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# Active Particle Diffusion in Convection Roll Arrays

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Undesired advection effects are unavoidable in most nano-technological applications involving active matter. However, it is conceivable to govern the transport of active particles at the small scales by suitably tuning the relevant advection and self-propulsion parameters. To this purpose, we numerically investigated the Brownian motion of active Janus particles in a linear array of planar counter-rotating convection rolls at high Péclet numbers. Similarly to passive particles, active microswimmers exhibit advection enhanced diffusion, but only for self-propulsion speeds up to a critical value. The diffusion of faster Janus particles is governed by advection along the array's edges, whereby distinct diffusion regimes are observed and characterized. Contrary to passive particles, the relevant spatial distributions of active Janus particles are inhomogeneous. These peculiar properties of active matter are related to the combined action of noise and self-propulsion in a confined geometry and hold regardless of the actual flow boundary conditions.

## 1 Introduction

The diffusion of a tracer (organic or artificial, alike) in a suspension fluid is a standard problem of classical transport theory<sup>1</sup>. This paper combines two distinct aspects of this phenomenon, which recently attracted widespread interdisciplinary interest, each for its own merit: (i) the persistent (or time-correlated) random motion of self-propelling particles and (ii) colloidal dispersion in laminar flows.

The most tractable example of persistent Brownian motion is represented by artificial micro-swimmers, namely tiny Brownian particles capable of self-propulsion in an active medium<sup>2,3</sup>. Such particles are designed to harvest environmental energy and convert it into kinetic energy. A class of artificial swimmers widely investigated in the current literature is the so-called Janus particles (JP), mostly spherical colloidal particles with two differently coated hemispheres, or “faces”. Their axial propulsion is sustained by the dipolar near-flow-field they generate by interacting with the surrounding active (mostly highly viscous) medium. Indeed, depending on their operating conditions, JPs can induce either concentration gradients, by catalyzing some chemical re-

action on their active surface, or thermal gradients, by inhomogeneous light absorption (self-thermophoresis) or magnetic excitation (magnetically induced self-thermophoresis)<sup>4,5</sup>. Moreover, experiments demonstrated their ability to perform guided motions through periodic arrays<sup>6</sup>.

Recently, artificial micro- and nano-swimmers of this class have been the focus of pharmaceutical (e.g., smart drug delivery<sup>7</sup>) and medical research (e.g., robotic microsurgery<sup>8</sup>). These peculiar Brownian particles change direction randomly as usual, but with finite time scale; persistence makes their diffusion extremely sensitive to geometric confinement and other constraints<sup>9–12</sup>. Technological applications involving sub-millimeter artificial swimmers thus require accurate control of their diffusive properties in non-homogeneous environments<sup>1,6</sup>.

On the other hand, Brownian diffusion in an advective medium is also a nanotechnological issue, for instance, in the design and operation of microfluidic devices<sup>13–15</sup> or chemical reactors<sup>16</sup>. We consider for simplicity a Brownian tracer of free diffusion constant  $D_0$ , advected by a planar stationary laminar flow, like in Fig. 1(a). Let the velocity field of the suspension fluid be formulated as<sup>17</sup>,  $\vec{v}_\psi = (\partial_y, -\partial_x)\psi$ , where

$$\psi(x, y) = (U_0 L / 2\pi) \sin(2\pi x / L) \sin(2\pi y / L), \quad (1)$$

is a stream function extensively studied in the context of Rayleigh-Bénard convection<sup>18</sup>. On combining the two constants,  $L$ , the flow's spatial period, and  $U_0$ , the maximum advection speed, one defines the advection diffusion scale,  $D_L = U_0 L / 2\pi$ , and the maximum roll vorticity,  $\Omega_L = 2\pi U_0 / L$  (Appendix A).

At high Péclet numbers,  $Pe = D_L / D_0 \gg 1$ , a passive tracer

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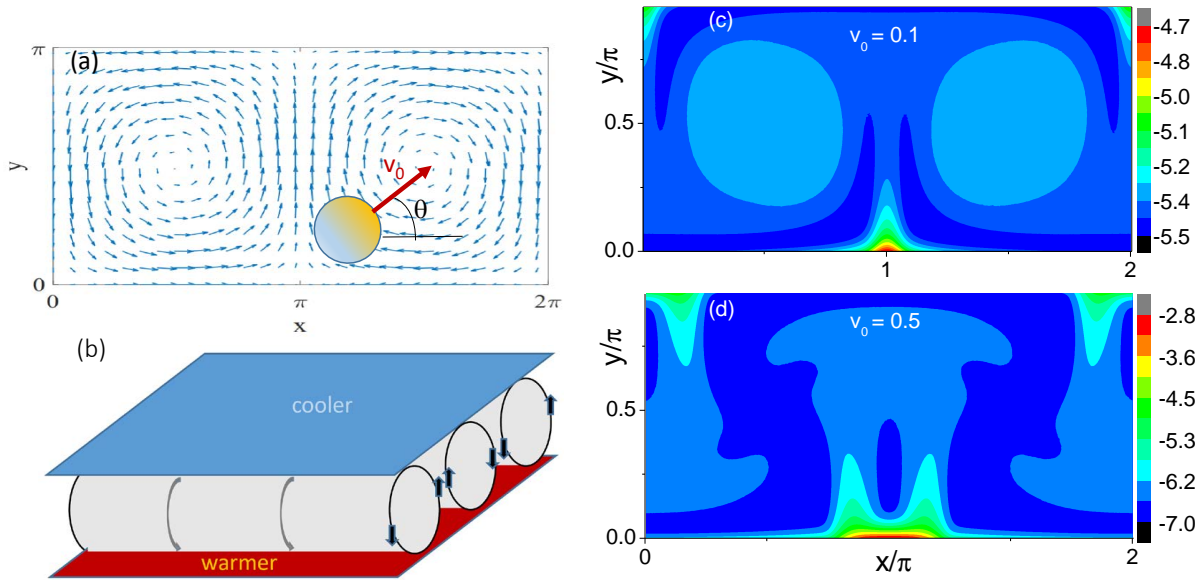
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**Fig. 1** Spatial distributions of a Janus particle in the laminar flow of Eq. (1), sketched in (a)-(b), for  $v_0 = 0.1$  (c) and  $0.5$  (d). The chart levels are color-coded on natural logarithmic scales as indicated. Other simulation parameters are:  $D_0 = 0.01$ ,  $D_\theta = 0.01$ ,  $U_0 = 1$  and  $L = 2\pi$ . According to Eq. (3), here  $v_c = 0.4$ . A practical realization of a linear convection array is represented by the Rayleigh-Bénard rolls sketched in (b); the JP self-propulsion model of Eq. (2) is illustrated in (a).

undergoes normal diffusion with enhanced diffusion constant  $D = \kappa\sqrt{D_L D_0}$  with  $\kappa = 1.07$ , that is  $D > D_0$ <sup>19</sup>. This advection effect, termed advection enhanced diffusivity (AED), has been explained<sup>19–22</sup> by noticing that for  $D_0 < D_L$  an unbiased particle jumps between convection rolls while being advected along their separatrices. Narrow flow boundary layers (FBL) of estimated width  $\delta = (D_0/\Omega_L)^{1/2}$ , form a network of advection channels centered around the  $\psi(x, y)$  cell separatrices, thus enabling a large-scale particle's diffusion.

