

Active particle transport in pulsating three-dimensional geometries

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We study the transport of active Brownian particles (ABPs) in three-dimensional (3D) spatially periodic oscillatory geometries. We establish a generalized Fick-Jacobs approach that reduces a 3D system to an effective one-dimensional (1D) system, assuming that particles quickly reach a steady state in the transverse directions of the geometry. The resulting 1D framework connects passive, static, and pulsating limits and provides robust predictions. The transport characteristics of ABPs are computed semianalytically and corroborated by numerical simulations. At the optimal frequency of the geometry oscillation, particles exhibit higher average velocity $\langle v \rangle$ and effective diffusion coefficient D_{eff} , resembling the phenomena of stochastic resonance. This effect is further enhanced by the self-propelled velocity of ABPs and the amplitude of geometry oscillations. These findings have significant implications for the development of micro- and nanofluidic devices with enhanced control over particle transport and precise manipulation of small-scale biomedical devices.

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I. INTRODUCTION

Biological systems offer rich examples of fluctuating geometries used for directed transport in various natural processes. For instance, cilia-lined pathways in the respiratory and reproductive systems generate rhythmic oscillations that expel mucus and pathogens from the lungs and propel egg cells through the fallopian tubes, respectively [1,2]. Similarly, peristaltic motion in the gastrointestinal tract—caused by wavelike muscular contractions—moves food and nutrients efficiently along the digestive system, resembling an oscillating tube [3]. Additionally, the pulsatile expansion and contraction of blood vessels during blood flow aid in distributing oxygen and nutrients throughout the body [4,5]. These natural systems highlight how oscillatory motion can optimize the transport of mesoscopic entities, inspiring the design of synthetic microfluidic structures that mimic such mechanisms.

In the scenarios mentioned above, geometric structural agitation can strongly influence particle transport. In these thermally or actively fluctuating three-dimensional (3D) structures (see Fig. 1), the irregular geometry induces spatial variations along the length of the geometry, leading to the emergence of entropic barriers [6–12] that dictate the diffusive behavior of the particles. Such entropic effects can lead to nontrivial transport properties [13–15], including

rectification, enhanced diffusion, and resonancelike transport phenomena in structured geometries [16–18]. This effect is well captured by the Fick-Jacobs (FJ) approximation [11,19–25], which maps the higher-dimensional problem to an effectively one-dimensional (1D) one. Recent work suggests that this approach is also well suited for studying fluid flow through biological membranes [26], where the entropic effect significantly modifies transport in both microfluidic [14] and biological channels [27]. Similar confinement effects have also been reported for active particles near surfaces and walls [28–31]. Related effective descriptions have also been used to study escape dynamics of active particles from static traps, yielding good agreement with microscopic simulations and theory [32–34].

While diffusion and transport of passive particles confined in time-dependent geometries [35–37] have been explored in several contexts, the quantitative analysis of surface agitation on active particle transport has not yet been systematically investigated. The fundamental question of whether these geometric fluctuations enhance or hinder transport is surprisingly complex. Under certain conditions, this agitation can sometimes accelerate transport, while at other times it may impede it. Understanding the precise conditions and mechanisms governing these contrasting effects remains a challenge. Moreover, most existing studies on active particle transport focus on scenarios involving proximity to a single boundary, leaving unexplored the role of 3D confinement, where particles interact continuously with the curved geometry of the enclosing surfaces. In this article, we study the motion of diffusing, noninteracting ABPs confined to an oscillating, three-dimensional, symmetric tube. The oscillatory boundaries of the tube drive the particles. The primary objective of this work is to investigate the correlation between tube oscillations and active Brownian particles (ABPs) diffusion using a semianalytical approach, complemented by Brownian dynamics simulations.

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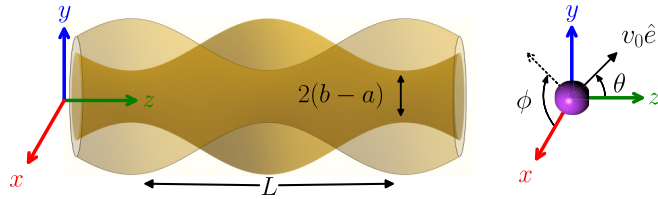


FIG. 1. (Left) Schematic illustration of the shape of a 3D oscillating tube, with time-dependent radius $W(z, t)$ [Eq. (2)], at time $t = 0$ (darker opacity) and at $t = T/2$ (lighter opacity). The tube is spatially periodic along the z direction with a periodicity of L and a bottleneck diameter of $2(b - a)$. (Right) Schematic of an active particle with the velocity v_0 and the orientation $\hat{e}$. θ and ϕ are the corresponding polar and azimuthal angles, respectively.

The article is organized as follows. In Sec. II, we introduce the Langevin model describing overdamped active Brownian particles in a 3D pulsating tube. In Sec. III, we develop the reduced semianalytical framework based on the FJ approximation. In Sec. IV, we present the numerical simulation methods used to validate the theoretical predictions. The transport properties of the system, including the mean velocity $\langle v \rangle$ and the effective diffusion coefficient D_{eff} , are analyzed in Sec. V and supported by numerical simulations. Section VI provides a detailed discussion of the obtained results and highlights the transport characteristic of active Brownian particles. Finally, Sec. VII summarizes the key findings of this work and outlines possible directions for future research.

