

Active particle motion in Poiseuille flow through rectangular channelsRahil N. Valani ^{1,3,*} Brendan Harding ² and Yvonne M. Stokes ¹¹*School of Computer and Mathematical Sciences, University of Adelaide, South Australia 5005, Australia*²*School of Mathematics and Statistics, Victoria University of Wellington, Wellington 6012, New Zealand*³*Rudolf Peierls Centre for Theoretical Physics, Parks Road, University of Oxford, OX1 3PU, United Kingdom*

(Received 2 June 2024; accepted 1 August 2024; published 5 September 2024)

We investigate the dynamics of a pointlike active particle suspended in fluid flow through a straight channel. For this particle-fluid system, we derive a constant of motion for a general unidirectional fluid flow and apply it to an approximation of Poiseuille flow through channels with rectangular cross-sections. We obtain a 4D nonlinear conservative dynamical system with one constant of motion and a dimensionless parameter describing the ratio of maximum flow speed to intrinsic active particle speed. Applied to square channels, we observe a diverse set of active particle trajectories with variations in system parameters and initial conditions which we classify into different types of swinging, trapping, tumbling, and wandering motion. Regular (periodic and quasiperiodic) motion as well as chaotic active particle motion are observed for these trajectories and quantified using largest Lyapunov exponents. We explore the transition to chaotic motion using Poincaré maps and show “sticky” chaotic tumbling trajectories that have long transients near a periodic state. We briefly illustrate how these results extend to rectangular cross-sections with a width-to-height ratio larger than one. Outcomes of this paper may have implications for dynamics of natural and artificial microswimmers in experimental microfluidic channels that typically have rectangular cross sections.

DOI: [10.1103/PhysRevE.110.034603](https://doi.org/10.1103/PhysRevE.110.034603)**I. INTRODUCTION**

Active particles are entities that take energy from the environment and convert it into persistent motion. Examples include macroscopic living organisms, such as birds, fish, and mammals, which consume energy from food and self-propel via various modes of locomotion. Active particles are also ubiquitous in the microscopic living world such as bacteria, cells, algae, and other microorganisms [1]. Although persistent motion is a visible feature that is commonly associated with life, active particles also emerge in several nonequilibrium inanimate physical and chemical systems [2–6].

Active particles immersed in a fluid medium at the microscale, also known as microswimmers, are a commonly studied class of active particles [7]. These microswimmers ubiquitously interact with external fluid flows in various situations. For example, microswimmers routinely experience unidirectional flows in confined channels such as sperm cells swimming in fallopian tubes [8,9], pathogens moving through blood vessels [10], and microrobots programmed for targeted drug delivery applications [11]. In these scenarios, the coupling between external flow fields and intrinsic velocity of the active particle can lead to rich dynamical behaviors [12].

Understanding the active particle dynamics arising from coupling with external fluid flows is not only interesting from a biological perspective, but is also crucial for design of artificial microswimmers for biomedical applications of cell manipulation, targeted drug delivery and cargo transport [13]. Further, it can aid design of industrial and biomedical microfluidic devices aimed at focusing, sorting, and filtering of microorganisms in a fluid suspension [14,15].

Zöttl and Stark [16] studied the motion of a microswimmer in unidirectional confined flows by modeling the active particle as a spherically symmetric point with constant intrinsic velocity. For 2D planar Poiseuille flow, they showed that the equation of motion for the active particle can be mapped onto the mathematical equation of a simple pendulum, where the oscillating and circling solutions of the pendulum motion correspond to two different types of active particle motion, swinging and tumbling, respectively. In swinging motion, the upstream-oriented active particle performs oscillations about the channel centerline, whereas in tumbling motion, the active particle oscillates near the edges of the channel with fluctuating orientation and does not cross the channel centerline. Variations of this model that include additional attributes to the active particle and/or fluid flow have been investigated in detail for 2D channel flows [17–22]. For 3D cylindrical Poiseuille flow, Zöttl and Stark [16] showed that the particle-fluid dynamical system is Hamiltonian with enough conserved quantities to make the system integrable. In this case, they showed that the active particle exhibits periodic motion with 3D generalizations of swinging and tumbling trajectories. The effect of flow anisotropy was also studied by Zöttl and Stark [22] who showed, for an elliptical channel cross section,

*Contact author: rahil.valani@physics.ox.ac.uk

Published by the American Physical Society under the terms of the [Creative Commons Attribution 4.0 International](https://creativecommons.org/licenses/by/4.0/) license. Further distribution of this work must maintain attribution to the author(s) and the published article's title, journal citation, and DOI.

that the active particle motion is much more complex with, typically, quasiperiodic trajectories. Using Poincaré maps, a few examples of chaotic motion were also reported by Zöttl [23].

Although the axisymmetric fluid flow profile in a cylindrical channel results in simplified equations for the active particle motion, in many microfluidic applications concerned with natural and artificial microswimmers, microchannels with rectangular cross sections are more commonly used since they are relatively easy to fabricate [24]. Motivated by this, herein we apply the model of Zöttl and Stark [16] to explore the dynamics of a simple active particle suspended in Poiseuille flow through a straight channel having a square or rectangular cross section. The introduction of a square or rectangular cross section introduces anisotropy, by breaking the continuous rotational symmetry of fluid flow that exists in a circular cross section, and makes the system nonintegrable. We observe a rich variety of active particle motion with both quasiperiodic and chaotic trajectories. These motions are explored in detail as a function of system parameters and initial conditions.

The paper is organized as follows. In Sec. II, we present the equations of motion for the particle-fluid system and derive general constants of motion for an active particle in unidirectional fluid flow. We then, in Sec. III, identify equilibrium states for an active particle suspended in Poiseuille-like flow through a rectangular cross section and determine their stability. After briefly reviewing the special case of active particle motion in a channel with a circular cross section in Sec. IV, we present a detailed exploration of active particle dynamics in a channel with a square cross section in Sec. V. This includes a classification of trajectories, comparison with dynamics in a circular cross section, a detailed parameter space exploration of cross-sectional active particle dynamics, as well as an investigation of the transport of an active particle along the channel. In Sec. VI, we briefly explore the effect of the width-to-height ratio of the rectangular cross section on active particle motion. We provide our conclusions in Sec. VII.

II. EQUATIONS OF MOTION

Consider the pointlike active particle model of a spherical microswimmer illustrated in Fig. 1. The active particle has a constant intrinsic swimming speed v_0 in the direction of its orientation $\hat{\mathbf{e}} = e_x \hat{\mathbf{i}} + e_y \hat{\mathbf{j}} + e_z \hat{\mathbf{k}}$, is located at $\mathbf{r} = x\hat{\mathbf{i}} + y\hat{\mathbf{j}} + z\hat{\mathbf{k}}$, and is suspended in a steady unidirectional flow $u(x, y)\hat{\mathbf{k}}$ through a straight 3D channel. The equations of motion for the active particle are given by [16]

$$\frac{d\mathbf{r}}{dt} = v_0 \hat{\mathbf{e}} + u(x, y)\hat{\mathbf{k}}, \quad (1a)$$

$$\frac{d\hat{\mathbf{e}}}{dt} = \frac{1}{2}(\nabla \times u(x, y)\hat{\mathbf{k}}) \times \hat{\mathbf{e}}. \quad (1b)$$

Equation (1a) describes the translational motion of the active particle as a combination of its intrinsic velocity $v_0 \hat{\mathbf{e}}$ and the local velocity of the background fluid flow $u(x, y)\hat{\mathbf{k}}$, whereas Eq. (1b) describes the evolution of the active particle's orientation based on the local flow vorticity. We assume that the active particle is small compared to the cross-sectional

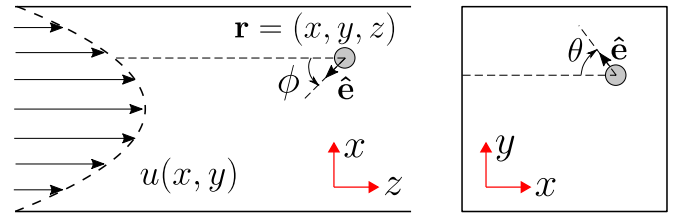


FIG. 1. Schematic of the particle-fluid system. A simple pointlike active particle located at $\mathbf{r} = (x, y, z)$ and having a constant intrinsic speed in the direction of its orientation $\hat{\mathbf{e}}$ is suspended in a unidirectional channel flow $u(x, y)$ through a straight 3D rectangular channel with width-to-height aspect ratio \mathcal{A} . The particle's orientation is represented using spherical coordinates with polar angle $\theta \in (-\pi/2, \pi/2)$ measuring the orientation relative to the $x-z$ plane, and azimuthal angle $\phi \in (-\pi, \pi]$ measuring the angle within the $x-z$ plane relative to the (negative) z axis. The left panel shows the top view of the channel in the $x-z$ plane while the right panel shows the cross-sectional view of the channel in the $y-x$ plane.

dimensions of the channel, and hence the particle does not disturb the fluid flow. Further, we assume that the active particle stays away from bounding walls, so we can neglect interactions and collisions between the active particle and the walls.

Nondimensionalizing Eqs. (1) with a characteristic length scale H of the cross section and timescale H/v_0 , we obtain the following dimensionless equations:

$$\frac{d\bar{\mathbf{r}}}{d\bar{t}} = \hat{\mathbf{e}} + \bar{u}(\bar{x}, \bar{y})\hat{\mathbf{k}}, \quad (2a)$$

$$\frac{d\hat{\mathbf{e}}}{d\bar{t}} = \frac{1}{2}(\bar{\nabla} \times \bar{u}(\bar{x}, \bar{y})\hat{\mathbf{k}}) \times \hat{\mathbf{e}}. \quad (2b)$$

Here, the dimensionless variables are denoted with an overbar and the dimensionless flow field $\bar{u}(\bar{x}, \bar{y})$ is scaled with the active particle speed v_0 . We now drop the overbars on dimensionless variables for convenience. In component form, we get a system of six nonlinear ordinary differential equations (ODEs) as follows:

$$\begin{aligned} \dot{x} &= e_x, & \dot{e}_x &= -\frac{1}{2}e_z \frac{\partial u}{\partial x}, \\ \dot{y} &= e_y, & \dot{e}_y &= -\frac{1}{2}e_z \frac{\partial u}{\partial y}, \\ \dot{z} &= e_z + u(x, y), & \dot{e}_z &= \frac{1}{2}e_x \frac{\partial u}{\partial x} + \frac{1}{2}e_y \frac{\partial u}{\partial y}. \end{aligned}$$

We note from the component form that the dynamical flow is divergence-free, that is,

$$\frac{\partial \dot{x}}{\partial x} + \frac{\partial \dot{y}}{\partial y} + \frac{\partial \dot{z}}{\partial z} + \frac{\partial \dot{e}_x}{\partial e_x} + \frac{\partial \dot{e}_y}{\partial e_y} + \frac{\partial \dot{e}_z}{\partial e_z} = 0.$$

Hence, the dynamical system is conservative and phase-space volumes are preserved under the dynamical flow. We further note that the z variable can be decoupled, i.e., the \dot{z} equation can be integrated separately, thus reducing our dynamical system to five differential equations. The effective dimension of our dynamical system is further reduced by identifying constants of motion, i.e., quantities that remain constant during the evolution of the system. A trivial constant of motion for

our system is

$$|\hat{\mathbf{e}}|^2 = e_x^2 + e_y^2 + e_z^2 = 1, \quad (3)$$

since the orientation vector maintains unit magnitude. We have also identified a second constant of motion as (see Appendix A for a proof)

$$H_g = -\frac{1}{2}u(x, y) + e_z. \quad (4)$$

With these two constants of motion, our five-dimensional dynamical system reduces to three effective dimensions. We can implicitly use the constant of motion in Eq. (3) and reduce our system to four nonlinear ODEs by parametrizing the Euler axis using spherical coordinate angles θ and ϕ as follows:

$$e_x = -\cos\theta \sin\phi,$$

$$e_y = \sin\theta,$$

$$e_z = -\cos\theta \cos\phi.$$

Here, $\theta \in (-\pi/2, \pi/2)$ is the polar angle measuring the orientation relative to the $x-z$ plane, while $\phi \in (-\pi, \pi]$ is the azimuthal angle measuring the orientation component within the $x-z$ plane relative to the negative z axis (see Fig. 1). This parametrization gives us the following four coupled nonlinear ODEs:

$$\dot{x} = -\cos\theta \sin\phi, \quad (5a)$$

$$\dot{y} = \sin\theta, \quad (5b)$$

$$\dot{\theta} = \frac{1}{2} \frac{\partial u}{\partial y} \cos\phi, \quad (5c)$$

$$\dot{\phi} = \frac{1}{2} \frac{\partial u}{\partial y} \tan\theta \sin\phi - \frac{1}{2} \frac{\partial u}{\partial x}, \quad (5d)$$

along with the constant of motion in Eq. (4), which is rewritten in the above parametrization as

$$H_g = -\frac{1}{2}u(x, y) - \cos\phi \cos\theta. \quad (6)$$

We note that up to this point, our consideration of the fluid flow field $u(x, y)$ has been general and hence the constant of motion in Eq. (4) exists independent of the specific flow profile.