Peculiar effects due to the combination of self-propulsion and advection are expected to emerge when one considers an active JP suspended in a one dimensional (1D) array of counter-rotating convection rolls. An ideal experimental setup is sketched in Fig. 1(b). An array of stationary Rayleigh-Bénard cells can occur in a plane horizontal layer of fluid heated from below<sup>23,24</sup>. Assuming that they are counter-rotating cylinders parallel to the  $z$ -axis, the  $z$  coordinate of a suspended tracer is ignorable; hence the reduced two dimensional (2D) flow pattern of Eq. (1). Advection enhanced diffusivity of passive colloidal particles in arrays of Rayleigh-Bénard rolls<sup>18</sup> has already been demonstrated experimentally<sup>25,26</sup>. Experimental data on the dispersion of self-propelling microswimmers in convective laminar flows are scarce. Recent reports mostly addressed the hydrodynamic effects of laminar flows on the self-propulsion of finite-size microswimmers of various geometries<sup>27</sup>, either artificial<sup>28</sup> or of biological nature<sup>29,30</sup>. In this regard, active JPs are ideal tracers for this kind of measurements because their shape and size minimize hydrodynamic effects and their self-propulsion speed can be conveniently tuned with respect to the advection drag established in the convection cell.

This paper is organized as follows. In Sec. 2 we present our model and briefly discuss the dynamical significance of the rel-

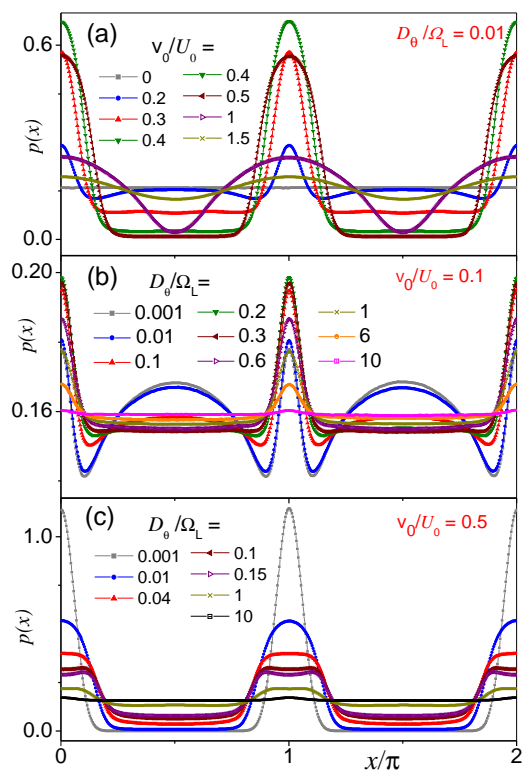
evant parameters. Our derivation of the relevant time scales is detailed in Appendix A. Our main numerical results are analysed in Secs. 3 and 4, where we show that: (i) The interplay of advection and self-propulsion causes the nonuniform spatial distribution of a confined active JP. For self-propulsion speeds below a certain threshold, its distribution tends to accumulate along the roll boundaries (Sec. 3 and Appendix B); (ii) Under these conditions, its self-propulsion and advection velocities tend to line up, so that, contrary to the 2D case of Ref.<sup>31</sup>, the large-scale diffusion of an active JP is insensitive to self-propulsion itself (Sec. 4); (iii) Active tracers with self-propulsion speeds larger than the above threshold, attain a maximum diffusion constant for an optimal persistence time, which we relate to advection at the array's edges (Sec. 4 and Appendix C). In Sec. 5 we stress the role of geometric confinement on the diffusion properties of an active JP in a convection array and show that the picture above holds also for rigid (i.e., no-slip) edge flows.

## 2 Model

By (linear) convection array we mean here a stationary laminar flow with periodic stream function like  $\psi(x, y)$  of Eq. (1), confined between two parallel edges,  $y = 0$  and  $y = L/2$ , which act as dynamical reflecting boundaries. The unit cell of the array consists of two counter-rotating convection rolls [Fig. 1(a)]. The dynamics of an overdamped active JP can then be formulated by means of two translational and one rotational Langevin equation (LE),

$$\begin{aligned}\dot{\vec{r}} &= \vec{v}_\psi + \vec{v}_0 + \sqrt{D_0} \xi(t) \\ \dot{\theta} &= (\alpha/2) \nabla \times \vec{v}_\psi + \sqrt{D_\theta} \xi_\theta(t),\end{aligned}\quad (2)$$

where  $\vec{r} = (x, y)$ ,  $\vec{v}_\psi$  is the advection velocity introduced above, and the self-propulsion vector,  $\vec{v}_0 = v_0(\cos \theta, \sin \theta)$ , has constant



**Fig. 2** Stationary longitudinal distributions,  $p(x)$ , of a Janus particle in the laminar flow of Eq. (1) for (a)  $D_\theta = 0.01$  and different  $v_0$ ; (b)  $v_0 = 0.1$  and (c)  $v_0 = 0.5$  and different  $D_\theta$  (see legends). Other simulation parameters are:  $D_0 = 0.01$ ;  $U_0 = 1$  and  $L = 2\pi$ , with  $D_L = \Omega_L = 1$ .