II. MODEL

Consider the dynamics of noninteracting ABPs suspended in a thermal bath and confined to diffuse within a 3D symmetric tube with time-oscillating boundaries, which is periodic in space along the z direction with period L , as shown in Fig. 1. An ABP self-propels with a constant velocity v_0 in the direction of its orientation vector $\hat{e}$, which is expressed in terms of the polar and azimuthal angles θ and ϕ , as shown in Fig. 1. The dynamics of ABP is governed by the overdamped Langevin equation as [38–40]

$$\dot{\vec{r}}(t) = v_0 \hat{e}(t) + \sqrt{2D_0} \vec{\eta}(t), \quad (1a)$$

$$\dot{\hat{e}}(t) = \sqrt{2D_r} \vec{\xi}(t) \times \hat{e}(t). \quad (1b)$$

Equation (1) describes the translational and rotational motion of ABP. Here, a dot over a variable denotes a derivative with respect to time, and $\vec{r}$ represents the position vector of ABP. $D_0 = k_B \Phi / \gamma_t$ and $D_r = k_B \Phi / \gamma_r$ are the translational and rotational diffusion constants that obey the Einstein relations. k_B is the Boltzmann constant, Φ is the temperature of the surrounding medium, and γ_t and γ_r denote the corresponding translational and rotational friction coefficients, respectively. $\vec{\eta}(t)$ and $\vec{\xi}(t)$ are independent, zero-mean, unit-variance Gaussian white noises, $\langle \eta_i(t) \eta_j(t') \rangle = \delta_{ij} \delta(t - t')$ and $\langle \xi_i(t) \xi_j(t') \rangle = \delta_{ij} \delta(t - t')$, where the indices $i, j \in \{x, y, z\}$. The oscillatory tube radius is defined as (see Fig. 1)

$$W(z, t) = a \sin\left(\frac{2\pi z}{L} - \omega t\right) + b, \quad (2)$$

where a is the amplitude of the tube oscillation, b is a constant, ω is the frequency given by $\omega = 2\pi/T$, and T is the time period of oscillation. The parameters a and b control the curvature and diameter of the tube (see Fig. 1). To enable particle movement from one cell to another along the length of the tube (z direction), the condition $b > a$ must be met. Otherwise, the bottlenecks of the tube are closed.

III. REDUCED 1D DESCRIPTION: FICK-JACOBS APPROXIMATION

The Fokker-Planck equation corresponding to Eq. (1) is given by

$$\begin{aligned} \frac{\partial P(\vec{r}, \hat{e}, t)}{\partial t} = & -v_0 \hat{e} \cdot \nabla P(\vec{r}, \hat{e}, t) \\ & + D_0 \nabla^2 P(\vec{r}, \hat{e}, t) + D_r \mathcal{L} P(\vec{r}, \hat{e}, t), \end{aligned} \quad (3)$$

where $P(\vec{r}, \hat{e}, t)$ is the probability density of ABPs [41] and $\mathcal{L} \equiv \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \frac{\partial}{\partial \theta}) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2}$ is the Laplace-Beltrami operator [41,42]. Solving Eq. (3) with the no-flux boundary conditions at the tube walls is not possible analytically. However, by assuming that the diffusion time for particles along the transversal directions (x, y) is much shorter compared to the diffusion time along z direction, Eq. (3) can be integrated along x and y directions [11], and obtain an effective 1D equation analogous to the Fick-Jacobs equation for ABPs in 3D oscillatory tube (see Appendix A for the detailed derivation). The 1D probability density $P(z, \hat{e}, t)$ along the z axis reads

$$\begin{aligned} \frac{\partial P(z, \hat{e}, t)}{\partial t} = & -v_0 \cos(\theta) \frac{\partial P(z, \hat{e}, t)}{\partial z} \\ & + \frac{\partial}{\partial z} \left[D(z, t) e^{\frac{-A(z, t)}{k_B \Phi}} \frac{\partial}{\partial z} \left(e^{\frac{A(z, t)}{k_B \Phi}} P(z, \hat{e}, t) \right) \right] \\ & + D_r \mathcal{L} P(z, \hat{e}, t), \end{aligned} \quad (4)$$

where $\hat{e}$ is expressed in terms of θ and ϕ . $D(z, t)$ is the position- and time-dependent diffusion coefficient incorporating the curvature of the tube geometry [19,20]:

$$D(z, t) = D_0 (1 + (W'(z, t))^2)^{-\alpha}, \quad (5)$$

where d is the dimension of the geometry, and $\alpha = 1/3$ for a 2D geometry and $\alpha = 1/2$ for a 3D geometry. Thus, the coefficient $D(z, t)$ represents a purely geometry-induced correction to the translational diffusivity (D_0) [43]. While self-propulsion (v_0) is accounted for separately via orientational dynamics [see Eqs. (10), (12), and (13)]. $A(z, t)$ is the free energy of the system, which is obtained as

$$A(z, t) = E - \Phi S = -k_B \Phi \ln h(z, t), \quad (6)$$

where $E = 0$ in our case, as there is no energetic contribution in our system, and $S = k_B \ln h(z, t)$ is the entropy due to the geometric variation in the tube's shape with respect to space and time. The transverse cross section is given by $h(z, t) = \pi[W(z, t)/L]^2$ in 3D and the width $h(z, t) = 2W(z, t)/L$ in 2D. In the case of passive Brownian particles (PBP), i.e., $v_0 = 0$, the probability density is simply $P(z, t)$, recovering the standard FJ equation for PBPs [11],

$$\frac{\partial P(z, t)}{\partial t} = \frac{\partial}{\partial z} \left[D(z, t) e^{\frac{-A(z, t)}{k_B \Phi}} \frac{\partial}{\partial z} \left(e^{\frac{A(z, t)}{k_B \Phi}} P(z, t) \right) \right]. \quad (7)$$