We now consider the specific fluid flow profile of Poiseuille flow in a 3D straight channel having a rectangular cross section with width W and height H . With H as the length scale and defining the aspect ratio $\mathcal{A} = W/H$, we approximate the dimensionless flow profile by

$$u(x, y) = U \left(1 - \left(\frac{x}{\mathcal{A}} \right)^2 \right) (1 - y^2), \quad (7)$$

where $U = u(0, 0)$ is the maximum velocity in the channel scaled with the intrinsic particle speed v_0 . This expression provides a good approximation to the exact solution of Poiseuille flow in rectangular channels expressed as an infinite series (see Appendix B). Substituting this flow field in Eqs. (5), we get the following 4D dynamical system [along

with the constant of motion in Eq. (6)]:

$$\dot{x} = -\cos\theta \sin\phi, \quad (8a)$$

$$\dot{y} = \sin\theta, \quad (8b)$$

$$\dot{\theta} = -Uy \cos\phi \left(1 - \frac{x^2}{\mathcal{A}^2} \right), \quad (8c)$$

$$\dot{\phi} = -Uy \tan\theta \sin\phi \left(1 - \frac{x^2}{\mathcal{A}^2} \right) + U \frac{x(1-y^2)}{\mathcal{A}^2}, \quad (8d)$$

where $-\mathcal{A} < x < \mathcal{A}$, $-1 < y < 1$, $-\pi/2 < \theta < \pi/2$ and $-\pi < \phi \leq \pi$.

We solve the dynamical system in Eqs. (8) up to $t = 1000$ (unless stated otherwise) using the ode45 solver in MATLAB with relative and absolute tolerance of 10^{-10} . These very small tolerances ensure that numerical variations in the constants of motion are less than 10^{-8} for the duration of simulations.

III. EQUILIBRIUM STATES AND STABILITY

We start by finding equilibrium states of the dynamical system that would correspond to an active particle with a fixed cross-sectional location and a fixed orientation. This is done by making the time derivatives zero in Eqs. (8) and solving the resulting nonlinear algebraic equations. We find the following two equilibrium states:

$$(x^*, y^*, \theta^*, \phi^*) = (0, 0, 0, 0) \text{ and } (0, 0, 0, \pi).$$

The first equilibrium (with $\phi^* = 0$) corresponds to an active particle oriented upstream at the center of the channel, while the second (with $\phi^* = \pi$) corresponds to an active particle oriented downstream, also at the center of the channel.

To understand the stability of these equilibrium states, we perform a linear stability analysis, thus perturbing the equilibrium states: $(x, y, \theta, \phi) = (x^*, y^*, \theta^*, \phi^*) + \epsilon(x_1, y_1, \theta_1, \phi_1)$, where $0 < \epsilon \ll 1$ is a perturbation parameter. Substituting this in Eqs. (8) and comparing $O(\epsilon)$ terms, we get a matrix equation for the evolution of the perturbation variables $(x_1, y_1, \theta_1, \phi_1)$.

A. Upstream-oriented equilibrium state

For the upstream-oriented equilibrium state $(x^*, y^*, \theta^*, \phi^*) = (0, 0, 0, 0)$, we obtain the following linear equation that governs the evolution of perturbations:

$$\begin{bmatrix} \dot{x}_1 \\ \dot{y}_1 \\ \dot{\theta}_1 \\ \dot{\phi}_1 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & -U & 0 & 0 \\ U/\mathcal{A}^2 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \\ \theta_1 \\ \phi_1 \end{bmatrix}.$$

The stability of the equilibrium state is determined by the nature of the eigenvalues of the right-hand-side matrix [25]. We obtain the following characteristic polynomial equation for eigenvalues λ :

$$\lambda^4 + U \left(1 + \frac{1}{\mathcal{A}^2} \right) \lambda^2 + \frac{U^2}{\mathcal{A}^2} = 0.$$

The roots of this quartic polynomial give the eigenvalues

$$\lambda = \pm i\sqrt{U}, \pm i\frac{\sqrt{U}}{\mathcal{A}}.$$

All the eigenvalues being purely imaginary, this upstream-oriented active particle equilibrium may correspond to a center, a stable spiral or an unstable spiral [25]. However, the conservative nature of our dynamical system makes this equilibrium a center. We will revisit this numerically in Sec. VC. Furthermore, for nonsquare cross sections having an aspect ratio differing from $\mathcal{A} = 1$, the oscillation frequency differs along the two eigenvector pairs corresponding to the two conjugate eigenvalue pairs.

I. Downstream-oriented equilibrium state

For the downstream-oriented equilibrium state $(x^*, y^*, \theta^*, \phi^*) = (0, 0, 0, \pi)$, we obtain the following linear equation describing the evolution of perturbations:

$$\begin{bmatrix} \dot{x}_1 \\ \dot{y}_1 \\ \dot{\theta}_1 \\ \dot{\phi}_1 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & U & 0 & 0 \\ U/\mathcal{A}^2 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \\ \theta_1 \\ \phi_1 \end{bmatrix},$$

with the characteristic equation

$$\lambda^4 - U \left(1 + \frac{1}{\mathcal{A}^2} \right) \lambda^2 + \frac{U^2}{\mathcal{A}^2} = 0.$$

Solving this quartic polynomial gives us the eigenvalues

$$\lambda = \pm\sqrt{U}, \pm\frac{\sqrt{U}}{\mathcal{A}}.$$

Since the eigenvalues are all real, with two positive and two negative, this equilibrium state is an unstable saddle point having both stable and unstable manifolds which are two-dimensional. Again, due to the different magnitudes of eigenvalues for nonsquare cross sections, the rate of instability from the saddle point differs in the directions of the corresponding eigenvectors. We will numerically revisit the dynamics of an active particle starting near this equilibrium state in Sec. VC.

IV. DYNAMICS IN A CYLINDRICAL CHANNEL

Zöttl and Stark [16] studied the nonlinear dynamics of an active particle suspended in fluid flow through a cylindrical channel. For a circular cross section, the flow field is axisymmetric and takes the dimensionless form

$$u_c(x, y) = U(1 - (x^2 + y^2)), \quad (9)$$

(with length variables scaled with the duct radius). For this special case, they identified two constants of motion:

$$H_c = \frac{1}{2}U(x^2 + y^2) + 1 - \cos\phi \cos\theta, \quad (10a)$$

$$L_z = x \sin\theta + y \cos\theta \sin\phi. \quad (10b)$$

Here H_c is a linear transform of the general constant of motion identified in Eq. (6). The new constant of motion L_z arises from the continuous rotational symmetry of the circular cross section and is proportional to the angular momentum of

the active particle in the z direction. This additional constant of motion further reduces the effective dimension of the dynamical system in Eqs. (5) from three to two dimensions. By making a change of coordinates, Zöttl and Stark [16] obtained three nonlinear ODEs with the two constants of motion H_c and L_z , and showed that the active particle motion in a cylindrical channel results in an integrable Hamiltonian system where the motion in the three-dimensional phase space is restricted to a curve formed by the intersection of two surfaces corresponding to H_c and L_z .

V. DYNAMICS IN A SQUARE CHANNEL

We now explore in detail the dynamics of an active particle suspended in fluid flow through a 3D straight channel with a square cross section, i.e., $\mathcal{A} = 1$. We explore the active particle dynamics as a function of the dimensionless parameter U as well as the initial conditions, i.e., the initial position in the cross section $(x(0), y(0))$ and the initial orientation angles $(\theta(0), \phi(0))$.

A. Classification of active particle trajectories

A large diversity of trajectories are observed for the active particle in a square channel by varying the system parameter U as well as the initial conditions. Some typical trajectories and the corresponding orientations are shown in Fig. 2 for $U = 10$. We choose to classify the trajectories into the following six types based on the region they occupy (shown in gray in Fig. 2) at long times within the square cross section: (i) Central swinging motion (green) with trajectories undergoing swinging motion about the channel centerline (similar to swinging motion in cylindrical channel [16]) and confined near the center of the channel to the cross-sectional domain $-0.25 < x, y < 0.25$. (ii) Vertical swinging motion (cyan) with trajectories undergoing swinging motion in the vertical y direction and confined in the x direction to the vertical band $-0.25 < x < 0.25$. (iii) Horizontal swinging motion (blue) with trajectories undergoing swinging motion in the horizontal x direction and confined in the y direction to the horizontal band $-0.25 < y < 0.25$. (iv) Off-centered trapping (yellow) with trajectories confined within a rectangular region of the cross section having an area less than half the area of the cross section; this region may cross at most one centerline of the cross section ($x = 0$ or $y = 0$ or neither) but not both. (v) Tumbling motion (purple) with trajectories that stay outside the central region of the cross section as defined for central swinging, and wander near the channel walls. (vi) Wandering motion (red) with trajectories not in classes (i)–(v) and which, therefore, visit both the central region defined for central swinging motion, as well as the outer region defined for tumbling motion. Numerically, the classification is implemented by only analyzing the latter half of the trajectory to remove any transient dynamical behaviors at short times.

B. Comparison with cylindrical channel

For a square cross section ($\mathcal{A} = 1$), we have the approximate dimensionless fluid velocity from Eq. (7):

$$u_s(x, y) = U(1 - x^2)(1 - y^2) = U(1 - (x^2 + y^2) + x^2y^2).$$

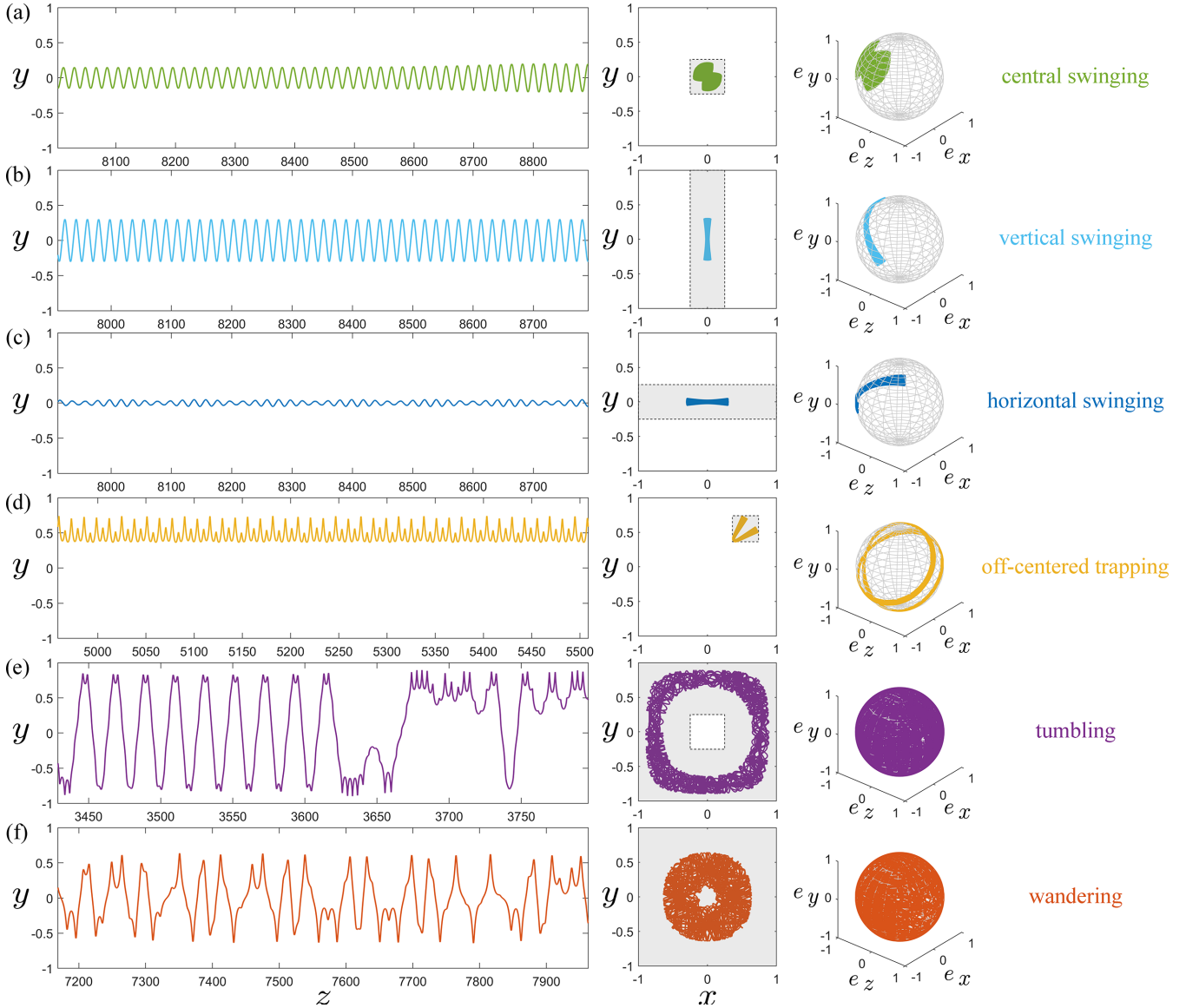


FIG. 2. Classification of active particle motion. Different trajectories of the active particle in a straight channel with square cross section are shown in the (z, y) plane and (x, y) plane based on different initial positions for (a) $(x(0), y(0)) = (0.15, 0.15)$, (b) $(x(0), y(0)) = (0.05, 0.30)$, (c) $(x(0), y(0)) = (0.30, 0.05)$, (d) $(x(0), y(0)) = (0.58, 0.70)$, (e) $(x(0), y(0)) = (0.75, 0.75)$, and (f) $(x(0), y(0)) = (0.55, 0.40)$. At right, the shaded region of the spherical surface shows the time evolution of the particle's orientation. Different colors denote the classification of trajectories based on the region occupied in the cross section (gray shading with dashed boundaries). (a) Central swinging motion (green); trajectories that stay near the center of the channel $-0.25 < x, y < 0.25$. (b) Vertical swinging motion (cyan); trajectories that are confined in the x direction, i.e., inside the vertical band $-0.25 < x < 0.25$. (c) Horizontal swinging motion (blue); trajectories that are confined in the y direction, i.e., inside the horizontal band $-0.25 < y < 0.25$. (d) Off-centered trapping (yellow); trajectories that are confined in a rectangular region of the cross section having an area less than half the area of the cross section and which may cross either centerline ($x = 0, y = 0$), or neither, but not both. (e) Tumbling motion (purple); trajectories that stay near the walls of the channel, i.e., outside the region of central swinging motion. (f) Wandering motion (red); trajectories that explore both the central as well as outer regions of the cross section. Other parameters were fixed to $U = 10, z(0) = 0, \theta(0) = 0$, and $\phi(0) = 0$. See also Supplemental Material Videos S1–S6 [26] for videos of particle trajectories and orientations corresponding to (a)–(f), respectively.