modulus,  $v_0$ , and is oriented at an angle  $\theta$  with respect to the longitudinal  $x$ -axis. The translational (thermal) noises in the  $x$  and  $y$  directions,  $\xi(t) = (\xi_x(t), \xi_y(t))$ , and the rotational noise,  $\xi_\theta(t)$ , are stationary, independent, delta-correlated Gaussian noises,  $\langle \xi_i(t) \xi_j(0) \rangle = 2\delta_{ij} \delta(t)$ , with  $i, j = x, y, \theta$ .  $D_0$  and  $D_\theta$  are the respective noise strengths, which for generality we assume to be unrelated<sup>10</sup>. To avoid uncontrolled hydrodynamic effects, the particle is taken to be pointlike<sup>15</sup>. Other effects due to its actual geometry and chemical-physical characteristics are encoded in the model dynamical parameters. The reciprocal of  $D_\theta$  coincides with the angular persistence (or correlation) time,  $\tau_\theta$ , of  $\vec{v}_0$ ; accordingly,  $l_\theta = v_0/D_\theta$  quantifies the persistence length of the particle's self-propelled random motion. The flow shear exerts a torque on the particle proportional to the local fluid vorticity,  $\nabla \times \vec{v}_\psi$ <sup>31,32</sup>. For simplicity, we adopt Faxén's second law, which, for an ideal no-stick spherical particle, yields  $\alpha = 1$ <sup>33</sup>. In the high Péclet number regime addressed here,  $Pe \gg 1$  or  $D_0 \ll D_L$ , particle diffusion is strongly influenced by advection (appendix A).

The Langevin equation (2) can be conveniently reformulated in dimensionless units by rescaling  $(x, y) \rightarrow (\tilde{x}, \tilde{y}) = (2\pi/L)(x, y)$  and  $t \rightarrow \tilde{t} = \Omega_L t$ . The three remaining independent parameters get rescaled as follows:  $v_0 \rightarrow v_0/U_0$ ,  $D_0 \rightarrow D_0/D_L$  and  $D_\theta \rightarrow D_\theta/\Omega_L$ . This means that, without loss of generality, we can set  $L = 2\pi$  and  $U_0 = 1$  and the ensuing simulation results can be regarded as expressed in dimensionless units and easily scaled back to arbitrary

dimensional units. The stochastic differential Eqs. (2) were numerically integrated by means of a standard Milstein scheme<sup>34</sup>. Particular caution was exerted when computing the asymptotic diffusion constant,  $D = \lim_{t \rightarrow \infty} [x(t) - x(0)]^2 / 2t$ , because for low values of the noise strengths,  $D_0$  and  $D_\theta$ , the transients of the diffusion process grow exceedingly long<sup>32,35</sup>. For asymptotically large running times, our estimates of  $D$  are independent of the starting point  $(x(0), y(0))$ .

### 3 Spatial distributions

In sharp contrast with the noiseless limit,  $D_0 = D_\theta = 0$ , investigated in Ref.<sup>32</sup>, the spatial distribution of a noisy active JP is not uniform. The outcome of our numerical simulations is summarized in Figs. 1(c),(d) and 2. The laminar flow acts upon the particle through both an advection drag and an advection torque. Along the roll boundaries the drag is maximum (with speed approaching  $U_0$ , except at the "stagnation" corners), but the torque vanishes. At low self-propulsion speeds, this favours the orientation of  $\vec{v}_0$  parallel to the advection velocity  $\vec{v}_\psi$ . The JP thus undergoes a large-scale intra-roll circulation motion, which causes its accumulation along the outer layers of the rolls. The less pronounced particle accumulation at the roll centers is attributable to the higher vorticity there<sup>35</sup>. These two areas of accumulation are separated by a circular depletion region. Indeed, in Figs. 1(c) and Figs. 2(a),(b) (see also Appendix B) the particle appears to be sucked in by the ascending ( $x = L/2$ ) and descending boundary flows ( $x = 0, L$ ), an effect that seems to increase with increasing  $v_0$ .

This picture changes abruptly as  $v_0$  is raised above a critical value  $v_c$  [Fig. 2(a)], which we established to depend on the strength of the thermal noise,  $D_0$  (Appendix C). The intra-roll circulation of Fig. 1(c) is suppressed and the roll interior gets depleted [Fig. 2(a),(c)]; as a result, the particle piles up symmetrically at the base of the ascending (bottom edge) and descending flows (top edges). Moreover, for  $v_0 U_0$ , the particle seems to diffuse mostly along the array's edges, which explains why the longitudinal distributions,  $p(x)$ , turn uniform again with increasing  $v_0$ , while the transverse distributions,  $p(y)$ , remain peaked at  $y = 0, L/2$  (Appendix B). One also notices that the peaks of  $p(x)$  widen with increasing  $v_0$  [Fig. 2(a)] and  $D_\theta$  [Fig. 2(c)].

The relevance of these results can be best appreciated by comparison with the diffusion of a passive particle in the same 1D convection array. In that case, the flow boundary layers still control the particle's large-scale diffusion, but all stationary distributions,  $p(x, y)$ , remain uniform<sup>35</sup>. This conclusion applies also to noiseless self-propelling JPs in 1D convection arrays, as proven in Ref.<sup>32</sup>, but is no longer true in the presence of thermal noise. Indeed, upon hitting either array edge, the particle will persist pointing against it for a time  $\tau_\theta$ ; hence the angular correlation of  $\vec{v}_0$  and  $\vec{v}_\psi$ . [Note that in most simulations presented here  $\tau_\theta$  is larger than the circulation characteristic time, ie,  $D_\theta < \Omega_L$ .] Accordingly, no probability density accumulation at the roll boundaries was detected for an active JP in the 2D laminar flow of Eq. (1) with periodic boundary conditions, regardless of the noise strengths,  $D_0$  and  $D_\theta$  (Appendix B). This leads to the conclusion that the FPL structure we detected in the stationary distributions

$p(x, y)$  of an active JP diffusing in a 1D convection array is a combined effect of noise and geometric confinement.

The self-propulsion threshold,  $v_c$ , can be estimated as follows. When the vector  $\vec{v}_0$  points inwards, the particle pulls away from the edge a length of the order of  $v_0/4\Omega_L$ , before being swept into a vertical flow layer. As such length grows comparable to the width of an unbiased flow boundary layers, i.e., for  $v_0 > v_c$  with