By solving Eq. (4) using the initial probability density $P(z, \hat{e}, 0) = \delta(z - z_0)\delta(\theta - \theta_0)\delta(\phi - \phi_0)$, where z_0, θ_0 , and ϕ_0 are the corresponding initial values, the translational current can be identified as

$$J(z, \hat{e}, t) = v_0 \cos(\theta) P(z, \hat{e}, t) - D(z, t) e^{\frac{-A(z,t)}{k_B \Phi}} \frac{\partial}{\partial z} \left(e^{\frac{A(z,t)}{k_B \Phi}} P(z, \hat{e}, t) \right). \quad (8)$$

The corresponding continuity equation [44] reads

$$\frac{\partial P(z, \hat{e}, t)}{\partial t} + \frac{\partial J(z, \hat{e}, t)}{\partial z} = D_r \mathcal{L} P(z, \hat{e}, t). \quad (9)$$

The mean velocity $\langle v \rangle$ of ABPs can be calculated by averaging over all possible orientations, space, and time to improve the accuracy of the estimate. $\langle v \rangle$ can be obtained as [43]

$$\langle v \rangle = \frac{1}{T} \int_0^T dt \int_{-\frac{L}{2}}^{\frac{L}{2}} dz \int_0^\pi d\theta \int_0^{2\pi} d\phi J(z, \theta, \phi, t) \sin \theta. \quad (10)$$

The effective diffusion coefficient D_{eff} is calculated as

$$D_{\text{eff}} = \frac{\langle z^2(t) \rangle - \langle z(t) \rangle^2}{2T}, \quad (11)$$

where $\langle z \rangle$ is the mean position and $\langle z^2 \rangle$ is the mean-squared position of ABPs computed as

$$\langle z(t) \rangle = \int_{-\frac{L}{2}}^{\frac{L}{2}} dz \int_0^\pi d\theta \int_0^{2\pi} d\phi z P(z, \theta, \phi, t) \sin \theta, \quad (12)$$

$$\langle z^2(t) \rangle = \int_{-\frac{L}{2}}^{\frac{L}{2}} dz \int_0^\pi d\theta \int_0^{2\pi} d\phi z^2 P(z, \theta, \phi, t) \sin \theta. \quad (13)$$

Note that the FJ approximation requires smooth boundary variations, i.e., $|W'(z, t)| \ll 1$. This condition ensures that ABPs quickly reach the steady state along the transversal directions of the geometry (as discussed in Appendix A), allowing the system to be effectively described by a 1D equation along the z axis, even for moderately corrugated tubes. For simplicity, we use dimensionless quantities; we scale all lengths by the periodicity of the tube L and time by the diffusive timescale $\tau = \gamma_t L^2 / k_B \Phi$. Now, the dimensionless variables are defined as $\vec{r} \rightarrow \vec{r}/L$, $t \rightarrow t/\tau$, $v_0 \rightarrow v_0 \tau / L$, $D_0 \rightarrow D_0 \tau / L^2$, and $D_r \rightarrow D_r \tau$. The dimensionless tube parameters are $a \rightarrow a/L$, $b \rightarrow b/L$, and $\omega \rightarrow \omega \tau$. In the rest of the paper, we use dimensionless quantities.

IV. NUMERICAL SIMULATIONS

As ABPs confined in the transversal direction of the tube, we can numerically compute $\langle v \rangle$ and D_{eff} along the length of the tube (z direction). These quantities can be calculated using the Brownian dynamics simulations performed by solving the overdamped Langevin equation [Eq. (1)] using the standard stochastic Euler algorithm over 2×10^4 trajectories with the integration step time of 10^{-4} . The ABPs are treated as point-sized entities initially located in the middle of the tube, in a cell [see Figs. 3(a) and 3(d)]. When an ABP approaches the tube boundary, it essentially slides along the boundary until a thermal fluctuation in the orientational vector $\hat{e}(t)$ redirects

it toward the interior of the tube [10,45–48]. Since we considered point particles, we can safely neglect hydrodynamic interactions between the particles and the tube boundaries. In the long-time limit, $\langle v \rangle$ and D_{eff} along the z direction can be calculated as

$$\langle v \rangle = \lim_{t \rightarrow \infty} \frac{\langle z(t) \rangle}{t}, \quad (14)$$

$$D_{\text{eff}} = \lim_{t \rightarrow \infty} \frac{\langle z^2(t) \rangle - \langle z(t) \rangle^2}{2t}. \quad (15)$$

The diffusive behavior of the particles is verified by analyzing the mean squared displacement (MSD) as a function of time (t). As shown in Appendix D (Fig. 8), the MSD grows linearly in time in the long-time regime, indicating normal diffusion.

