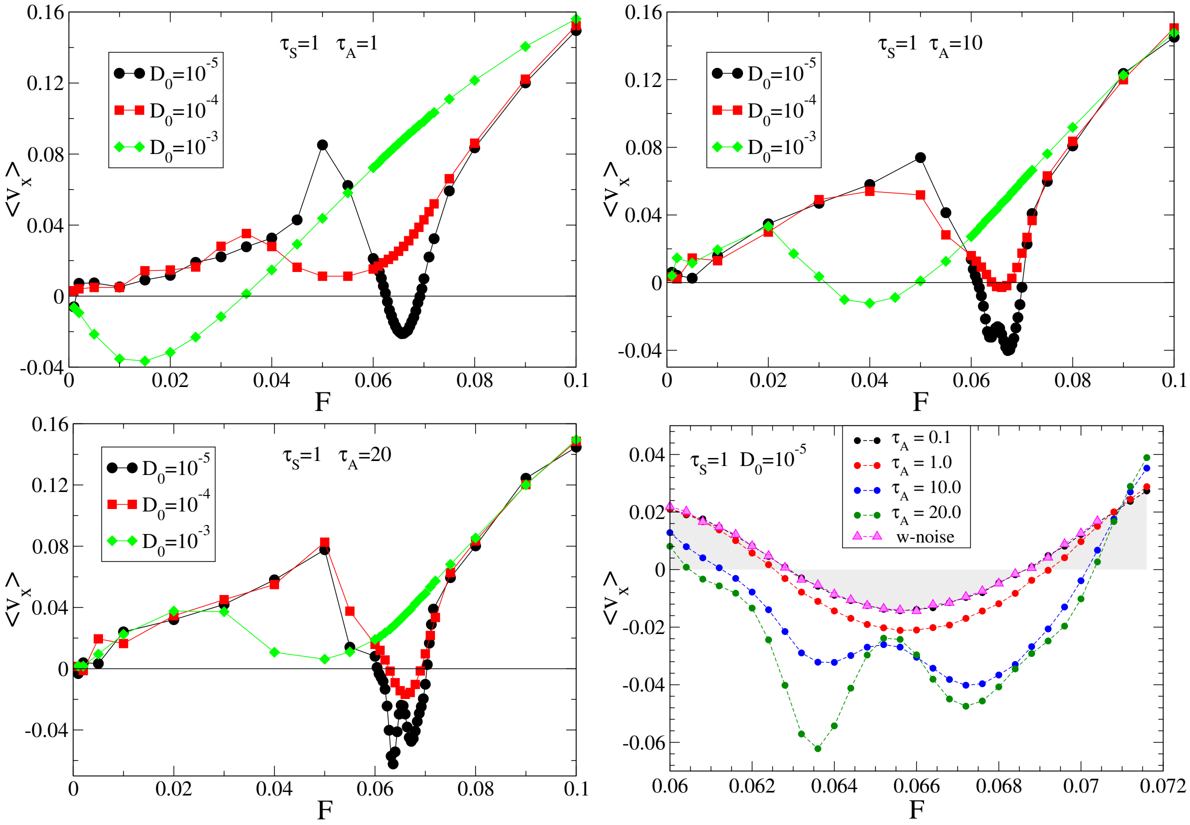

Figure 2. Force–velocity relation $\langle v_x\rangle(F)$ for $\tau_S = 1$, and several values of $D_0 = 10^{-5}$ and τ_A. In some cases absolute negative mobility is observed. Bottom right panel: zoom of a ANM region, showing a complex behavior characterized by two minima (the grey area represents the regions where the average velocity for the white noise case, $\tau_A = 0$, changes sign).

Table 1. Table showing the regions of the parameter space where ANM and NDM is observed, for $\tau_S = 1$ (ST means standard, i.e. $\mathrm{d}\langle v_x\rangle/\mathrm{d}F > 0$ in all the range of explored values of F).

$\tau_S = 1$	$\tau_A = 0$	$\tau_A = 1.0$	$\tau_A = 10$	$\tau_A = 20$
$D_0 = 10^{-3}$	ANM	ANM	ANM	NDM
$D_0 = 10^{-4}$	NDM	NDM	ANM	ANM
$D_0 = 10^{-5}$	ST	ANM	ANM	ANM

deterministic dynamics governs the behavior observed in the presence of noise. This explanation has been carefully described in [59] for a one-dimensional system.