By introducing the following velocity field:

$$u_{cs}(x, y) = U(1 - (x^2 + y^2) + \alpha x^2 y^2), \quad \alpha \in [0, 1],$$

we can continuously transform from the Poiseuille flow of a circular cross section as in Eq. (9) ($\alpha = 0$) to the approximate Poiseuille flow of a square cross section $u_s(x, y)$ ($\alpha = 1$). The corresponding nonlinear ODEs for an active particle within

the flow field $u_{cs}(x, y)$ are

$$\dot{x} = -\cos \theta \sin \phi, \quad (11a)$$

$$\dot{y} = \sin \theta, \quad (11b)$$

$$\dot{\theta} = -Uy \cos \phi + \alpha Ux^2 y \cos \phi, \quad (11c)$$

$$\dot{\phi} = U(-y \tan \theta \sin \phi + x) + \alpha Uxy(x \tan \theta \sin \phi - y). \quad (11d)$$

It can be seen from Eqs. (11) that the equilibrium states and their linear stability are the same for a square cross section (refer to Sec. III for $\mathcal{A} = 1$) and a circular cross section [16]. Specifically, since the α terms present in the $\dot{\theta}$ and $\dot{\phi}$ components of (11) contribute at an order $O(\epsilon^3)$ near the equilibrium points, their effects are not felt at order $O(\epsilon)$.

For our square channel, we only have the constant of motion H_g in Eq. (6) [i.e., having implicitly utilised Eq. (3)]. For ease of comparison with the quantity used by Zöttl and Stark [16] for a circular cross section, H_c of Eq. (10a), we define $H_s = 1 + \frac{1}{2}U + H_g \geq 0$, and express the constant of motion here as

$$H_s = \frac{1}{2}U(x^2 + y^2 - x^2y^2) + 1 - \cos \phi \cos \theta.$$

Furthermore, the time derivative of the second constant of motion L_z for the cylindrical channel in Eq. (10b) has the following form for a square cross section ($\alpha = 1$):

$$\frac{dL_z}{dt} = Uxy \cos \theta \cos \phi (x^2 - y^2). \quad (12)$$

We see that this quantity will not vary significantly when either x or y (or both) are small or when $y \approx \pm x$. Thus, for motion in a square cross section confined near the channel center, along x or y axis or along diagonals, we expect the dynamics of the system to be regular (periodic or quasiperiodic) since the system is close to the cylindrical channel system which is both Hamiltonian and integrable. The central, vertical, and horizontal swinging motions shown in Fig. 2 are examples of this type of motion. Conversely, for general motion that is not restricted to these above regions such that the particle explores regions away from the center of the channel cross section, the system deviates from a Hamiltonian integrable system and chaotic motion may arise. Tumbling and wandering motions (see Fig. 2) are examples of this. A comparison of active particle dynamics between circular and square cross sections for a typical tumbling motion with the same initial conditions $(x(0), y(0), \theta(0), \phi(0)) = (0.55, 0.58, \pi/24, \pi/24)$ is shown in Supplemental Material Video S7 [26].

C. Motion near equilibrium states

Since the equilibrium states of the particle-fluid system are located at the center of the cross section ($x = 0, y = 0$) and the additional nonlinear x^2y^2 term in the square channel flow field is small near these equilibrium points, we expect the motion near the equilibrium states to be similar to that of the circular cross section [16].

The eigenvectors corresponding to eigenvalues $\lambda_{1,2} = \pm i\sqrt{U}$ for the upstream-oriented particle equilibrium are

$$\mathbf{v}_1 = a_1 \begin{bmatrix} 1 \\ 0 \\ 0 \\ -i\sqrt{U} \end{bmatrix} + b_1 \begin{bmatrix} 0 \\ 1 \\ i\sqrt{U} \\ 0 \end{bmatrix}$$

and

$$\mathbf{v}_2 = a_2 \begin{bmatrix} 1 \\ 0 \\ 0 \\ i\sqrt{U} \end{bmatrix} + b_2 \begin{bmatrix} 0 \\ 1 \\ -i\sqrt{U} \\ 0 \end{bmatrix},$$

respectively. Here, $a_1, b_1, a_2,$ and b_2 are complex constants with $\bar{a}_1 = a_2$ and $\bar{b}_1 = b_2$, where the overbar denotes the complex conjugate. For small perturbations around this equilibrium point, we numerically observe periodic and quasiperiodic active particle motion confined near the center of the channel [e.g., see Fig. 2(a) and Supplemental Material Video S1]. We further find that the motion decouples in the (x, ϕ) and (y, θ) variables near this equilibrium point and we obtain the following system for the linearized equations of motion:

$$\begin{aligned} \ddot{\theta}_1 + U\theta_1 &= 0, \\ \dot{y}_1 &= \theta_1, \\ \ddot{\phi}_1 + U\phi_1 &= 0, \\ \dot{x}_1 &= -\phi_1. \end{aligned}$$

Thus, the evolution of active particle orientations θ and ϕ follow simple harmonic motion with oscillating frequency \sqrt{U} and these oscillating orientations drive the translational motion of the active particle near this equilibrium point. Hence, the response to general small perturbations around this equilibrium point is a superposition of the above two decoupled oscillatory motions.

The eigenvectors corresponding to eigenvalues $\lambda_{3,4} = \pm\sqrt{U}$ for the downstream-oriented equilibrium point are

$$\mathbf{v}_3 = a_3 \begin{bmatrix} 1 \\ 0 \\ 0 \\ \sqrt{U} \end{bmatrix} + b_3 \begin{bmatrix} 0 \\ 1 \\ \sqrt{U} \\ 0 \end{bmatrix}$$

and

$$\mathbf{v}_4 = a_4 \begin{bmatrix} 1 \\ 0 \\ 0 \\ -\sqrt{U} \end{bmatrix} + b_4 \begin{bmatrix} 0 \\ 1 \\ -\sqrt{U} \\ 0 \end{bmatrix},$$

respectively, with real constants $a_3, b_3, a_4,$ and b_4 . This equilibrium is a saddle point with its unstable manifold tangent to the hyperplane spanned by the two basis vectors defining \mathbf{v}_3 while its stable manifold is tangent to the hyperplane spanned by the two basis vectors defining \mathbf{v}_4 . To understand the nature of trajectories with small perturbations around this equilibrium point, we simulated motion with different initial perturbations. Some typical trajectories starting near this unstable equilibrium are shown in Fig. 3 for perturbations in the directions of the stable and unstable manifolds as well as a general perturbation. We see that for a perturbation in the direction of the unstable manifold of the saddle, Fig. 3(a) and Supplemental Material Video S8, we obtain a cross-shaped trajectory in the channel cross section that switches aperiodically between the four diagonals. The chaos here appears to be low-dimensional since the trajectory traces a well-defined

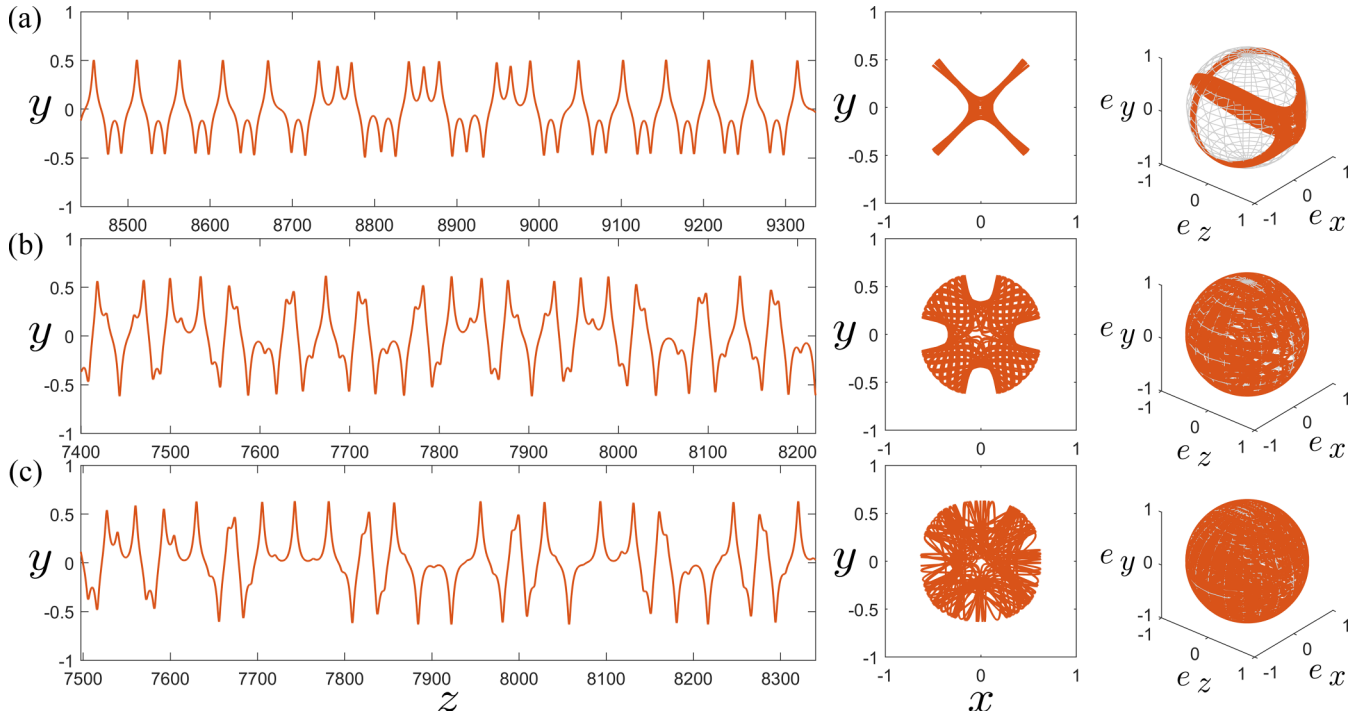


FIG. 3. Active particle motion for small perturbations near the unstable saddle equilibrium. Different trajectories are shown in the (z, y) plane and (x, y) plane for small perturbations (a) in the direction of the unstable manifold $(x(0), y(0), \theta(0), \phi(0)) = (0, 0, 0, \pi) + (0.02, 0.02, 0.02\sqrt{U}, 0.02\sqrt{U})$, (b) in the direction of the stable manifold $(x(0), y(0), \theta(0), \phi(0)) = (0, 0, 0, \pi) + (0.02, 0.02, -0.02\sqrt{U}, -0.02\sqrt{U})$, and (c) a small general perturbation $(x(0), y(0), \theta(0), \phi(0)) = (0, 0, 0, \pi) + (0.01, 0.02, 0.015, -0.005)$. The parameter $U = 10$ was fixed and $z(0) = 0$. See also Supplemental Material Videos S8–S10 [26] for videos of (a)–(c), respectively.

path on the cross shape with unpredictability only in the selection of the branches it traverses. For a perturbation in the direction of the stable manifold, Fig. 3(b) and Supplemental Material Video S9 [26], we obtain a fan-shaped apparently quasiperiodic trajectory, while for a general perturbation as shown in Fig. 3(c) and Supplemental Material Video S10 [26], we obtain a chaotic trajectory with no clear structure. In all cases, we find that a small perturbation from this unstable saddle equilibrium leads to wandering-type trajectories that move away from the equilibrium and explore both the inner and outer regions of the square cross section.