V. TRANSPORT PROPERTIES

A. Frequency-dependent transport

The behavior of $\langle v \rangle$ and D_{eff} as a function of frequency ω of the oscillatory tube for different values of the self-propulsion speed v_0 is depicted in Fig. 2. Surprisingly, there is a very good agreement between analytical predictions and the numerical results up to a higher value of ω . This indicates

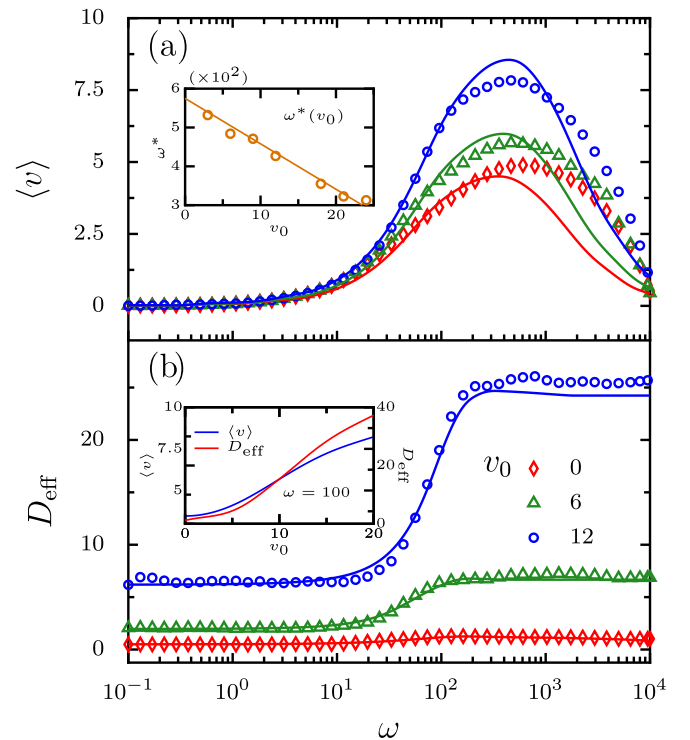


FIG. 2. (a) The mean velocity $\langle v \rangle$ and (b) the effective diffusion coefficient D_{eff} as a function of the tube oscillation frequency ω for various values of the self-propulsion speed v_0 of the particles. Symbols correspond to numerical simulation results [Eqs. (14) and (15)], whereas solid lines indicate the semianalytical results [Eqs. (10) and (11)] obtained by using the FJ approximations. The inset in panel (a) shows the peak position ω^* as a function of v_0 , while the inset in panel (b) presents the semianalytical $\langle v \rangle$ and D_{eff} vs v_0 at $\omega = 100$. Here, we set $D_0 = D_r = 1$. The tube parameters are $L = 1$, $a = 1/2\pi$, and $b = 2/2\pi$.

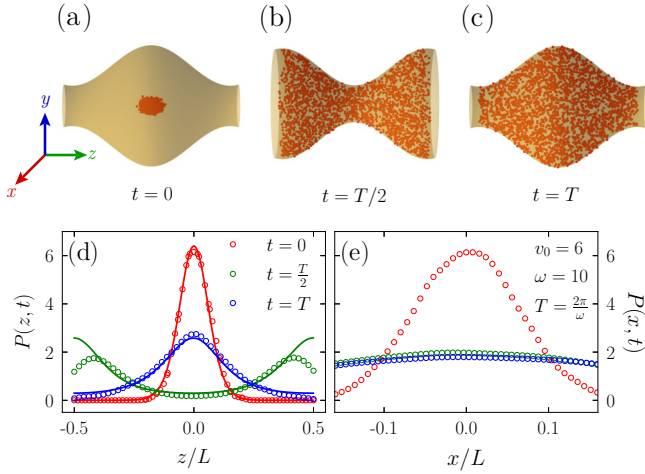


FIG. 3. Snapshots of active particles (with $v_0 = 6$) inside an oscillating tube at time (a) $t = 0$, (b) $t = T/2$, and (c) $t = T$ for $\omega = 10$. Time evolution of probability density (d) $P(z, t)$ along the tube axis z and (e) $P(x, t)$ along the transversal direction of the tube x at the same time intervals as snapshots were recorded. Here, we set $D_0 = D_r = 1$. The parameters of the tube boundary are $a = 1/2\pi$, $b = 2/2\pi$, and $L = 1$.