Figure 4 reports $M = 5 \times 10^4$ points sampled from a deterministic (noiseless) trajectory of the particle with $\tau_S = 1$ and re-folded into the fundamental cell $C = [-L/2, L/2] \times [-L/2, L/2]$, for forces $F = 0.063$ (left panel) and $F = 0.065$ (right panel). The figures indicate that the dynamics for $F = 0.063$ is regular/periodic while for $F = 0.065$ it looks 'chaotic'; however, in both cases the trajectory spends more time in the regions $R = \{(x, y) \in C \mid U_x(x, y) + F\tau_S \leqslant 0\}$ marked by green-shaded domains. The extension and the contour of these regions is obtained by solving the inequality for the explicit form of $U_x(x,y)$:

$$\sin(kx)\cos(ky) \leqslant -\frac{F\tau_S}{U_0} \equiv -W.$$

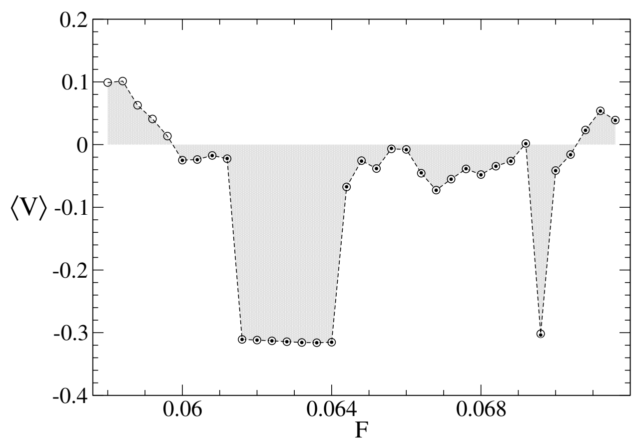

Figure 3. Force–velocity relation for $\tau_S = 1$ in the zero-noise ($\tau_A \to \infty$) limit.

The results are the two domains represented in figure 4:

$$D_1 = \begin{cases} x \in [-L/2, 0] \\ |y| \leqslant \frac{1}{k} \arccos\left[\frac{W}{|\sin(kx)|}\right] \end{cases}$$

and

$$D_2 = \begin{cases} x \in [0, L/2] \\ |y| \geqslant \frac{1}{k} \arccos\left[\frac{-W}{|\sin(kx)|}\right]. \end{cases}$$