$$v_c/U_0 = 4\sqrt{D_0/D_L}, \quad (3)$$

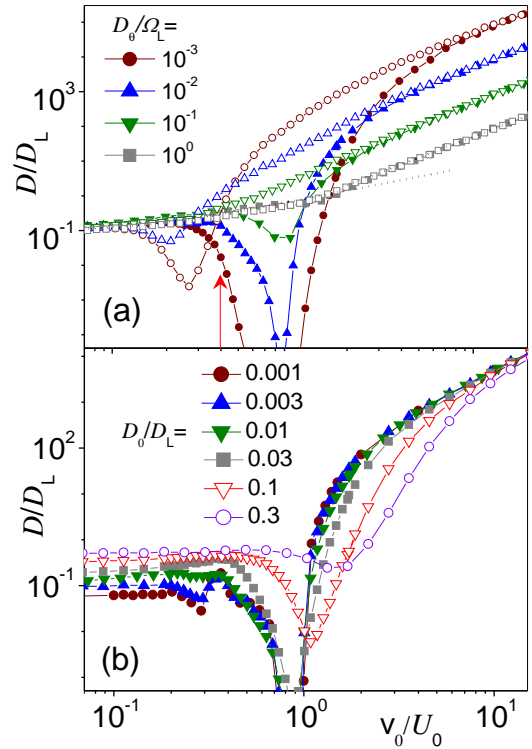
the particle exits the FBL and its circulation along the roll separatrix is interrupted. This estimate of  $v_c$  is consistent with our simulation data for  $p(x)$  and  $p(y)$  at low angular noise,  $D_\theta \ll \Omega_L$  [compare Figs. 1 and 2; see Appendices B and C for more details]. Note, for instance, that in Fig. 2 the  $p(x)$  regions delimited by the peaks at  $x = 0, \pi$  and  $2\pi$  get depleted only for  $v_0 = 0.5$ , that is for  $v_0 > v_c$ . Moreover, being confined in a FBL, a JP with  $v_0 < v_c$  ought to behave like a passive colloidal particle, ie, undergo advection enhanced diffusivity as an effect of the sole thermal noise. The diffusion data presented in the next section (Fig. 3) confirm this conclusion.

As the FBL circulation breaks up, the JP tends to accumulate against the array edges, provided that the self-propulsion length is larger than the array width,  $l_\theta > L/2$ , or, equivalently,  $D_\theta/\Omega_L < v_0/U_0$ . However, its motion along the edges is not advection-free. The coordinate  $x$  in Eq. (2) then obeys the approximate LE,  $\dot{x} = U_0 \langle \cos(2\pi y/L) \rangle \sin(2\pi x/L) + v_0 \cos \theta + \xi_x(t)$ , which describes the dynamics of a Brownian particle pinned to a washboard potential<sup>36</sup> (advection term) and subjected to a colored, non-Gaussian tilting noise,  $v_0 \cos \theta(t)$ , with correlation time  $\tau_\theta$ <sup>10</sup> (self-propulsion term). The average  $\langle \cos(2\pi y/L) \rangle$  depends on all three free parameters  $v_0, D_\theta$  and  $D_0$ ; in particular, its modulus increases with increasing  $v_0$  and decreasing  $D_\theta$ . This simple observation explains: (i) the non-monotonic  $v_0$ -dependence of the  $p(x)$  peaks, whereby a larger  $v_0$  implies not only higher washboard potential barriers, but also a stronger tilting term; (ii) the flattening of the longitudinal distributions for  $v_0 U_0$ , as self-propulsion wins over the advection pinning action at the edges; (iii) the broadening and double-peaked profile of the  $p(x)$  peaks in Fig. 2(c) on increasing  $D_\theta$  which is a well-known effect of colored noise<sup>37</sup>.

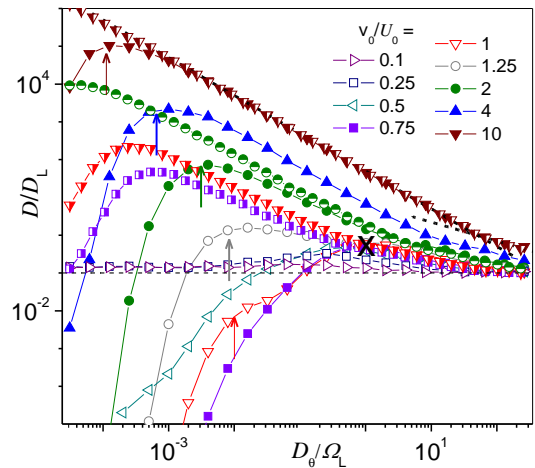
On increasing  $D_\theta$ , the JP self-propulsion length eventually grows shorter than the roll size,  $l_\theta < L/2$ ; the active particle then tends to behave like a passive Brownian particle, except its free diffusion constant,  $D_0$ , must be now incremented by the extra term  $D_s = v_0^2/2D_\theta$ . Accordingly, both its spatial distributions,  $p(x)$  and  $p(y)$ , become uniform [see Figs. 2(b),(c) and Appendix B].

## 4 Longitudinal diffusion

Based on the qualitative arguments of Sec. 3, we expect to observe distinct diffusion regimes for a JP with  $l_\theta > L/2$ . Our expectation are supported by the simulation data reported in Fig. 3(a,b). Indeed, the curves  $D$  versus  $v_0$  exhibit distinct behaviors for  $v_0 < v_c$ ,  $v_c < v_0 U_0$  and  $v_0 \gg U_0$ . For  $v_0 \gg U_0$ , advection is negligible compared to self-propulsion; since we assumed reflecting boundaries at the array's edges, not surprisingly,  $D \rightarrow D_0 + D_s$ <sup>31</sup>. This behavior is in sharp contrast with the sce-



**Fig. 3** (a) Longitudinal diffusion of a JP in the laminar flow of Eq. (1) (solid symbols) and (5) (empty symbols);  $D/D_L$  vs.  $v_0/U_0$  for  $D_0 = 0.01$  and different  $D_\theta$  (see legends). Dashed curves represent the estimates,  $D = \kappa\sqrt{D_L(D_0 + D_s)}$  and  $D = D_0 + D_s$ , with  $D_s = v_0^2/2D_\theta$ , respectively, for low and high  $v_0$  (see text). Our estimate for  $v_c$ , Eq. (3), is marked by a vertical arrow. (b)  $D/D_L$  vs.  $v_0/U_0$  for  $D_\theta = 0.01$  and different  $D_0$ . Flow parameters are  $U_0 = 1$  and  $L = 2\pi$ , with  $D_L = \Omega_L = 1$ .