that the FJ approximation remains valid in the presence of oscillatory boundaries, provided the boundary dynamics are not too rapid. In a static tube, or a tube with weak oscillatory boundaries, $\langle v \rangle$ is nearly zero and D_{eff} is finite, as they should be, because there is no external force acting on the particles. In this case, particles have sufficient time to explore the space available in the transversal directions (x and y), satisfying the FJ approximation. As ω increases, due to the movement of the tube boundaries in a particular direction, both $\langle v \rangle$ and D_{eff} increase. Interestingly, the FJ approximation still provides accurate results. It is observed that the magnitude of $\langle v \rangle$ and D_{eff} increases with the self-propelled velocity v_0 of ABPs, as the diffusive nature of ABPs increases with v_0 , allowing particles to explore the available space inside the tube more effectively (see Movie S2 of the Supplemental Material [49]). For intermediate values of ω , particles exhibit maximum $\langle v \rangle$ and higher D_{eff} . This is where the oscillatory boundaries of the tube most effectively enhance the particle movement. This situation resembles the stochastic resonance [50] phenomena

observed in the case of confined channels [9], where optimal transport results from the interplay between intrinsic particle dynamics and the oscillation frequency. The FJ nearly captures these maximum values. As shown in the inset of Fig. 2(a), the peak position shifts slightly toward lower frequencies as the self-propulsion speed v_0 increases, which can be well described by a linear fit $\omega^* \simeq 575 - 11.7 v_0$. When the ω value is further increased, particles do not have enough time to explore the space available in the transversal directions. Effectively, particles are restricted to the bottleneck regions (see Fig. 2). As a result, the FJ approximation fails [8, 11].

In the limit, $\omega \rightarrow \infty$, i.e., when the tube boundaries are rapidly changing with a timescale much smaller than the diffusion timescale of the particles, particles do not feel the oscillations of the tube boundaries and particle movement is restricted around the bottleneck region (see Fig. 4 and Movie S2 of the Supplemental Material [49]). This situation is analogous to the case of particles in a cylindrical tube, and as one would expect, $\langle v \rangle \rightarrow 0$ and D_{eff} satisfies [51]

$$D_{\text{eff}} = D_0 + \frac{v_0^2}{d(d-1)D_r}. \quad (16)$$

Interestingly, the FJ approximation nearly captures this result.

B. Axial and transverse probability density

To understand how particles explore the oscillating channel and to verify the Fick-Jacobs assumption that particles reach a steady state faster in the transverse direction than along the axial direction (see Sec. III and Appendix A), we analyze the time evolution of probability densities of the particles along the tube axis, $P(z, t)$, and along a transverse direction, $P(x, t)$. The time evolution of these distributions is shown in Figs. 3(d) and 3(e), respectively. Initially ($t = 0$), all the particles were placed in the middle of the tube [see Figs. 3(a) and 3(d)]. As time progresses, the particles diffuse throughout the tube, exploring all available space and responding to the oscillatory motion of the tube boundaries (see Movies S1 and S2 of the Supplemental Material [49]). These behaviors are nearly captured by the FJ approximation [see Figs. 3(b) and 3(c)]. Furthermore, the transverse probability density is nearly uniform across the tube cross section, as shown in Fig. 3(e), supporting the assumption of the 1D reduction. Note that, at lower ω , the diffusion time is much shorter than the

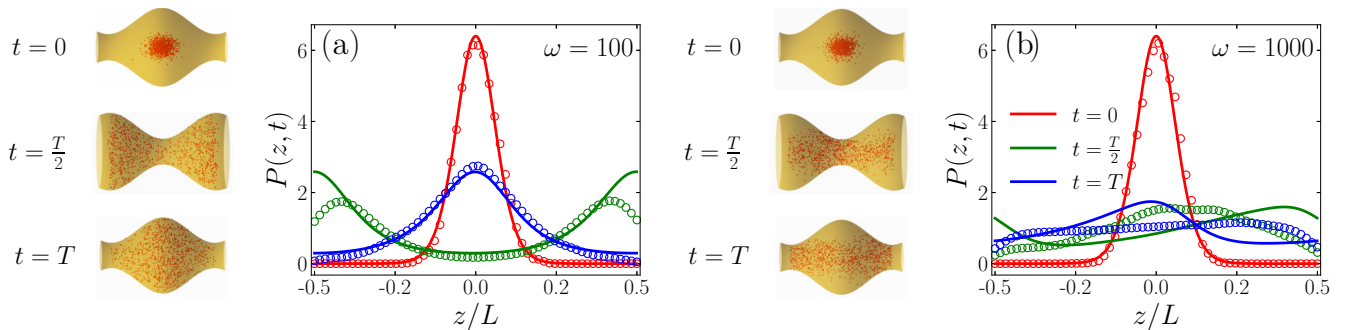


FIG. 4. Axial probability density $P(z, t)$ of active particles at three different times $t = 0$, $T/2$, and T within one oscillation period $T = 2\pi/\omega$ for (a) $\omega = 100$ and (b) $\omega = 1000$. The left panels correspond to $\omega = 100$, while the right panels correspond to $\omega = 1000$. Parameters: $D_0 = D_r = 1$, $v_0 = 6$, $a = 1/2\pi$, $b = 2/2\pi$, and $L = 1$.