D. Exploration of the parameter space

We have observed that both the initial conditions and the system parameters can greatly influence the type of active particle trajectory that is realized, and have classified these in Fig. 2. In this section, we explore the effects of the initial position and orientation, as well as the parameter U on the active particle motion.

The active particle dynamics are described by the 4D nonlinear dynamical system in Eqs. (8), which requires four initial conditions: two position coordinates $x(0)$ and $y(0)$, and two orientation angles $\theta(0)$ and $\phi(0)$. To explore the solution space across the four initial conditions, we fix two of them and examine the types of active particle trajectories realized in the initial-condition plane formed by the remaining two.

1. Effect of initial position

We first fix the initial orientation of the active particle to point upstream, i.e., $\theta(0) = \phi(0) = 0$, and explore the

variation in active particle trajectories across different initial positions $(x(0), y(0))$. We restrict the domain of initial positions to $x, y \in [-0.8, 0.8]$. This is done to exclude trajectories that get too close to the wall where interactions of the active particle with the wall may become important. A plot depicting the classification of trajectories realized for different initial positions in the cross section when $U = 10$ is shown in Fig. 4(a). We find that for an initial position near the center of the channel, the motion remains confined near the center of the channel as indicated by the green region of Fig. 4(a), and that central swinging motion occurs [see Fig. 2(a)]. An active particle starting out farther away from the center of the channel but near an axis remains confined near the same axis as indicated by the cyan and blue regions of Fig. 4(a), which corresponds to vertical and horizontal swinging motions as in Figs. 2(b) and 2(c). Along the diagonals and/or beyond the central region, Fig. 4(a) shows a red region corresponding to wandering trajectories [see Fig. 2(f)]. Near the edges of the square cross section of Fig. 4(a), we have a purple region corresponding to tumbling trajectories [as in Fig. 2(e)]. Lastly, near the corners, Fig. 4(a) shows islands of yellow in the sea of purple corresponding to off-centered confined motion [as in Fig. 2(d)].

The above trajectory classification in the initial-condition space is based on the region occupied by the trajectory in the cross section and does not necessarily capture information about the regular (periodic and quasiperiodic) or chaotic nature of trajectories. However, we typically find that trajectories which are confined near the center of the channel exhibit regular motion whereas active particles that travel near the edges

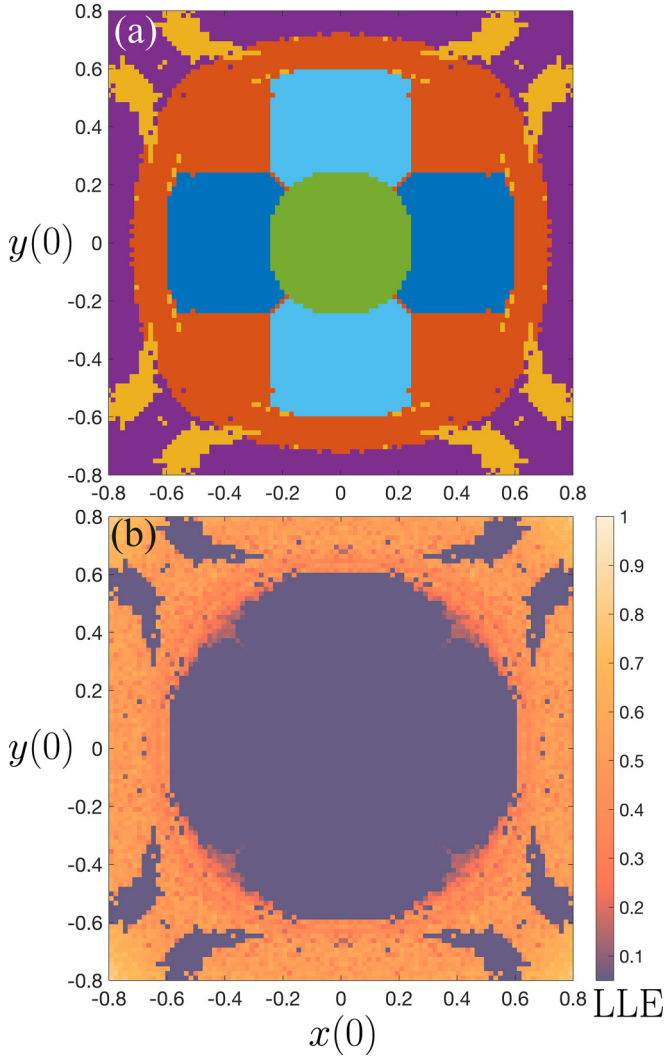


FIG. 4. (a) Classification of active particle trajectories for the types of trajectories shown in Fig. 2, and (b) largest Lyapunov exponent (LLE), each in the initial position $(x(0), y(0))$ plane with fixed $U = 10$, $\theta(0) = 0$ and $\phi(0) = 0$. For trajectory classification, green (●) is central swinging motion, cyan (●) is vertical swinging motion, blue (●) is horizontal swinging motion, yellow (●) is off-centered trapping motion, purple (●) is tumbling motion, and red (●) is wandering motion.

of the cross section show aperiodic motion and hints of chaos. Furthermore, the trajectories that travel near the edges can flip direction of motion around the origin between clockwise and counterclockwise (e.g., see tumbling trajectory in Supplemental Material Videos S5 and S7 [26]). The presence of chaos in these trajectories can be quantified by calculating the largest Lyapunov exponent (LLE) of the underlying nonlinear dynamical system [25,27]. If the LLE is zero, then the active particle motion is either periodic or quasiperiodic, whereas a positive LLE indicates chaos (with the degree of sensitivity to initial conditions given by the magnitude of the LLE). To numerically calculate the LLE, we used the algorithm given in Wolf *et al.* [28]. The magnitude of the LLE in the plane of initial conditions $(x(0), y(0))$ is shown in Fig. 4(b) for the same domain of parameter values as Fig 4(a). We typically find that particles starting in the central region of the square

cross section have regular motion, whereas particles starting near the walls of the channel [outer red and purple regions of Fig. 4(a)] are chaotic. However, we also find anomalous periodic regions near corners (within the chaotic sea); a particle starting in these small regions shows regular dynamics. These anomalous periodic regions correspond to the yellow region in Fig. 4(a) of off-centered trapping motion.

2. Effect of initial orientation

We now explore how the classification of trajectories in the $(x(0), y(0))$ initial-position plane varies with small changes in the (fixed) initial orientation angles $\theta(0)$ and $\phi(0)$ from the upstream orientation.

First, we explore the effect of variations in $\phi(0)$ for fixed $\theta(0) = 0$. For a small positive value of $\phi(0) = \pi/24$, we find that the blue and cyan regions shrink marginally from those shown in Fig. 4(a) (where $\phi(0) = 0$) to those of the top panel of Fig. 5(a). Further increasing to $\phi(0) = \pi/12$, we find that the cyan region corresponding to vertically swinging motion vanishes as shown in Fig. 5(b). This is because the value of $\phi(0)$ is large enough that, regardless of initial position, the active particle cannot remain confined to the vertical strip which classifies vertical swinging motion. Further increasing $\phi(0)$ to $\pi/6$ and $\pi/3$ leads to the shrinkage and disappearance, respectively, of the green region of central swinging motion [see Figs. 5(c) and 5(d)]. Again, with a large value of $\phi(0)$, the active particle is unable to remain confined near the channel center. Further, we see that parts of the red region of wandering motion are increasingly replaced by purple tumbling motion with trajectories largely confined near the channel walls. In terms of the chaotic nature of the trajectories, the bottom panels of Figs. 5(a)–5(d) show a progressive vertical stretching of the regular region as $\phi(0)$ increases. However, structure indicating chaotic motion also persists within this vertical band of regular motion. The black regions near the corners of Fig. 5(d) correspond to trajectories that came too close to the channel walls, i.e., trajectories that went outside the square domain $(x, y) \in [-0.95, 0.95] \times [-0.95, 0.95]$. We note that although initial nonzero values of ϕ break symmetry in the x direction, we do largely see a persistent left-right symmetry in Fig. 5. This is probably due to fact that only long-time behavior is captured in the classification of trajectories.

We see a similar trend as $\theta(0)$ is increased for fixed $\phi(0) = 0$, but with the blue regions vanishing instead of the cyan regions, see Figs. 5(e)–5(h). The green region also disappears for large $\theta(0)$. Even reasonably small but nonzero values of $\theta(0)$ cannot give rise to a horizontally swinging motion and large $\theta(0)$ also precludes trajectories confined to the central region. Again the presence of up-down symmetry for initial nonzero values of θ is probably due to fact that only long-time behavior is captured in the classification of trajectories.

We note that the yellow periodic islands present near the corner of the square cross section in Fig. 4(a) are not seen in Fig. 5 when one of the orientation angles is nonzero. Nevertheless, such islands do persist for sufficiently small nonzero values of both orientation angle.

3. Effect of U

We now examine the variations in active particle dynamics with respect to the dimensionless parameter U , the ratio of

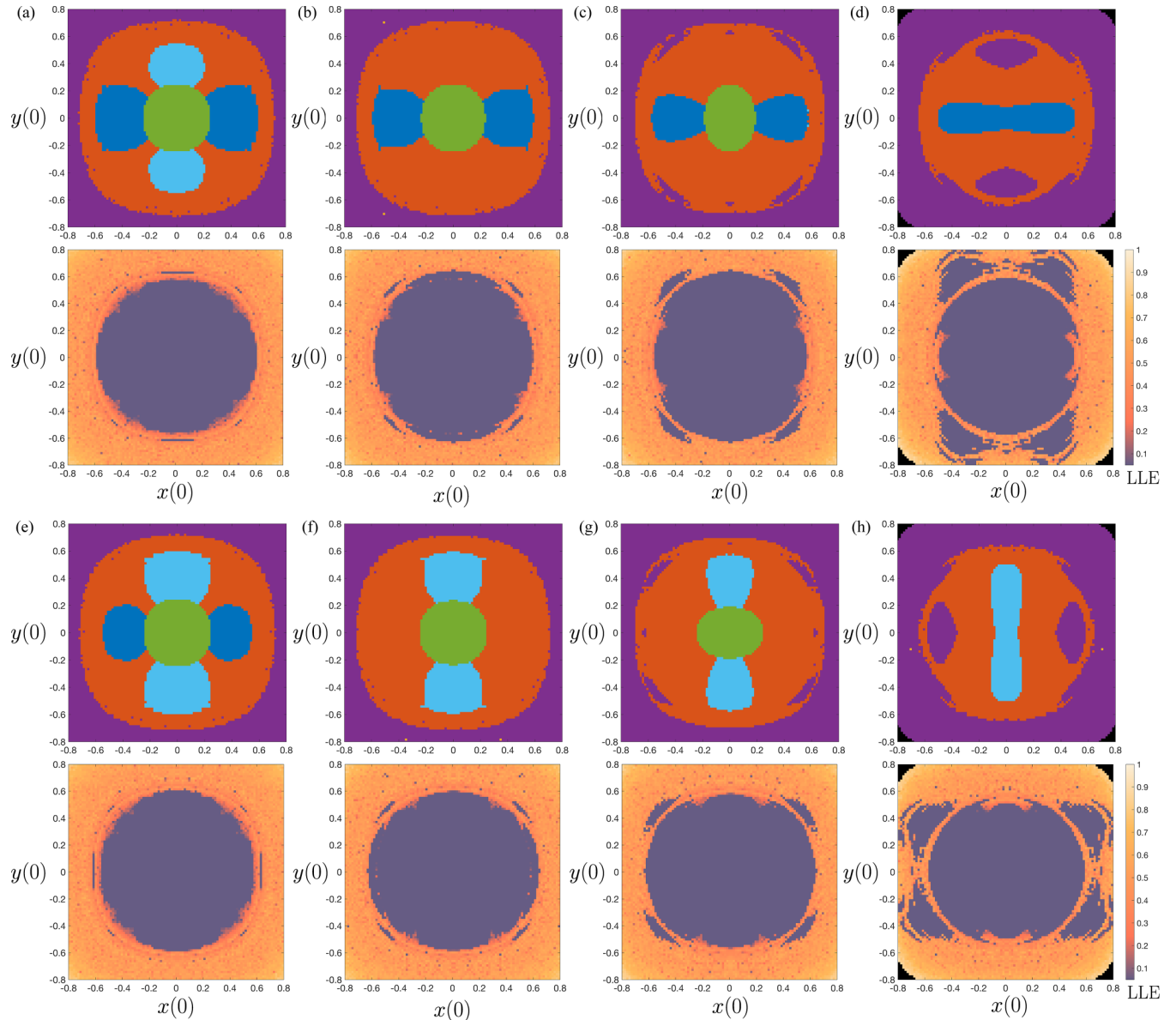


FIG. 5. Trajectory classification (top panels) and LLE (bottom panels) in the initial position $(x(0), y(0))$ plane for fixed $U = 10$ and varying initial orientations $\theta(0)$ and $\phi(0)$. For fixed $\theta(0) = 0$ and (a) $\phi(0) = \pi/24$, (b) $\phi(0) = \pi/12$, (c) $\phi(0) = \pi/6$, and (d) $\phi(0) = \pi/3$. For fixed $\phi(0) = 0$ and (e) $\theta(0) = \pi/24$, (f) $\theta(0) = \pi/12$, (g) $\theta(0) = \pi/6$, and (h) $\theta(0) = \pi/3$. For trajectory classification, green (●) is central swinging motion, cyan (●) is vertical swinging motion, blue (●) is horizontal swinging motion, purple (●) is tumbling motion, and red (●) is wandering motion. Black regions in (d) and (h) correspond to trajectories that came too close to the channel walls, i.e., trajectories that went outside a square of $[-0.95, 0.95] \times [-0.95, 0.95]$.

the maximum flow speed to the intrinsic active particle speed. For $U \ll 1$, the active particle intrinsic velocity dominates the flow field and, hence, the particle will readily encounter the walls. Moreover, the active particle's self-generated flow fields would need to be captured to understand its dynamics. Since the simple model used in this paper does not capture these two effects, we do not explore this regime of active particle motion in a quiescent fluid within a rectangular duct. For a recent detailed numerical exploration of this regime, see Radhakrishnan *et al.* [29].