**Fig. 4** Longitudinal diffusion of a JP in the laminar flow of Eq. (1):  $D/D_L$  vs.  $D_\theta/\Omega_L$  for different values of  $v_0$  (filled and empty symbols, see legends). We remind that here Eq. (3) yields  $v_c = 0.4$ . Dashed curves represent the limiting cases  $D = \kappa\sqrt{D_L D_0}$  (passive particle with  $Pe \gg 1$ ),  $D = D_0 + D_s$  (free JP) and  $D = \kappa\sqrt{D_L(D_0 + D_s)}$  (advection enhanced diffusivity of a JP in 2D<sup>31</sup>), with  $D_s = v_0^2/2D_\theta$  (see text). Vertical arrows mark our estimates for  $D_\theta^*$ , Eq. (4), and a cross the maxima,  $D/D_L = 0.5$ , of the curves with  $v_c < v_0 U_0$ . Other simulation parameters are:  $D_0 = 0.01$ ,  $U_0 = 1$  and  $L = 2\pi$ , hence  $D_L = \Omega_L = 1$ . A few curves for the same JP in the rigid-boundary flow of Eq. (5) are plotted for a comparison (half-filled symbols of the corresponding shape and color).

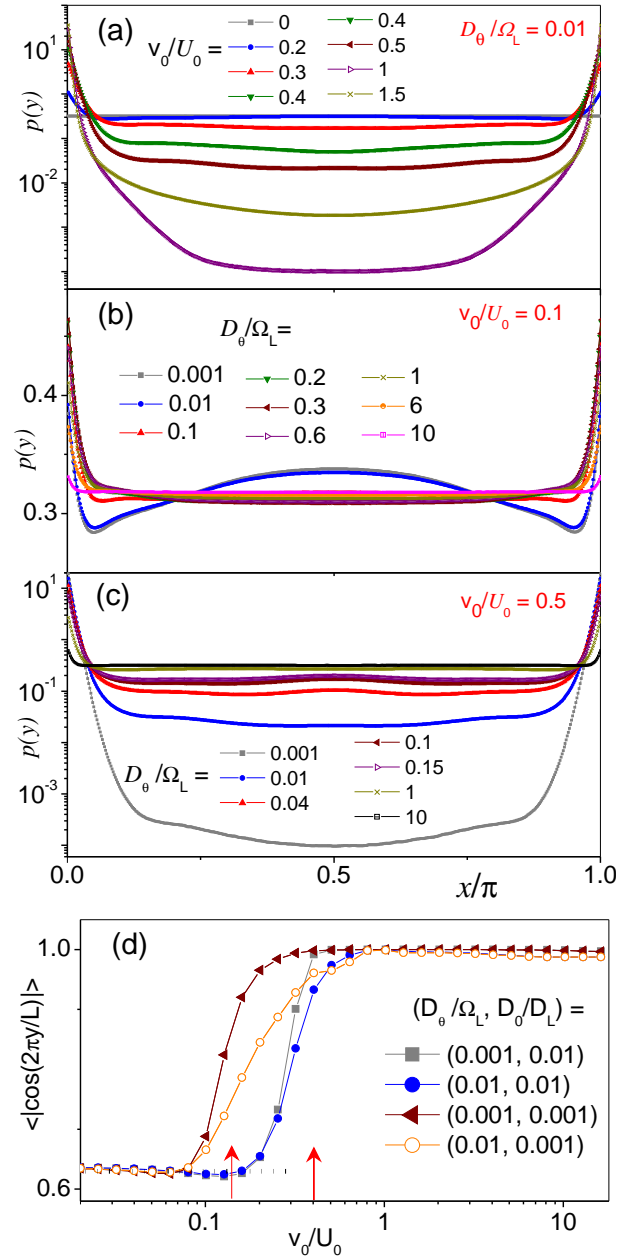
nario suggested by the  $D$  curves in the limit  $v_0/U_0 \rightarrow 0$ . All curves overlap, insensitive to  $D_\theta$ , and, more remarkably, tend to the advection enhanced diffusivity estimate,  $D = \kappa\sqrt{D_L D_0}$ , for passive pointlike particles<sup>19</sup>. Such a behavior persists for  $v_0$  up to an upper value, which appears to agree well with our estimate for  $v_c$  in Eq. (3). This picture holds also at lower thermal noise strengths, Fig. 3(b) and Appendix C (though not with as good statistics). This result confirms that for  $v_0 < v_c$  the array's edges make the JP self-propulsion velocity,  $\bar{v}_0$ , to line up with the advection drag,  $\bar{v}_\psi$ , so that the JP diffuses only through the FBL network due to thermal fluctuations, .

The intermediate regime,  $v_c < v_0 U_0$ , is characterized by a sharp drop of the particle's diffusivity. This is a signature of its pinning to the array's edges. For  $D_\theta/\Omega_L \ll v_0/U_0$ , the particle can slide along the edges only by overcoming the advection washboard potential of amplitude  $D_L|\langle\cos(2\pi y/L)\rangle|$ . In the limit of very low noises,  $D_0/D_L, D_\theta/D_L \rightarrow 0$ , this occurs for  $v_0 \sim U_0$ . For  $D_0/D_L \ll \{|\langle\cos(2\pi y/L)\rangle|, v_0/U_0\}$ , its diffusion constant drops to exponentially small values<sup>36</sup>, which could not be computed numerically. On increasing  $D_0$  and (or)  $D_\theta$ , the amplitude of the pinning potential diminishes, and the particle's diffusivity becomes numerically appreciable; eventually, the diffusion dips because pinning becomes negligible.

Interesting is the shift of the  $D$  minima to higher  $v_0$  values with increasing  $D_0$  (inset of Fig. 3). This counterintuitive effect, is due to the fact that for  $D_\theta/\Omega_L < D_0/D_L \ll 1$ , the JP self-propulsion velocity,  $\bar{v}_0$ , changes direction owing to the combined action of thermal noise (pulling the particle away from its pinning site) and advection (exerting a torque on it). A larger dispersion of the JP orientation angle,  $\theta$ , with thermal noise, implies a higher depinning value of  $v_0$ . We stress here, once again, the role of advection along the array's edges. In a periodic 2D convection array of stream function (1), the  $v_0$ -dependence of  $D$  is quite different<sup>31,32</sup>. In the noiseless limit, a spherical JP gets trapped for  $v_0$  lower than the threshold  $v_{th} \simeq 2.2 U_0$ <sup>32</sup>. After a generally long transient, during which it keeps roll jumping, the particle eventually ends being uniformly distributed inside a single convection roll (i.e., with  $v_c = 0$ ). Here, instead, advection at the array's edges lowers the trapping threshold down to  $U_0$ .