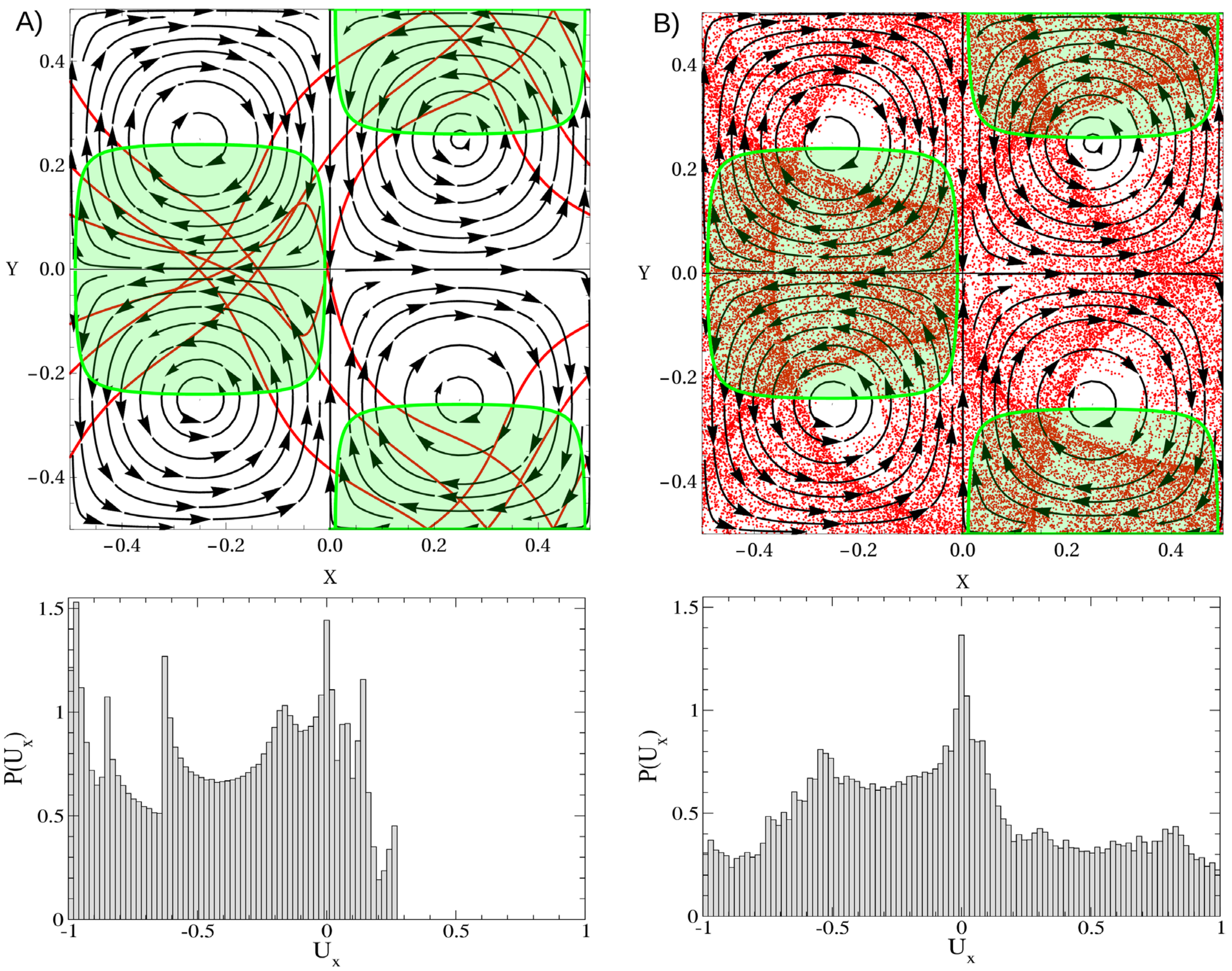

Figure 4. Deterministic (noiseless) trajectory (red dots) sampled every $t_s = 2000\Delta t$ and folded into the fundamental cell $C = [-L/2, L/2] \times [-L/2, L/2]$ for two cases: $\tau_S = 1, F = 0.063$ (left panel) and $\tau_S = 1, F = 0.065$ (right panel). Left: the folded trajectory is periodic and mainly visits the regions of C where $U_x(x, y) + F\tau_S \leqslant 0$ (shaded green areas). Right: the folded trajectory looks chaotic but again points are denser in the regions where $U_x(x, y) + F\tau_S \leqslant 0$. Bottom panels reports the normalized histograms of the values $U = U_x(x,y)$ collected along the trajectories showing the asymmetry with respect to the origin: $P(-|U|) > P(|U|)$. This dynamical symmetry breaking is another signature of the presence of negative mobility states.

Table 2. Table showing the regions of the parameter space where ANM and NDM is observed, for $\tau_S = 0.65$.

$\tau_S = 0.65$	$\tau_A = 0$	$\tau_A = 1.0$	$\tau_A = 10$	$\tau_A = 20$
$D_0 = 10^{-3}$	ANM	NDM	NDM	NDM
$D_0 = 10^{-4}$	NDM	NDM	NDM	NDM
$D_0 = 10^{-5}$	ANM	NDM	NDM	NDM

For the values of F for which ANM is observed, figure 3, the dynamics preferentially occupies these domains so that the average (10) turns to be certainly negative.

The bottom panels of figure 4 show the corresponding histograms of the set of values $U_k = U_x[x(t_k), y(t_k)]$, $k = 1, ..., M$ evaluated over the sampled points. Both histograms exhibit a neat asymmetry with respect to the origin, $P(-|U|) > P(|U|)$, indicating that in equation (10) the average $\langle U_x(x, y)\rangle$ gets mainly negative contributions and dominates over $F\tau_S$.

We have performed the same analysis also for $\tau_S = 0.65$: table 2 summarizes our results. In particular, note that for $\tau_S = 0.65 < \tau^*$ we do not observe ANM, but only NDM, at variance with the white-noise case $\tau_A = 0$, where ANM occurs for some values of D_0.

4. Conclusions

In this paper, we have studied the nonlinear response to an external force of an active particle, with persistence time τ_A, in the presence of a laminar flow. We have focused on the behavior of the average velocity of the particle as a function of the applied force, exploring a region of the model parameter space, (τ_S, τ_A, D_0), where τ_S is the Stokes time of the particle and D_0 the amplitude of the active noise. We found that the force–velocity relation of the particle can show non-monotonic behaviors, including negative differential and absolute mobility. Our results indicate that the response of active matter in the presence of an underlying velocity field can show counterintuitive phenomena, such as NDM or ANM. In particular, this can be applied for sorting and selection of particles with different activity (defined via the active time τ_A), exploiting the different response to an external force.

In general, anomalous response behavior can be expected in the nonlinear response regime, or/and out of equilibrium, namely in the presence of currents, when the time-reversal symmetry and detailed balance are violated by the dynamics. This happens in our model, where, even for zero external force, the system does not satisfy detailed balance, due to the non-gradient form of the velocity field and due to the active nature of the tracer.

It could be also interesting the study of more complex situations where several interacting active particles are considered, or including the effect of the particle motion on the structure of the surrounding fluid, or the presence of particular boundary conditions. Moreover, the investigation of the diffusion properties in the absence and in the presence of the external force requires further analysis, in particular in the light of the non-equilibrium fluctuation-dissipation relations, connecting mobility and diffusion coefficient.

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