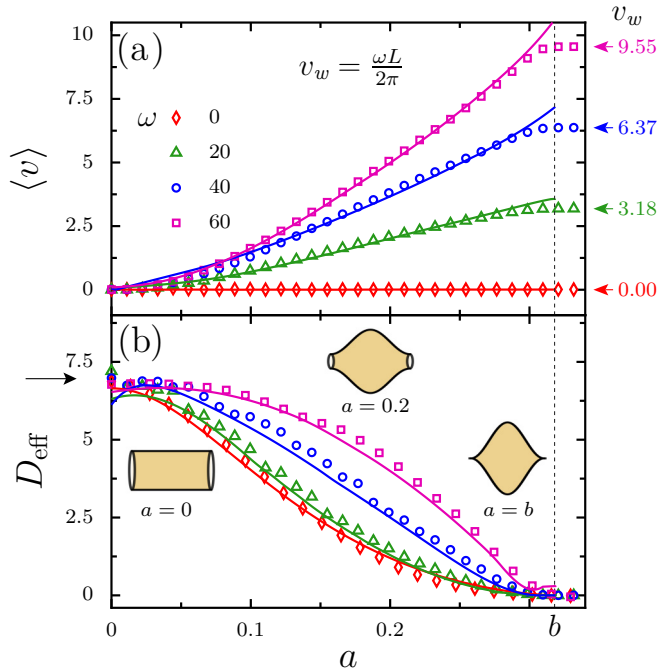


FIG. 5. (a) The magnitude of the mean velocity $\langle v \rangle$. The left arrows indicate the values of saturated mean velocity $\langle v \rangle = v_w = \frac{\omega L}{2\pi}$ beyond $a = b$. (b) The effective diffusion coefficient D_{eff} as a function of the corrugation amplitude a for different values of boundary oscillation frequency ω . The right arrows denote the value of D_{eff} calculated using Eq. (16) for a given v_0 . Here, we set $D_0 = D_r = 1$ and $L = 1$. The other parameters are $v_0 = 6$ and $b = 2/2\pi$.

oscillations of the tube, and particles get enough time to explore the available space inside the tube.

Figure 4 shows the axial probability density $P(z, t)$ at three representative times within one oscillation period for higher frequencies. At $\omega = 100$ [Fig. 4(a)], particles are able to follow the time-dependent geometry of the tube and adapt to its instantaneous shape, resulting in a smoothly modulated distribution that reflects the local tube structure (see Movies S1 and S2 of the Supplemental Material [49]). In this regime, the FJ approximation accurately reproduces the numerical results, consistent with the assumption of fast transverse equilibration. In contrast, at $\omega = 1000$ [Fig. 4(b)], the rapid boundary oscillations prevent particles from responding to the instantaneous geometry, placing the system in the nonadiabatic regime, as illustrated in Movies S1 and S2 of the Supplemental Material [49]. Consequently, the axial distribution becomes nearly uniform, and the spatial modulation associated with entropic barriers is strongly suppressed, indicating a breakdown of the FJ approximation at high frequencies.

C. Effect of oscillation amplitude

Figure 5 shows $\langle v \rangle$ and D_{eff} as a function of the amplitude of the tube oscillation a [see Eq. (2)] for different values of frequency ω . FJ approximation results are in good agreement with the numerical simulation results. When $a = 0$, the tube is a cylinder with radius b , and as expected, $\langle v \rangle$ is zero and D_{eff} satisfies Eq. (16). However, in the case of a static corrugated

tube ($\omega = 0$ and $a \neq 0$), due to symmetry of the tube, $\langle v \rangle$ is zero. However, D_{eff} decays monotonically as a increases. The tube expands in the transversal directions with increasing a , and as a result, particles explore the available space as they diffuse, which leads to a decrease in D_{eff} along the tube axis. In this situation, the entropic barriers play a vital role [11,52] (see Fig. 5). In this static limit ($\omega = 0$), the D_{eff} curve in panel (b) (red solid line) is well described by the classical Lifson-Jackson analytical formula [42,44,53,54],

$$D_{\text{eff}} = \left[\frac{1}{L^2} \int_{-\frac{L}{2}}^{\frac{L}{2}} dz e^{\frac{A(z)}{k_B \Phi}} \int_{-\frac{L}{2}}^{\frac{L}{2}} dz \frac{e^{-\frac{A(z)}{k_B \Phi}}}{D_b(z)} \right]^{-1}, \quad (17)$$

where $A(z)$ is defined in Eq. (6). $D_b(z)$ is given by the activity-renormalized bulk diffusion [42],

$$D_b(z) = \left(D_0 + \frac{v_0^2}{d(d-1)D_r} \right) [1 + (W'(z))^2]^{-\alpha}, \quad (18)$$

where the scaling exponent $\alpha = 1/2$ for the case of a 3D tube. Note that $D_b(z)$ entering in the Lifson-Jackson formula [Eq. (17)] differs from the diffusivity $D(z, t)$ appearing in the FJ equation [Eq. (4)]. The latter purely accounts for the curvature of the tube boundaries. Additionally, $D_b(z)$ includes the v_0 contribution [42], and it corresponds to strictly an effective 1D representation of the 3D system.

When the tube boundaries oscillate ($\omega > 0$), the tube boundaries squeeze the particles along the z direction. As a result, both $\langle v \rangle$ and D_{eff} increase. When $a \approx b$, $\langle v \rangle$ saturates at the phase velocity of the tube boundaries ($v_{\text{wall}} = \frac{\omega L}{2\pi}$). At $a = b$, i.e., when the pore radius $b - a = 0$, the bottlenecks of the tube are closed, and particles are confined without moving from one cell to another. Particles move together as a wave packet, and $\langle v \rangle$ matches the phase velocity of the tube walls. This confinement leads to vanishing D_{eff} because the particles are unable to spread between adjacent cells in the tube. In this situation, the FJ approximation fails because there is no accessible transverse domain, preventing ABPs from reaching the steady state in the transverse direction. Consequently, both the free energy $A(z, t)$ and the translational current $J(z, t)$ diverge (see the explanation in Appendix C and Fig. 7).