As anticipated above and illustrated in Fig. 4,  $D_\theta$ , is an important control parameter, because it governs orientation and persistence of self-propulsion. When  $D_\theta$  is so large that  $D_s$  is negligible compared to  $D_0$ ,  $D_\theta/\Omega_L \gg (D_L/D_0)(v_0/U_0)^2$ , the passive particle regime is recovered, no matter the value of  $v_0$ . In Fig. 4 we set  $D_0 < D_L$ , i.e.,  $Pe \gg 1$ : therefore, for  $D_\theta/\Omega_L \rightarrow \infty$ , all  $D$  curves plotted there tend to the same (high Péclet number) advection enhanced diffusivity value,  $D = \kappa\sqrt{D_L D_0}$ . More remarkably, the two curves with  $v_0 < v_c$  only slightly deviate from that value throughout the entire  $D_\theta$  domain. This result is a further evidence of the particle's confined circulation inside the FBLs.

The curves for  $v_c < v_0 U_0$  overshoot the advection enhanced diffusivity value, with overlapping maxima at  $D_\theta \sim \Omega_L$ . This effect is due to the synchronized action of angular diffusion and advection torque. The two, combined, optimize the mechanism of edge switching, whereby the JP moves from one pinning site at the bottom to a pinning site at the top, and vice versa. As such



**Fig. 5** Stationary transverse distributions: (a)-(c) transverse density functions,  $p(y)$ , corresponding to the longitudinal distributions,  $p(x)$ , of Fig. 2; (d)  $\langle|\cos(2\pi y/L)|\rangle$  vs.  $v_0/U_0$ . Simulation parameters in (a)-(c) are the same as in the corresponding panels of Fig. 2; if not specified otherwise in the legend, the same parameters have been adopted in (d). Vertical arrows mark our estimates for  $v_c$  at  $D_0 = 0.01$  and  $0.001$ , Eq. (3).

pinning sites are (at least) a distance  $L/2$  apart, edge switching enhances lateral diffusion against edge pinning. Under these conditions (Fig. 4), the leading contribution to the diffusion constant is  $D = (L/2\pi)^2 \Omega_L/2$ , i.e.,  $D/D_L \simeq 1/2$ , independent of  $v_0$  and  $D_0$  (Appendix A).

The curves for  $v_0 \gg U_0$ , as anticipated above, are mostly governed by self-propulsion. For a wide  $D_\theta$  range, they closely follow the free diffusion law,  $D = D_0 + D_s$ , like in a straight zero-flow channel, even when  $l_\theta > L/2$  (as a consequence of the reflecting boundaries). However, having chosen  $D_0 \ll D_L$ , at larger  $D_\theta$  the JP free diffusion constant,  $D_0 + D_s$ , grows smaller than  $D_L$ : Particle's diffusion then takes place at effective high Péclet numbers and the advection enhanced diffusivity mechanism applies, hence  $D = \kappa \sqrt{D_L(D_0 + D_s)^{31}}$ . These two distinct diffusion laws are both illustrated in Figs. 3 and 4.

All  $D$  curves with  $v_0 > v_c$  in Fig. 4 share a surprising property: Upon lowering  $D_\theta$ , they drop below the free diffusion value,  $D_0$ . This suggests that for  $v_0 > v_c$  and large  $\tau_\theta$  advection at the array edges is never negligible. We already noticed that a JP with  $l_\theta > L/2$  trapped at the array's edges can free itself either by sliding against the advection drag or by switching edge. We also know that in the limit  $D_0/D_L, D_\theta/D_L \rightarrow 0$ , a particle pointing against an edge with  $|\cos \theta| < U_0/v_0$  ends up sitting in a stagnation corner, i.e., sliding can be suppressed even for  $v_0 \gg U_0$ . Diffusion is then activated by autonomous edge switching, which, for a JP, can occur through either angular reorientation, with time constant  $\tau_\theta$ , or translational diffusion, with time constant  $\tau_D = (L/2\pi)^2/2D_0$  (Appendix A). For  $v_0 \gg U_0$ , depinning from the edge washboard potential requires  $|\theta| > U_0/v_0$ , therefore, angular diffusion ceases driving edge switching when  $2D_\theta \tau_D < (U_0/v_0)^2$ , or  $D_\theta < D_\theta^*$ , with

$$D_\theta^*/\Omega_L = (U_0/v_0)^2 (D_0/D_L). \quad (4)$$

As shown in Fig. 4, lowering  $D_\theta$  below  $D_\theta^*$  causes a sharp drop of the  $D$  curves to values so small that they could not be numerically computed with acceptable accuracy. This effect is clearly due to geometric confinement, as confirmed by the fact that it was never detected in 2D flows<sup>31</sup>.

## 5 Concluding remarks

We have investigated the diffusion of an active JP in a 1D array of counter-rotating convection rolls. The JP considered here should be regarded as modeling a self-propelling micro-swimmer of biological or synthetic nature, alike. Our choice for the laminar flow is meant to mimic the Rayleigh-Bénard rolls occurring between two parallel (free-slip) surfaces: by varying the temperature difference between them it is possible to vary the advection speed of the suspension fluid with respect to the speed of the active JP and thus explore the parameter space investigated in the present paper.

We focused on effects due the combination of three key ingredients, namely, thermal noise, advection and self-propulsion, in a confined geometry. Such effects, not detectable in 2D arrays of convection rolls with same hydrodynamical parameters but no boundaries, can be summarized as follows:

(i) The large-scale circulation of a JP trapped in a convection roll

is confined to narrow flow boundary layers, whereby the particle self-propulsion velocity tends to line up with the advection drag, which results in an accumulation of the particle probability density.

(ii) The diffusion of an active JP with low self-propulsion speed is governed by its circulation along the roll boundaries, and is thus undistinguishable from that of a regular passive particle.

(iii) For larger self-propulsion speeds, the JP tends to sojourn in the vicinity of the array's edges and diffuses by sliding along them. Its diffusion is dominated by the advection drag parallel to the array's boundaries even for self-propulsion speeds much larger than the advection drag. This mechanism works for strengths of the angular noise above a certain threshold; below that threshold, the particle's diffusion constant drops to vanishingly small values.

Our emphasis on the above confinement effects is motivated by the widespread interest in controlling transport of diluted active matter<sup>3,4</sup> in microfluidic circuits<sup>13</sup>.

To this regard we note that, due to the large variability of the advection parameters in actual Rayleigh-Bénard cells<sup>14,25</sup> [ $L$  and  $U_0$  in the model of Eq. (1)] and the self-propulsion mechanisms<sup>5,8</sup> [ $v_0$  and  $D_\theta$  in the JP model of Sec. 2], all three diffusion regimes listed above are experimentally accessible. Both organic and synthetic microswimmers could be employed to investigate advection effects on the active diffusion in laminar flow patterns. Next focus of the present project is the self-assembly of advected JPs. Indeed, mixtures of both passive and active JPs are known to form a variety of superstructures<sup>2-4</sup> mostly because of the hydrodynamic effects associated with the particle self-propulsion and the particle-particle interactions, all effects which have been neglected in this first report.