Figure 6 shows the different types of trajectories (left panels) and LLE (right panels) in the initial position space for various values of U and fixed initial upstream orientation

$\theta(0) = 0$ and $\phi(0) = 0$. For $U \lesssim 1$, and as shown in Fig. 6(a) for $U = 0.5$, we observe regular swinging motion of the active particle about the channel center. Moreover, at these low values of U there is a net *upstream* migration of the particle, i.e., against the flow. For $U \gtrsim 1$, and as shown in Fig. 6(b) for $U = 2.5$, we again observe regular swinging motion but now U is sufficiently large that the net migration of the particle is downstream in the direction of the flow. Increasing to $U = 5$, Fig. 6(c), the classification of trajectories does not change qualitatively from that seen at lower values of U , but the plot of the LLE shows the emergence of chaotic motion for initial particle positions near the corners of the channel cross section. Further increasing U to 7.5, Fig. 6(d), we see the emergence of

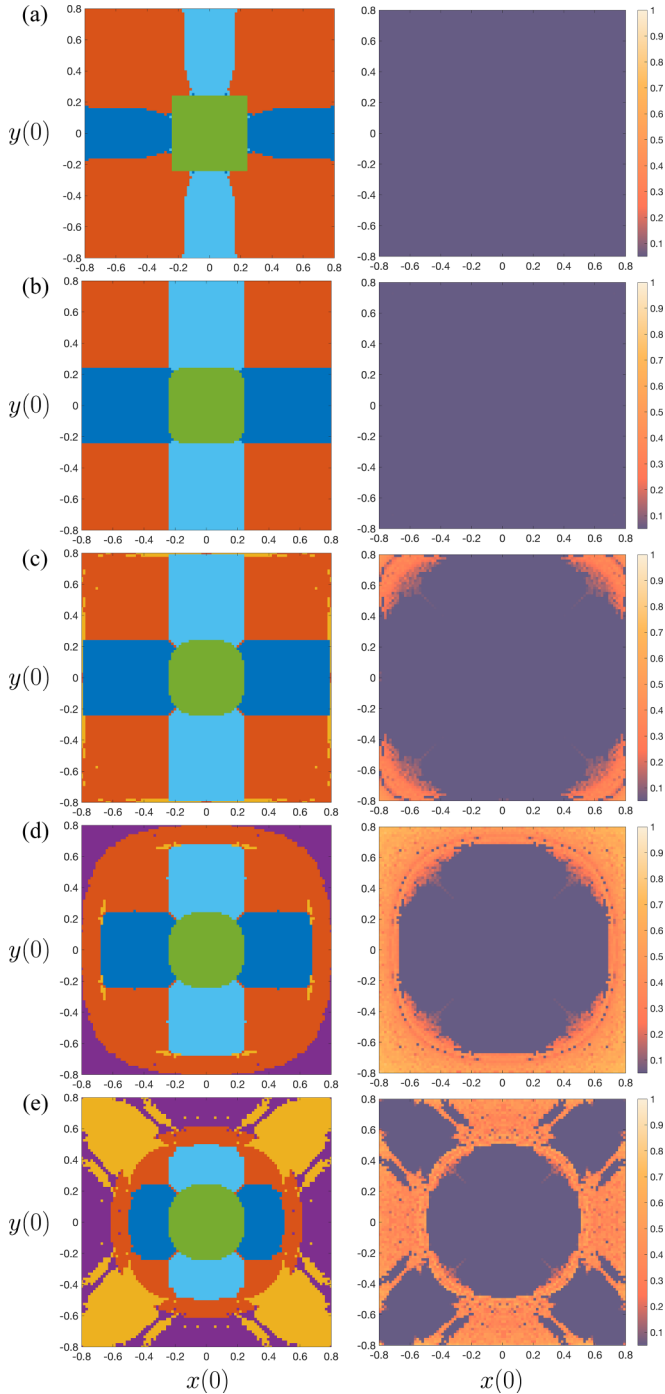


FIG. 6. Trajectory classification (left panels) and LLE (right panels) in the initial position $(x(0), y(0))$ plane for the types of trajectories shown in Fig. 2 and different values of U : (a) $U = 0.5$, (b) $U = 2.5$, (c) $U = 5$, (d) $U = 7.5$, and (e) $U = 15$. Initial orientation angles are fixed to $\theta(0) = 0$ and $\phi(0) = 0$. For trajectory classification, green (●) is central swinging motion, cyan (●) is vertical swinging motion, blue (●) is horizontal swinging motion, yellow (●) is off-centered trapping motion, purple (●) is tumbling motion, and red (●) is wandering motion.

purple regions of tumbling-motion trajectories near the walls of the channel where we also see an increase in the extent of chaotic regions. For a large value of $U = 15$, Fig. 6(e), we see

the appearance of regular trajectories near the corners of the channel cross section (yellow regions of the trajectory plot).

To summarize, for the parameter values and the range of U values shown in Fig. 6, we find that as U increases, the green region corresponding to central swinging motion does not change significantly while the cyan and blue regions of vertical and horizontal swinging shrink progressively. Further, with increasing U , the red region of wandering motion also shrinks with the appearance of tumbling and off-centered trapping motion near the edges and corners of the cross section. In terms of the chaotic nature, we see a progressive increase in chaotic trajectories up to $U = 7.5$, but further increase in U leads to the appearance of regions of regular motion near the corners.

4. Poincaré map and sticky trajectories

Since one constant of motion H_s remains for our 4D dynamical system in Eqs. (8), the effective dynamics of the system take place in 3D. We can further explore the nature of the system dynamics and transition to chaos by using Poincaré sections to visualize regular and chaotic regions of the system on a 2D plot. We construct a Poincaré map by sampling the active particle trajectory at times t_n that correspond to a crossing of the phase-space trajectory with the $\theta = 0$ (equivalently, $e_y = 0$) hyperplane in the positive direction, i.e., $\theta_n = \theta(t_n) = 0$ with $\dot{\theta}_n = \dot{\theta}(t_n) > 0$. At these times t_n , we store the values $\phi_n = \phi(t_n)$ and $x_n = x(t_n)$ and plot them against each other, giving us a Poincaré map. We repeat this for many active particle trajectories having different initial conditions but a common fixed value of the constant of motion H_s , i.e., the initial conditions satisfy

$$H_s = \frac{1}{2}U(x(0)^2 + y(0)^2 - x^2(0)y^2(0)) + 1 - \cos(\phi(0)) \cos(\theta(0)). \quad (13)$$

Several such Poincaré maps are shown in Fig. 7 for different values of the constant of motion H_s . We find that for small values of H_s , we observe regular behavior with ubiquitous quasiperiodic trajectories that correspond to closed curves on the Poincaré map [see Figs. 7(a) and 7(b)]. As H_s is increased, we observe that, due to nonlinear resonances, some of these orbits break into a chain of smaller orbits [see Fig. 7(c)]. Further increase in H_s gives rise to chaos as evident by the apparently random scatter of points in the Poincaré map [see Figs. 7(d) and 7(e)]. At these large values of H_s , we have a mixture of order and chaos where small islands of regular behaviors exist within the chaotic sea. Increase in the value of H_s can also be interpreted as initial positions going away from the center of the channel. For example, with fixed initial upstream orientation $\theta(0) = \phi(0) = 0$, Eq. (13) describes a closed curve:

$$x(0)^2 + y(0)^2 - x^2(0)y^2(0) = 2H_s/U.$$

These closed curves are the same shape as the level sets of the flow field $u(x, y)$. Small values of H_s correspond to circlelike closed curves near the center of the channel while increasing H_s leads to squarelike closed curves away from the center of the channel. Since near the center of the channel, the dynamics of the system are similar to a circular cross section and are hence integrable, this transition to chaos with increasing H_s

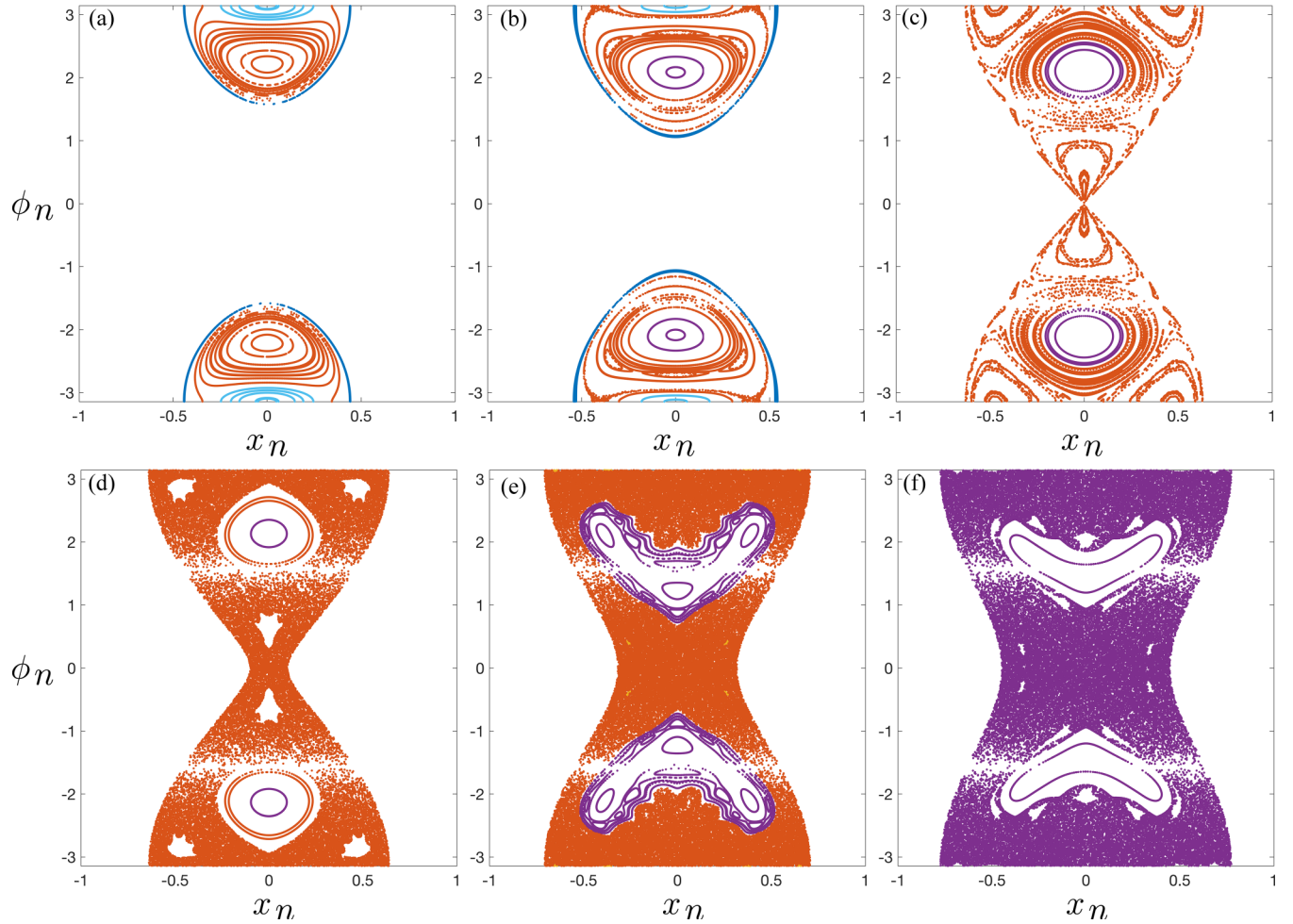


FIG. 7. Poincaré maps in the (x_n, ϕ_n) plane for $\theta(t_n) = 0$ ($\dot{\theta}(t_n) > 0$) and (a) $H_s = 1$, (b) $H_s = 1.5$, (c) $H_s = 2$, (d) $H_s = 2.05$, (e) $H_s = 2.5$, and (f) $H_s = 3$. The parameter $U = 10$ was fixed and many different initial conditions were chosen based on Eq. (13) while keeping H_s fixed. Cyan (●) is vertical swinging motion, blue (●) is horizontal swinging motion, purple (●) is tumbling motion, and red (●) is wandering motion.

may be understood in terms of the theory of nearly integrable Hamiltonian systems and KAM theory [30].