VI. DISCUSSION

Particle diffusion confined within the fluctuating boundaries or dynamic porous media shows transport behavior distinct from the case of static confinement [55–57]. For example, our semianalytical and numerical simulations reveal a resonancelike enhancement [58,59] in both $\langle v \rangle$ and D_{eff} of ABPs. In contrast with the intuition that transport increases (decreases) with high (low) oscillation frequency ω due to structural jiggling, we find enhancement peak at an optimal frequency. As shown in the inset of Fig. 2(a), the peak position shifts slightly toward lower frequencies as the self-propulsion speed v_0 increases, which can be described by the linear relation $\omega^* \simeq 575 - 11.7 v_0$. These observations are consistent with the experimental results of thin liquid films and oscillating microchannels, which show that frequency-dependent mobility is enhanced [60]. Additionally, studies on particles and macromolecules confined between oscillating surfaces report increased mobility and diffusion at a certain

frequency, supporting our findings [61,62]. These parallels between semianalytics, simulations, and experiments underscore the physical relevance of resonance-enhanced transport in confined systems. Importantly, the generalized Fick-Jacobs framework consistently connects several well-understood limiting cases, including passive and active particles, biased and unbiased conditions, and static and pulsating geometries [11,36,44], highlighting the robustness of the reduced description. To contextualize our dimensionless parameters in real units considered, particles moving in a 3D oscillating geometry with system parameters $a \sim 15.9 \mu\text{m}$, $b \sim 31.8 \mu\text{m}$, and period length $L \sim 100 \mu\text{m}$ filled with water at room temperature ($\Phi \sim 300 \text{ K}$), having viscous drag $\gamma_t \sim 2 \times 10^{-10} \text{ kg/s}$, characteristic diffusion time $\tau \sim 455 \text{ s}$, and self propulsion speed $v_0 \sim 1.3 \mu\text{m/s}$, which corresponds to the dimensionless propulsion speed $v_0 = 6$ used in our model, our dimensionless frequency range $\omega = 0.1\text{--}10\,000$ corresponds to a physical band of $\approx 3.5 \times 10^{-5}$ to 3.5 Hz .

VII. CONCLUSIONS

In conclusion, this work highlights the crucial role of confinement and the coupling between the particles' intrinsic activity and the dynamic oscillations of the tube boundaries. This coupling gives rise to nontrivial transport phenomena that are inaccessible in static systems, highlighting the universality of resonancelike mechanisms in particle transport. Our model more accurately captures natural and synthetic systems with 3D confinement. For instance, our generalized Fick-Jacobs framework for ABPs in a 3D pulsating tube consistently connects several well-understood limiting cases, including passive and active, biased and unbiased, and static-rigid and pulsating limits, and provides robust quantitative predictions for the transport properties. We have demonstrated that the transport properties have maximum values at an intermediate frequency ω of the tube oscillations, maximizing both $\langle v \rangle$ and D_{eff} of ABPs. This behavior is analogous to stochastic resonance [50], where optimal transport emerges from the competition between the time scales associated with intrinsic particle dynamics and the oscillation frequency. Furthermore, the amplitude of boundary oscillations enhances both $\langle v \rangle$ and D_{eff} . In the limit of tube bottleneck radius to zero, $\langle v \rangle$ approaches the phase velocity of the oscillating wall ($v_{\text{wall}} = \frac{\omega L}{2\pi}$) and D_{eff} is nearly zero, where particles are confined to individual cells. Our framework reveals key principles for controlling particle transport in confined systems with oscillatory boundaries. In the latter case, one needs to identify the appropriate length scale depending on the system of interest. These results suggest improved strategies for targeted drug delivery, microfluidic control, selective filtration, and precise biomolecular manipulation.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX A: DERIVATION OF THE FICK-JACOBS EQUATION

Here, we derive the reduced 1D Fick-Jacobs equation for active Brownian particles (ABPs) confined in a 3D tube with oscillatory boundaries (see Fig. 1). The corresponding Fokker-Planck equation for the dynamics given in Eq. (1) reads

$$\partial_t P(\vec{r}, \hat{e}, t) = -v_0 \hat{e} \cdot \nabla P(\vec{r}, \hat{e}, t) + D_0 \nabla^2 P(\vec{r}, \hat{e}, t) + D_r \mathcal{L}P(\vec{r}, \hat{e}, t), \quad (\text{A1})$$

where $P(\vec{r}, \hat{e}, t)$ is the probability density, $\vec{r} = (x, y, z)$ is the position vector, v_0 is the self-propelled velocity of the ABP with orientation vector $\hat{e} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ [41], and $\mathcal{L} \equiv [\frac{1}{\sin \theta} \partial_\theta (\sin \theta \partial_\theta) + \frac{1}{\sin^2 \theta} \partial_\phi^2]$ is the Laplace-Beltrami operator [41,42]. The following assumptions are made to map the 3D system to an effective 1D system:

(1) Diffusion across the transverse direction (x and y) is fast compared to the transport axis (z). It means that the associated timescale $\tau_\perp \sim W(z, t)^2/D_0$ in the transverse directions is much smaller than the timescale $\tau_z \sim L^2/D_0$ along the z direction. This separation of timescales implies that $\tau_\perp \ll \tau_z$ or, equivalently, $\frac{W(z, t)}{L} \ll 1$ corresponds to a narrow tube geometry.