Finally, we remark that the overall picture presented here holds for rigid (or no-slip) boundary arrays, as well. Numerical results for the stream function,

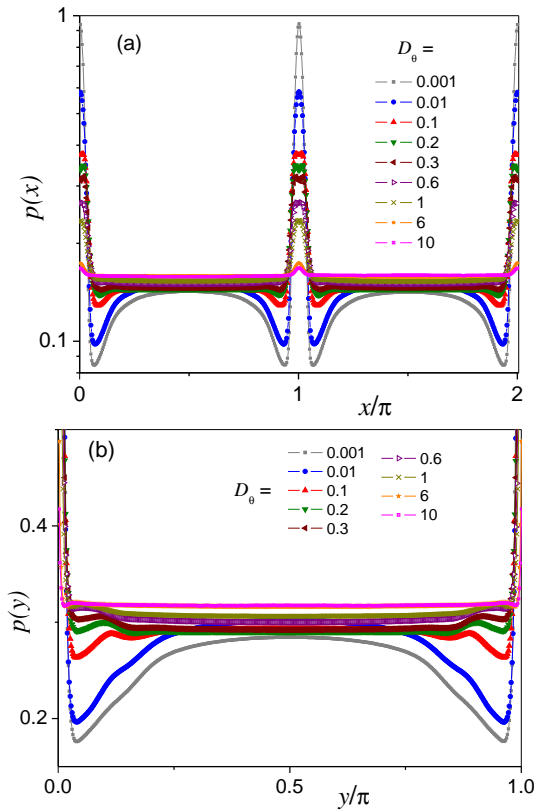
$$\psi(x, y) = (U_0 L/2\pi) \sin(2\pi x/L) \sin^2(2\pi y/L), \quad (5)$$

are reported in Figs. 3 and 4 for a comparison. The breakdown of the FBL circulation with increasing  $v_0$  is still detectable, though not as sharp as in free-boundary convection arrays. In Fig. 3 the dips of the  $D$  curves occur at lower values of  $v_0$  and are less pronounced. This happens because a particle moving against the edges of the array of Eq. (5) is advection free: it moves subjected to the sole thermal noise; correspondingly, the FBL width shrinks. For the same reason, in Fig. 4 the  $D$  curves never drop below  $D_0$ .

## A Model's time scales

The diffusion process of Eq. (2) is characterized by many dynamical parameters. In particular, in our analysis of the diffusion data we made use of various time scales, which we now recap for reader's convenience, with reference to the underlying dynamical mechanisms:

(i) *Angular diffusion.* In Eq. (2), the self-propulsion velocity vector,  $\vec{v}_0$ , was assumed to have constant modulus,  $v_0$ , and fluctuating orientation with angle  $\theta(t)$ . In the absence of advection,  $U_0 = 0$ , we know that<sup>10,38</sup>,  $\langle v_i(t)v_i(0) \rangle = (v_0^2/2) \exp(-D_\theta |t|)$ , with  $i = x, y$ . These autocorrelation functions prove that the angular



**Fig. 6** Stationary distributions,  $p(x)$  and  $p(y)$ , for different  $D_\theta$  with the same simulation parameters as in panels (b) of Figs. 2 and 5, except for  $D_0 = 0.001$ . Note that here Eq. (3) yields  $v_c = 0.13$ .

noise strength,  $D_\theta$ , plays the role of angular diffusion rate and, accordingly,

$$\tau_\theta = 1/D_\theta, \quad (6)$$

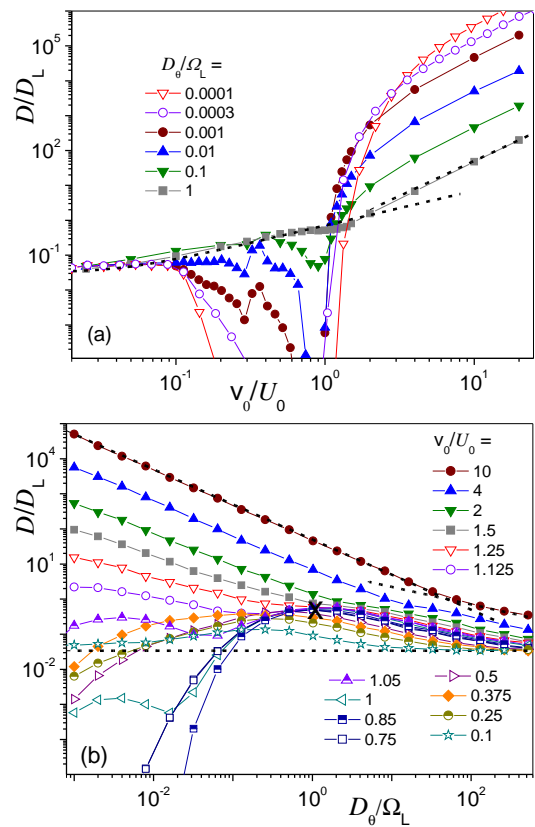
defines the persistence time of the ensuing active Brownian motion of the self-propelling JP. (ii) *Roll circulation*. Due to advection, a particle trapped in a convection roll, is dragged along a circular FBL of approximate radius  $L/4$  with speed  $U_0$ . This means that the particle circulates inside the trapping roll with period of the order of  $\tau'_L = \pi L/2U_0$  or, equivalently, angular frequency  $\Omega'_L = 4U_0/L = (2/\pi)\Omega_L$ . Therefore, consistently with the current literature, we agreed to use the standard definition of circulation time scale<sup>35</sup>, namely

$$\tau_L = 2\pi/\Omega_L = L/U_0. \quad (7)$$

(iii) *Thermal diffusion*. Subjected to thermal noise, the suspended particle diffuses across the array with mean first-passage time<sup>1</sup>  $\tau'_D = (L/2)^2/2D_0$ . Advection drag and thermal diffusion are comparable when  $\tau'_D/\tau'_L \sim 1$ . In the text, this condition has been reformulated more conveniently as  $\Omega_L\tau_D \sim 1$ , with

$$\tau_D = (L/2\pi)^2/2D_0. \quad (8)$$

(iv) *Ballistic self-propulsion*. In the absence of angular diffusion,  $D_\theta = 0$ , the JP crosses ballistically a unit flow cell with time constant  $\tau'_0 = L/|v_x| = \pi L/2v_0$ . In this regime, the action of advection and self-propulsion are comparable under the condition



**Fig. 7** Longitudinal diffusion of a JP in the laminar flow of Eq. (1): same as in Fig. 3, (a), and Fig. 4, (b), but for  $D_0 = 0.001$ .

that  $\tau'_0 \sim \tau'_L$ , or, equivalently,  $\tau_0 \sim \tau_L$ , with

$$\tau_0 = L/v_0. \quad (9)$$

It should be noted that ballistic effects due to self-propulsion are negligible with respect to advection and the array's geometry, respectively under the conditions  $\Omega_L\tau_0 \gg 1$  and  $D_\theta\tau_0 \gg 1$ , that is, for  $v_0 \ll U_0$  and  $D_\theta/\Omega_L \gg v_0/U_0$ <sup>31</sup>.