When islands of regular behaviors exist within the chaotic sea of a Poincaré map, sticky trajectories can arise where a long time is spent in the vicinity of these periodic islands [31]. An example of such a sticky tumbling trajectory is shown in Fig. 8 and Supplemental Material Video S11 [26]. Figures 8(a) and 8(b) show the trajectory in different planes while Fig. 8(c) shows a Poincaré map with the light green colored part in all

three panels representing the sticky behavior. On the Poincaré map, such trajectories spend a very long time near the boundaries of the periodic islands compared to the time spent in a domain of the chaotic sea of the same phase-space volume.

5. Dynamics in the large U limit

In the limit of large $U \gg 1$, Eqs. (8) approaches a singular limit for the evolution of θ and ϕ . Hence, to understand this

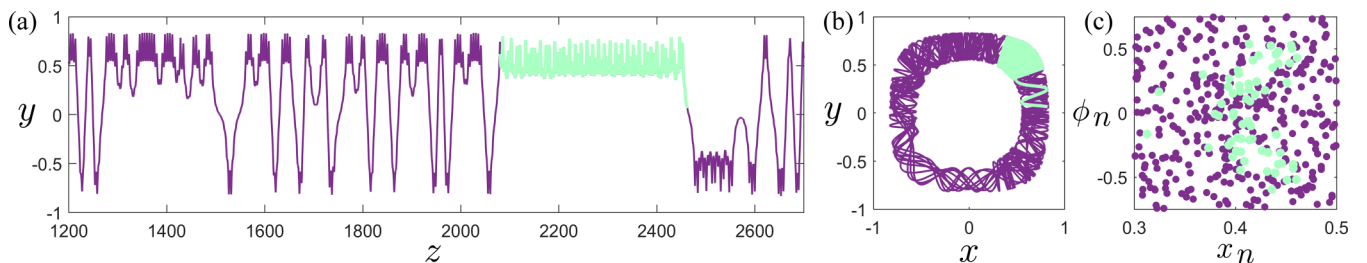


FIG. 8. Sticky trajectory for an active particle in a square cross section. Particle trajectory in the (a) (z, y) plane and (b) (x, y) plane, as well as (c) Poincaré map in the (x_n, ϕ_n) plane for $\theta_n = 0$ ($\dot{\theta}_n > 0$). Purple shows the entire trajectory of the particle while light green shows a typical sticky region for the trajectory. The parameter $U = 10$ and initial conditions were chosen such that $H_s = 3.5$ with $x(0) \approx 0.6861$, $y(0) \approx 0.6582$, $z(0) = 0$, $\theta(0) = 0$, and $\phi(0) = 0$. See also Supplemental Material Video S11 [26] for a video of the trajectory.

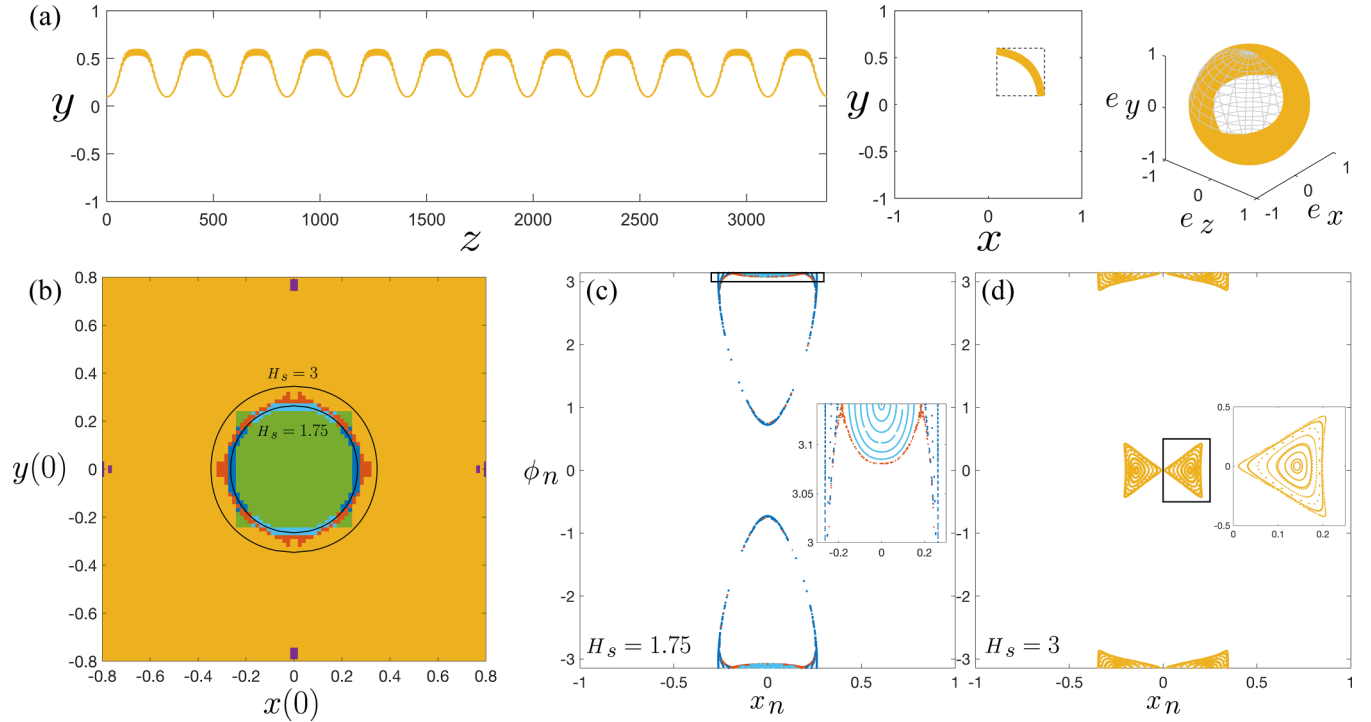


FIG. 9. Active particle dynamics for large $U = 50$ starting at $z(0) = 0$ with fixed initial upstream orientation angles $\theta(0) = 0$ and $\phi(0) = 0$. (a) A typical confined trajectory in the (z, y) (left) and (x, y) (middle) planes, as well as the orientation evolution (right) for initial position $x(0) = 0.6$, $y(0) = 0.1$. (b) Classification of behaviors in the $(x(0), y(0))$ initial-position plane using the color scheme of Fig. 2(c), (d) Poincaré maps in the (x_n, ϕ_n) plane for $\theta_n = 0$ with $\dot{\theta}_n > 0$ for the constants of motion (c) $H_s = 1.75$ and (d) $H_s = 3$. These values of the constant of motion are indicated by black curves in (b). The trajectory in (a) was simulated for $t = 100$, using the time scaling of Eqs. (8), which corresponds to $t = 100U$ using the timescaling of Eq. (14). See also Supplemental Material Video S12 [26] for a video of the active particle trajectory in (a).

regime, we rescale the dimensionless time in Eqs. (8) (with $\mathcal{A} = 1$) by U to obtain the following system:

$$\begin{aligned}\dot{x} &= -\frac{1}{U} \cos \theta \sin \phi, \\ \dot{y} &= \frac{1}{U} \sin \theta, \\ \dot{\theta} &= -y \cos \phi (1 - x^2), \\ \dot{\phi} &= -y \tan \theta \sin \phi (1 - x^2) + x(1 - y^2).\end{aligned}\quad (14)$$

This form of the system removes the singular terms and allows efficient numerical solution. A typical classification of trajectories at a large value of $U = 50$ along with an example trajectory and Poincaré maps are shown in Fig. 9. In this regime of large U , we find that chaos ceases and we have regular behaviors. A typical regular trajectory that confines itself to a quadrant of the channel is shown in Fig. 9(a). Simulating many different initial conditions with fixed initial upstream orientation $\theta(0) = \phi(0) = 0$ gives us the classification in the initial position plane $(x(0), y(0))$ as shown in Fig. 9(b). Compared to Fig. 6, we find that the central green region still exists while the cyan, blue, and red regions have almost vanished. Outside the central region, the behavior is dominated by off-centered trapped trajectories (yellow region). Two different Poincaré maps at $H_s = 1.75$ and $H_s = 3$ are shown in Figs. 9(c) and 9(d), respectively. These typically show closed loops, indicating quasiperiodic behavior of the

system in this regime. With variation in the initial orientation angles $\theta(0)$ and $\phi(0)$ from the upstream equilibrium state, we find that in the initial-position plane, some yellow regions transition to purple regions corresponding to regular tumbling trajectories.

Hence, from Figs. 6 and 9 we see that the active particle motion is regular for small and large U , whereas chaos emerges for intermediate U .

E. Active particle transport along the channel

The trajectories shown in Fig. 2 started at $z = 0$ and the time series is shown for $t = 900$ to $t = 1000$. We see that the transport of the active particle in the z direction, i.e., axially along with the flow, can vary significantly depending on the type of active particle motion realized in the channel cross section. Active particles that perform swinging motion near the center of the channel (e.g., green, blue, cyan, and some red trajectories) will travel farther along the channel compared to active particles whose motion is confined near the walls of the channel (e.g., purple trajectories). Figure 10 shows, for different U values, a contour plot of the z (axial) location at the end of the simulation ($t = 1000$) in the $(x(0), y(0))$ plane for initially upstream-oriented active particles (starting from $z = 0$). For a small value of $U = 0.5$, we see that the final axial positions are negative indicating that the active particle's intrinsic speed dominates the fluid flow speed resulting in a net upstream migration of the active particle. For a larger value

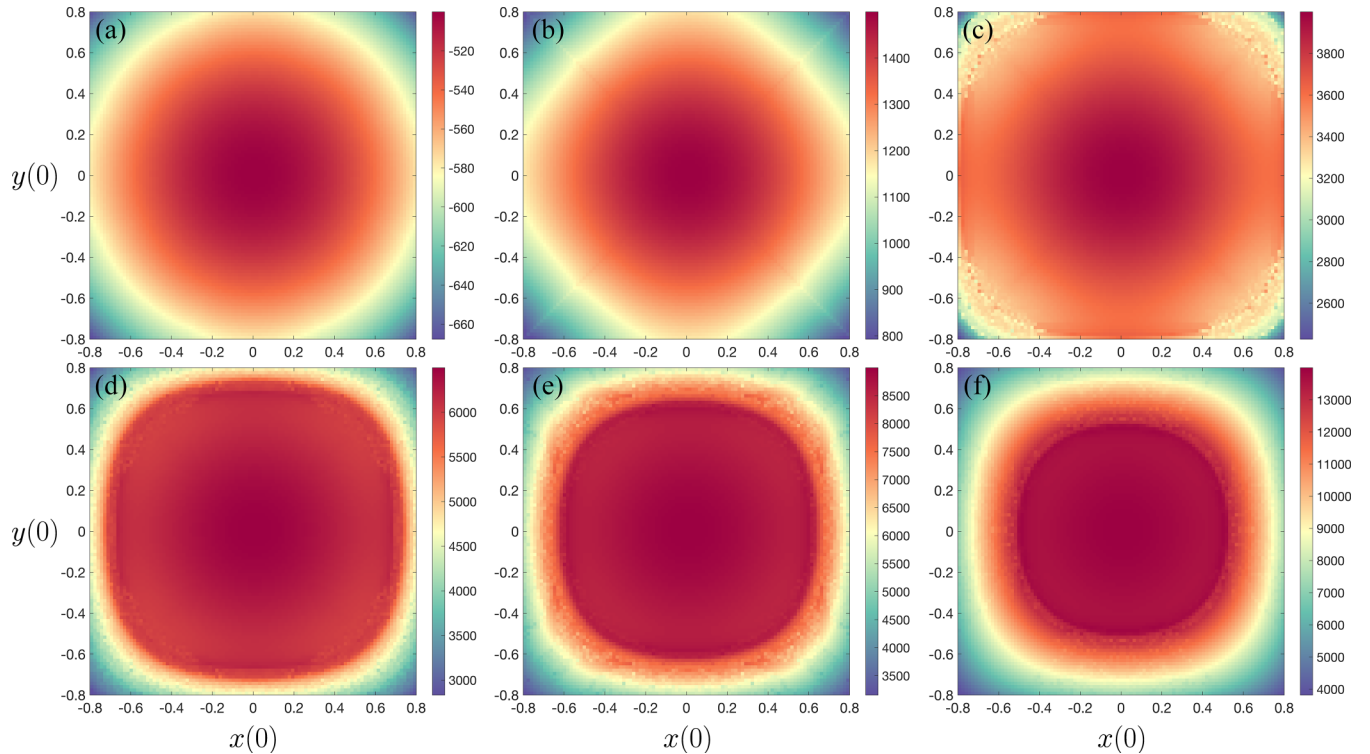


FIG. 10. Axial transport of the active particle along the straight channel based on the initial position in the $(x(0), y(0))$ plane for various U and fixed $\theta(0) = 0$ and $\phi(0) = 0$. The color bars indicate the final axial coordinate z of the active particle from an initial axial position of $z(0) = 0$ for values of (a) $U = 0.5$, (b) $U = 2.5$, (c) $U = 5$, (d) $U = 7.5$, (e) $U = 10$, and (f) $U = 15$.

of $U = 2.5$, the fluid speed dominates the particle speed and we obtain a net downstream migration. Further increase to $U = 5$ does not qualitatively change the axial transport profile near the center of the cross section, however, near the corners, we see fluctuations in this profile due to the appearance of chaotic wandering motion in this region [see Fig. 6(c)]. For even larger values of U , the active particle axial transport is dominated by the background fluid flow profile. We find a central plug region corresponding to large axial transport of the active particle undergoing swinging motion near the center of the channel where flow speed is large, while near the walls and corners we observe small axial transport corresponding to off-centered trapping or tumbling trajectories that stay near the outer regions of the cross section where the flow speed is small.

VI. DYNAMICS IN WIDER RECTANGULAR CHANNELS

In this section, we briefly explore the effects of the aspect ratio \mathcal{A} of the rectangular cross-section on the active particle dynamics. In Figs. 11(a) and 11(b), we plot the trajectory classification and LLE in the initial-position plane $(x(0), y(0))$, while keeping $\theta(0) = 0$, $\phi(0) = 0$, and $U = 10$ fixed, for two different rectangular cross sections with $\mathcal{A} = 2$ and $\mathcal{A} = 4$, respectively. We note that the classification criteria presented for square channels in Sec. V A has been scaled based on \mathcal{A} in the x direction for rectangular channels. So, for example, the classification of central swinging motion (green) has been modified to confinement in a rectangular box of domain $-0.25\mathcal{A} < x < 0.25\mathcal{A}$ and $-0.25 < y < 0.25$. For

the rectangular cross section with $\mathcal{A} = 2$, we find similar types of active particle trajectories at similar initial positions compared to the $\mathcal{A} = 1$ square channel (see Fig. 4) with some minor differences. Near the center of the channel, we obtain central swinging motion (green) as well as vertical (cyan) and horizontal (blue) swinging motion, but there is a horizontal stretching of these regions due to increasing the width of the channel. Moreover, the relative frequency of oscillations in the horizontal and vertical directions near the center of the channel will be scaled by \mathcal{A} as per the eigenvalues in Sec. III A. Beyond the central region, we find wandering motion (red) and tumbling motion (purple) similar to the square channel. We find that the yellow islands, corresponding to confined trajectories away from the channel center, have diminished in size compared to the square cross section, and these regions are more scattered. A typical trajectory in the yellow region is shown in Fig. 11(c), where the motion is trapped in an off-centered vertical band compared to the motion confined near the corner for a square cross section [see Fig. 2(d)]. For the $\mathcal{A} = 2$ channel, we also see the emergence of small horizontal swinging (blue) regions appearing near the left and right ends of the horizontal centerline that were not present for square channels. The LLE also shows a similar structure with regular trajectories near the central region of the channel and the dominance of chaos near the channel walls. The $\mathcal{A} = 4$ rectangular cross section shows similar features to the $\mathcal{A} = 2$ channel with a few noteworthy differences. The yellow regions for off-centered trapping motion increase in extent while the small regions for horizontal swinging present for the $\mathcal{A} = 2$ channel no longer exist. Moreover, the tumbling

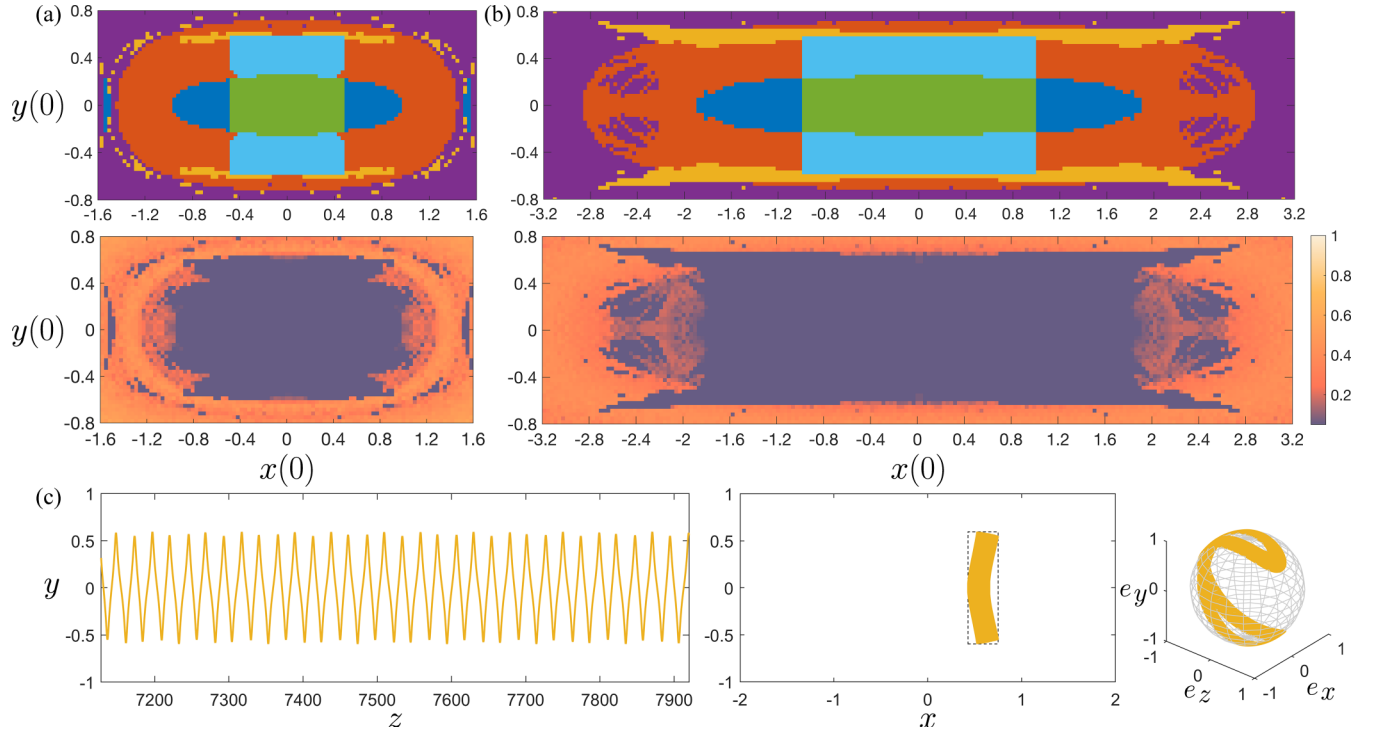


FIG. 11. (a), (b) Active particle trajectory classification (top) and LLE (bottom) in the initial position plane $(x(0), y(0))$ for motion in rectangular channels with (a) $\mathcal{A} = 2$ and (b) $\mathcal{A} = 4$. (c) A typical trajectory of a particle starting in the yellow region with $x(0) = 0.75$ and $y(0) = 0.55$ for the case $\mathcal{A} = 2$. Other parameters are fixed to $U = 10$, $z(0) = 0$, $\theta(0) = 0$, and $\phi(0) = 0$. See Supplemental Material Video S13 [26] for a video of the active particle trajectory in (c).

motion (purple) region penetrates the wandering motion (red) region near the left and right edges of the cross section. We also note that our simple flow field approximation in Eq. (7) will become poor near the left and right edges of the cross section as \mathcal{A} increases, and hence a more accurate flow field for Poiseuille flow in rectangular channels may be needed to accurately capture the active particle dynamics in these regions.

VII. CONCLUSIONS

We have studied in detail, theoretically and numerically, the motion of a pointlike active particle in a steady unidirectional fluid flow, specifically through a straight channel with rectangular cross section. We identified a general constant of motion that enabled the six equations of motion to be reduced to a 4D nonlinear dynamical system with one constant of motion. We identified two equilibrium states for this particle-fluid system located at the center of the rectangular cross section: (i) an upstream-oriented marginally stable equilibrium where small perturbations lead to oscillatory motion about this equilibrium point and (ii) a downstream-oriented unstable saddle equilibrium. By numerically solving the system, we observed a variety of active particle trajectories for different values of the maximum flow speed U and the channel width-to-height aspect ratio \mathcal{A} , as well as different initial particle positions and orientations. The trajectories were classified based on the regions they occupy in the channel cross section. Swinging trajectories, such as central swinging, vertical swinging, and horizontal swinging, were typical quasiperiodic motions near

the centerlines of the channel, whereas off-centered trapping motion was the typical form of confined quasiperiodic motion away from the channel centerlines. Tumbling trajectories stayed near the walls of the channel while wandering trajectories visited both the central and the outer regions of the cross section. By calculating the largest Lyapunov exponents, many of the tumbling and wandering trajectories were shown to be chaotic. Poincaré maps with increasing value of the constant of motion showed the transition to chaotic behavior and the persistence of small islands of regular behavior in the chaotic sea. The latter resulted in sticky chaotic tumbling trajectories due to the chaotic trajectory becoming trapped near a periodic state for a long time.

We have shown how the active particle motion varies with the system parameters and initial conditions. We focused on a square channel cross section ($\mathcal{A} = 1$) and also showed that qualitatively similar particle trajectories were obtained in cross sections with larger aspect ratio \mathcal{A} . Varying the maximum flow speed U revealed rich dynamics with nonchaotic motion at very small and large U and the emergence of chaos in an intermediate range of U . In this regime of U where chaos arises, we found that the active particle trajectories are generally very sensitive to initial conditions with a couple of robust regimes. The active particle oriented upstream and starting near the channel center typically undergoes regular swinging motion that is robust to small variations in the initial position and orientation. Similarly, the active particle oriented upstream and starting near the walls of the channel typically undergoes chaotic tumbling motion, which is again robust to small variations of the initial conditions. The present

paper highlights the importance of initial conditions on active particle motion. A comparison with careful microfluidic experiments quantifying the effects of initial conditions on active particle motion in channel flows would be of great interest.

The model used in this paper is simple and can be extended in various ways to more accurately capture the motion of natural and artificial microswimmers in channel flows. In the present formalism, the active particle is modeled simply with a constant self-propulsion whereas natural microswimmers exhibit more complex locomotion such as run-and-tumble motion [7]. It would be interesting to explore the dynamics of our particle-fluid system when an intrinsic tumbling mechanism is added for the active particle so that it reorients itself at certain times either stochastically or deterministically. Furthermore, the present model does not capture swimmer-swimmer interactions and they may become important when considering the motion and trajectories of multiple active particles in Poiseuille flow. In addition to swimmer-swimmer interactions, it would also be useful to explore the effects of swimmer-wall interactions to (i) understand motion of active particles in narrow channels and (ii) accurately capture the active particle trajectories that get very close to the channel walls. Simulations of microswimmers in 3D rectangular confinement with quiescent fluid have demonstrated that interactions of a microswimmer with channel walls can significantly influence its trajectory depending on the flow field generated by the microswimmer i.e., pusher, puller, or neutral [29]. By considering wall interactions using squirmer models for the active particle in 2D planar Poiseuille flow, Zöttl and Stark [16] showed that the conservative nature of the dynamical system is destroyed. They further showed that, when this happens, dissipative dynamical features emerge, such as a stable point attractor and a limit cycle attractor in the case of the upstream-oriented swinging motion. Choudhary *et al.* [20] explored the effects of adding fluid inertia for active particles in 2D planar Poiseuille flow and reported similar dynamical features. Our previous work on the dynamics of passive spheres in 3D channel flows with the presence of fluid inertia has revealed rich dynamical structure for inertial particle focusing behaviors [32–34]. In future work, we aim to use squirmer models of active particles to explore the effects of inertia, swimmer-wall, and swimmer-swimmer interactions

on the dynamics and focusing of active particles in 3D microfluidic channel flows.

ACKNOWLEDGMENTS

This research is supported under the Australian Research Council's Discovery Projects funding scheme (Project No. DP200100834). Some of the results were computed using supercomputing resources provided by the Phoenix HPC service at the University of Adelaide.