Equations (6)-(9) define the time scales used in our analysis of the simulation data displayed in Figs. 3 and 4. They can also be combined to obtain convenient estimates of the reference diffusion scales introduced in Sec. 4. Firstly, based on our derivation of  $\Omega'_L$ , the diffusing particle is advected across the array width  $L/2$  with effective speed  $(2/\pi)U_0$ <sup>39</sup>. This means that by hitting the roll boundaries it undergoes a large-scale diffusion with diffusion constant  $D = (1/2)(L/2)(2U_0/\pi) = D_L$ , which coincides with the diffusion scale associated with the stream function of Eq. (1). Secondly, in Sec. 3, the FBL of a convection roll has been modeled as an annulus of radius  $L/4$  and width  $\delta = (D_0/\Omega_L)^{1/2}$ ; accordingly, it covers a fraction  $\phi = 2\pi\delta/L$  of the roll's surface. We know that, for  $v_0 < v_c$ , the large-scale diffusion of a JP, with diffusion constant  $D_L$ , is restricted to the FBL network. Therefore, its effective diffusion constant is  $D = \phi D_L$ , that is,  $D = \sqrt{D_L D_0}$ . This simple argument reproduces the result of Ref.<sup>19</sup> with  $\kappa = 1$  instead of the more accurate  $\kappa = 1.07$ .



## B Transverse distributions

We present in Fig. 5 the transverse distributions,  $p(y)$ , corresponding to the longitudinal distributions,  $p(x)$ . Combined with Figs. 1(c),(d) and 2 of Sec. 3, this figure illustrates the large-scale circulation of a JP with  $v_0 < v_c$  and the break-up of the FBLs for  $v_0 > v_c$ . The depletion of the inner region of the convection rolls is the most pronounced for  $v_0 \simeq U_0$  [Fig. 5(a)], which corresponds to the strongest interplay of advection and self-propulsion. In Fig. 5(d), the FBL break-up causes the sharp jumps of  $\langle |\cos(2\pi y/L)| \rangle$ , from 0 to 1 at  $v_0 \sim v_c$ .

Moreover, we stated in Sec. 3 that the flattening of the  $p(x)$  for  $v_0 \gg U_0$  is due to the symmetric particle accumulation against both array's edges. That statement is supported here by the profile of the corresponding  $p(y)$  curves of Fig. 5(a), which, indeed, exhibit sharp maxima at  $y = 0$  and  $y = L/2$ .

We remind once again that the nonuniform distributions  $p(x)$  and  $p(y)$  are peculiar of 1D convection arrays. Indeed, particle accumulation inside the FBLs for  $v_0 < v_c$  and against the array's edges for  $v_0 > v_c$  is an effect of geometric confinement. Numerical simulations of an active JP in the 2D flow of Eq. (1), with periodic boundary conditions in the  $x$  and  $y$  direction, returned uniform longitudinal and transverse distribution for any value of  $v_0$  (not shown).

## C The role of thermal noise

For brevity, in Secs. 3 and 4 we did not dwell on the role thermal noise. We just stressed that its strength,  $D_0$ , was set much smaller than the advection diffusion scale,  $D_L$ . Accordingly, we defined the Péclet number as  $Pe = D_L/D_0$ . We then mentioned that  $D_0$  enters our estimates of both the FBL width,  $\delta = (D_0/\Omega_L)^{1/2}$ , and the break-up threshold,  $v_c$ , in Eq. (3).

To support those statements we present here simulation results for the 1D distributions,  $p(x)$  and  $p(y)$ , and the asymptotic diffusion constant,  $D$ , obtained for a value of  $D_0$  one order of magnitude smaller than in Figs. 2-4. On comparing Fig. 6(a) with Fig. 2(b), it is apparent that the FBL width shrinks with increasing  $D_0$ . Analogously, the existence of the threshold  $v_c$  and its dependence on  $D_0$  are confirmed by the curves  $D$  versus  $v_0$ , in Fig. 7(a), and  $D$  versus  $D_\theta$ , in Fig. 7(b) [see also Fig. 5(d)].

The overall behavior of the diffusion curves in Figs. 7 is consistent with that displayed in Figs. 3 and 4. For instance, in Fig. 7(b) all curves with  $v_c < v_0 U_0$  attain the same maximum,  $D/D_L \simeq 1/2$  at  $D_\theta/\Omega_L = 1$ , as in Fig. 4, i.e., independently of  $D_0$ . However, a few differences are worthy to note: (i) Diffusion in the pinning range,  $v_c < v_0 U_0$ , of Fig. 7(a) reveals additional details, which went unnoticed in Fig. 3; (ii) These details reflect into the non-monotonic  $D_\theta$ -dependence of the corresponding  $D$  curves in Fig. 7(b); (iii) The interplay between thermal,  $D_0$ , and angular noise,  $D_\theta$ , causes the double-peaked aspect of the  $p(x)$  maxima in Fig. 6(a) [absent in Fig. 2(b)]. These details do not affect the main conclusions of our work. We also remark here that obtaining simulation data with a good statistics at very low noise levels,  $D_0 \rightarrow 0$  and (or)  $D_\theta \rightarrow 0$ , would require exceeding computational resources. For this reason we could not push our numerical investigation to lower  $D_0$  values.

A more substantial difference between Figs. 4 and 7(b) regards the curves with  $v_0 \gg U_0$ . In Fig. 7(b) those curves seem to not bend downward upon decreasing  $D_\theta$ . This is due to the fact that, consistently with Eq. (4), for the simulation parameters of Fig. 7 the estimated position of their maxima,  $D_\theta^*$ , is not captured by the numerically accessible  $D_\theta$  range.

## Conflicts of interest

There are no conflicts to declare.

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