APPENDIX A: CALCULATION FOR GENERAL CONSTANT OF MOTION

For dynamics of the active particle suspended in a unidirectional flow field $u(x, y)$ as given by Eqs. (2), we show that the following is a constant of motion:

$$H_g = -\frac{1}{2}u(x, y) + e_z.$$

Differentiating the above equation with respect to time, we get

$$\frac{dH_g}{dt} = \frac{\partial H_g}{\partial x}\dot{x} + \frac{\partial H_g}{\partial y}\dot{y} + \frac{\partial H_g}{\partial z}\dot{z} + \frac{\partial H_g}{\partial e_x}\dot{e}_x + \frac{\partial H_g}{\partial e_y}\dot{e}_y + \frac{\partial H_g}{\partial e_z}\dot{e}_z.$$

Calculating the derivatives and using Eqs. (2), we get

$$\begin{aligned} \frac{dH_g}{dt} &= -\frac{1}{2}\frac{\partial u}{\partial x}e_x - \frac{1}{2}\frac{\partial u}{\partial y}e_y + 0 + 0 + 0 \\ &\quad + \left(\frac{1}{2}\frac{\partial u}{\partial x}e_x + \frac{1}{2}\frac{\partial u}{\partial y}e_y\right) = 0. \end{aligned}$$

Hence, H_g is a constant of motion. If angular variables θ and ϕ are used for the particle orientation in place of e_x , e_y and e_z , then the constant of motion transforms to

$$H_g = -\frac{1}{2}u(x, y) - \cos\theta \cos\phi.$$

APPENDIX B: COMPARISON OF EXACT VERSUS APPROXIMATE FLOW FIELD FOR POISEUILLE FLOW IN A SQUARE CROSS SECTION

The dimensionless flow field $u(x, y)$ used in this paper is an approximation to the following exact flow field for Poiseuille

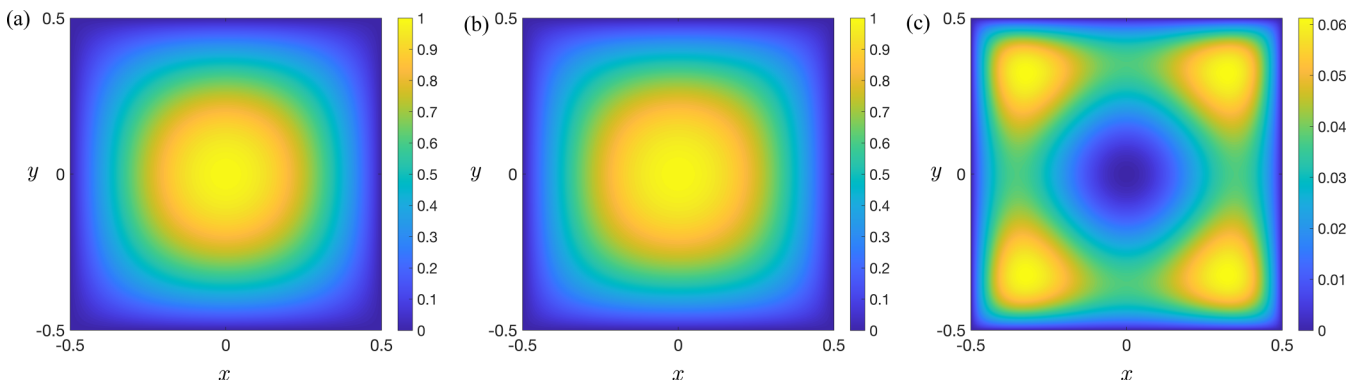


FIG. 12. Comparison of (a) the flow field $u(x, y)$ as in Eq. (7) used in this paper to approximate Poiseuille flow in a 3D rectangular channel (here setting $\mathcal{A} = 1$ for a square channel) with (b) the more accurate representation of the flow field $u_e(x, y)$ as in Eq. (B1) with $n = 100$ terms. The difference $u_e(x, y) - u(x, y)$ is shown in (c).

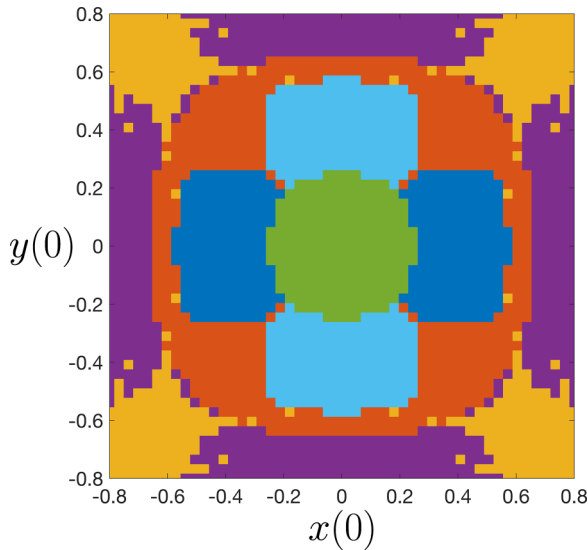


FIG. 13. Classification of active particle trajectories in the initial condition $(x(0), y(0))$ plane using the more accurate flow field in the square cross section $u_e(x, y)$ [as per Eq. (B1) with $n = 100$ terms]. This compares well with the classification shown in Fig. 4, obtained using the approximate flow field $u(x, y)$ with $\mathcal{A} = 1$. We note that the grid resolution here is 50×50 compared to the 100×100 resolution in Fig. 4. Other parameters were fixed to $\theta(0) = 0$, $\phi(0) = 0$ and $U = 10$.

flow in a straight duct with a square cross section [35]:

$$u_e(x, y) = U_e(1 - y^2) + \frac{32U_e}{\pi^3} \times \sum_{n=0}^{\infty} \frac{(-1)^{n+1} \cosh\left((2n+1)\frac{\pi x}{2}\right) \cos\left((2n+1)\frac{\pi y}{2}\right)}{(2n+1)^3 \cosh\left((2n+1)\frac{\pi}{2}\right)}. \quad (\text{B1})$$

Here $U_e = U / \max\{u_e(x, y)\} = U / u_e(0, 0)$, to match the maximum flow speed of U at the center of the channel. A comparison of the flow field u and u_e for $U = 1$ is shown in Fig. 12. We see that the overall qualitative flow field is captured well by our approximate flow field u and the difference between the two flow fields is small; at most 6% when scaled by the maximum flow speed at the center. Further, we note that the regions in the cross section where the most significant difference is observed in the flow field are near the corners of the square. For wider rectangular cross sections, the approximation becomes poorer with increasing \mathcal{A} . For a 2×1 rectangular cross section, the maximum difference between the two velocity fields is around 15% while for a 4×1 rectangular cross section it is around 35%.

Figure 13 shows the different types of active particle trajectories realized for the more accurate flow field $u_e(x, y)$ for Poiseuille flow in a straight channel with square cross section. Comparing with Fig. 4(a), which used the simpler approximation of the flow field $u(x, y)$, we find noticeable differences mainly in the yellow regions. This is to be expected since at these locations, the difference between the flow fields u_e and u is the largest [see Fig. 12(c)].

- [1] E. M. Purcell, Life at low Reynolds number, *Am. J. Phys.* **45**, 3 (1977).
- [2] J. Deseigne, O. Dauchot, and H. Chaté, Collective motion of vibrated polar disks, *Phys. Rev. Lett.* **105**, 098001 (2010).
- [3] R. Golestanian, T. B. Liverpool, and A. Ajdari, Designing phoretic micro- and nano-swimmers, *New J. Phys.* **9**, 126 (2007).
- [4] Y. Couder, S. Protière, E. Fort, and A. Boudaoud, Dynamical phenomena: Walking and orbiting droplets, *Nature (London)* **437**, 208 (2005).
- [5] R. N. Valani, A. C. Slim, and T. Simula, Superwalking droplets, *Phys. Rev. Lett.* **123**, 024503 (2019).
- [6] B. V. Hokmabad, R. Dey, M. Jalaal, D. Mohanty, M. Almukambetova, K. A. Baldwin, D. Lohse, and C. C. Maass, Emergence of bimodal motility in active droplets, *Phys. Rev. X* **11**, 011043 (2021).
- [7] J. Elgeti, R. G. Winkler, and G. Gompper, Physics of microswimmers—single particle motion and collective behavior: A review, *Rep. Prog. Phys.* **78**, 056601 (2015).
- [8] Marcos, H. C. Fu, T. R. Powers, and R. Stocker, Bacterial rheotaxis, *Proc. Natl. Acad. Sci. USA* **109**, 4780 (2012).
- [9] J. E. Simons and S. D. Olson, Sperm motility: Models for dynamic behavior in complex environments, in *Cell Movement: Modeling and Applications*, edited by M. Stolarska and N. Tarfulea (Springer International Publishing, Cham, 2018), pp. 169–209.
- [10] J. C. Conrad and R. Poling-Skutvik, Confined flow: Consequences and implications for bacteria and biofilms, *Annu. Rev. Chem. Biomol. Eng.* **9**, 175 (2018).
- [11] Z. Wu, Y. Chen, D. Mukasa, O. S. Pak, and W. Gao, Medical micro/nanorobots in complex media, *Chem. Soc. Rev.* **49**, 8088 (2020).
- [12] K. Ishimoto, Jeffery's orbits and microswimmers in flows: A theoretical review, *J. Phys. Soc. Jpn.* **92**, 062001 (2023).
- [13] A.-I. Bunea and R. Taboryski, Recent advances in microswimmers for biomedical applications, *Micromachines* **11**, 1048(2020).
- [14] D. Zhang, H. Bi, B. Liu, and L. Qiao, Detection of pathogenic microorganisms by microfluidics based analytical methods, *Anal. Chem.* **90**, 5512 (2018).
- [15] D. Matsunaga, F. Meng, A. Zöttl, R. Golestanian, and J. M. Yeomans, Focusing and sorting of ellipsoidal magnetic particles in microchannels, *Phys. Rev. Lett.* **119**, 198002 (2017).
- [16] A. Zöttl and H. Stark, Nonlinear dynamics of a microswimmer in Poiseuille flow, *Phys. Rev. Lett.* **108**, 218104 (2012).
- [17] R. Chacón, Chaotic dynamics of a microswimmer in Poiseuille flow, *Phys. Rev. E* **88**, 052905 (2013).
- [18] A. J. T. M. Mathijssen, T. N. Shendruk, J. M. Yeomans, and A. Doostmohammadi, Upstream swimming in microbiological flows, *Phys. Rev. Lett.* **116**, 028104 (2016).
- [19] M. Tarama, Swinging motion of active deformable particles in Poiseuille flow, *Phys. Rev. E* **96**, 022602 (2017).

- [20] A. Choudhary, S. Paul, F. Rühle, and H. Stark, How inertial lift affects the dynamics of a microswimmer in Poiseuille flow, *Commun. Phys.* **5**, 14 (2022).
- [21] A. Choudhary and H. Stark, On the cross-streamline lift of microswimmers in viscoelastic flows, *Soft Matter* **18**, 48 (2021).
- [22] A. Zöttl and H. Stark, Periodic and quasiperiodic motion of an elongated microswimmer in Poiseuille flow, *Eur. Phys. J. E* **36**, 4 (2013).
- [23] A. Zöttl, Hydrodynamics of microswimmers in confinement and in Poiseuille flow, Ph.D. Thesis, Technical University of Berlin, 2014.
- [24] Y. Xia and G. M. Whitesides, Soft lithography, *Annu. Rev. Mater. Sci.* **28**, 153 (1998).
- [25] S. H. Strogatz, *Nonlinear Dynamics and Chaos: With Applications to Physics, Biology, Chemistry, and Engineering*, 2nd ed. (CRC Press, Boca Raton, Florida, 2015).
- [26] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevE.110.034603> for videos S1 to S13.
- [27] A. Pikovsky and A. Politi, *Lyapunov Exponents: A Tool to Explore Complex Dynamics* (Cambridge University Press, Cambridge, UK, 2016).
- [28] A. Wolf, J. B. Swift, H. L. Swinney, and J. A. Vastano, Determining Lyapunov exponents from a time series, *Physica D* **16**, 285 (1985).
- [29] B. N. Radhakrishnan, A. Purushothaman, R. Dey, and S. P. Thampi, Confinement induced three-dimensional trajectories of microswimmers in rectangular channels, *Phys. Rev. Fluids* **9**, 083302 (2024).
- [30] G. M. Zaslavsky, *Hamiltonian Chaos and Fractional Dynamics* (Oxford University Press, London, 2005).
- [31] V. Afraimovich and G. M. Zaslavsky, Sticky orbits of chaotic Hamiltonian dynamics, in *Chaos, Kinetics and Nonlinear Dynamics in Fluids and Plasmas*, edited by S. Benkadda and G. M. Zaslavsky (Springer, Berlin, 1998), pp. 59–82.
- [32] B. Harding, Y. M. Stokes, and A. L. Bertozzi, Effect of inertial lift on a spherical particle suspended in flow through a curved duct, *J. Fluid Mech.* **875**, 1 (2019).
- [33] R. N. Valani, B. Harding, and Y. M. Stokes, Bifurcations and dynamics in inertial focusing of particles in curved rectangular ducts, *SIAM J. Appl. Dyn. Syst.* **21**, 2371 (2022).
- [34] R. N. Valani, B. Harding, and Y. M. Stokes, Bifurcations in inertial focusing of a particle suspended in flow through curved rectangular ducts, *Perspectives in Dynamical Systems II—Numerical and Analytical Approaches*, edited by J. Awrejcewicz (Springer International Publishing, Cham, 2024), pp. 667–683.
- [35] M. O. Deville, *An Introduction to the Mechanics of Incompressible Fluids* (Springer International Publishing, Cham, Switzerland, 2022).