(2) The tube radius $W(z, t)$ varies smoothly along the axial direction [9], i.e., $|\partial_z W(z, t)| \ll 1$.

(3) The probability density profile is nearly uniform in transverse directions [11]. Then, we can write $P(\vec{r}, \hat{e}, t) \approx P(z, \hat{e}, t)/h(z, t)$, where $h(z, t) = \pi[W(z, t)/L]^2$ is the cross-sectional area of the tube. Here, $P(z, \hat{e}, t)$ is the marginal probability density, which is written as $P(z, \hat{e}, t) = \iint_{\Omega(z, t)} P(\vec{r}, \hat{e}, t) dx dy$, where $\Omega(z, t)$ is the region in the xy plane defined by the tube's cross section at position z and time t .

(4) No-flux boundary conditions [42] for ABPs in a confined tube ensure that particles cannot escape through the tube walls, meaning the translational probability current normal to the tube wall is zero.

Using the above assumptions, we integrate the Fokker-Planck equation [Eq. (A1)] over the transverse cross section $\Omega(z, t)$,

$$\iint_{\Omega(z, t)} \partial_t P(\vec{r}, \hat{e}, t) dx dy = \iint_{\Omega(z, t)} [-v_0 \hat{e} \cdot \nabla P + D_0 \nabla^2 P + D_r \mathcal{L}P] dx dy. \quad (\text{A2})$$

The corresponding translational and rotational probability currents are given by

$$\vec{J}(\vec{r}, \hat{e}, t) = v_0 \hat{e} P(\vec{r}, \hat{e}, t) - D_0 \nabla P(\vec{r}, \hat{e}, t), \quad (\text{A3})$$

$$\vec{J}_r(\vec{r}, \hat{e}, t) = -D_r \left(\hat{\theta} \partial_\theta P + \frac{1}{\sin \theta} \hat{\phi} \partial_\phi P \right). \quad (\text{A4})$$

Each term in Eq. (A2) is evaluated separately. Integrating the left-hand side of Eq. (A2) over the cross section $\Omega(z, t)$ and applying Leibniz's rule for domains with dynamic boundaries at fixed z yields

$$\iint_{\Omega(z,t)} \partial_t P dx dy = \partial_t \left(\iint_{\Omega(z,t)} P dx dy \right) - \oint_{\partial\Omega(z,t)} P (\partial_t \vec{r} \cdot \hat{n}) d\ell. \quad (\text{A5})$$

Based on Assumption 3, the marginal probability density is

$$P(z, \hat{e}, t) = \iint_{\Omega(z,t)} P(\vec{r}, \hat{e}, t) dx dy, \quad (\text{A6})$$

which gives

$$\iint_{\Omega(z,t)} \partial_t P dx dy = \partial_t P(z, \hat{e}, t) - \oint_{\partial\Omega(z,t)} P(\vec{r}, \hat{e}, t) (\partial_t \vec{r} \cdot \hat{n}) d\ell, \quad (\text{A7})$$

where $d\ell$ denotes the length element along $\partial\Omega(z, t)$. Here, $\partial\Omega(z, t)$ denotes the boundary of the transverse cross section at fixed z and t . For an axisymmetric tube with radius $W(z, t)$, the boundary position can be written as

$$\vec{r} = (W(z, t) \cos \psi, W(z, t) \sin \psi, z), \quad (\text{A8})$$

where ψ is the azimuthal angle in the transverse (xy) plane. Differentiating with respect to time gives

$$\partial_t \vec{r} = (\partial_t W(z, t) \cos \psi, \partial_t W(z, t) \sin \psi, 0). \quad (\text{A9})$$

The outward unit normal vector reads

$$\hat{n} = \frac{(\cos \psi, \sin \psi, -\partial_z W(z, t))}{\sqrt{1 + (\partial_z W(z, t))^2}}. \quad (\text{A10})$$

It follows that $\partial_t \vec{r} \cdot \hat{n} = 0$, and hence the boundary term vanishes.

$$\oint_{\partial\Omega(z,t)} P(\vec{r}, \hat{e}, t) (\partial_t \vec{r} \cdot \hat{n}) d\ell = 0. \quad (\text{A11})$$

Hence, the left-hand side of Eq. (A2) reduces to

$$\iint_{\Omega(z,t)} \partial_t P(\vec{r}, \hat{e}, t) dx dy = \partial_t P(z, \hat{e}, t). \quad (\text{A12})$$

The first term on the right-hand side of Eq. (A2) can be written as

$$\begin{aligned} & - \iint_{\Omega(z,t)} v_0 \hat{e} \cdot \nabla P dx dy \\ & = -v_0 \left[\sin \theta \cos \phi \iint_{\Omega(z,t)} \partial_x P dx dy \right. \\ & \quad + \sin \theta \sin \phi \iint_{\Omega(z,t)} \partial_y P dx dy \\ & \quad \left. + \cos \theta \iint_{\Omega(z,t)} \partial_z P dx dy \right]. \end{aligned} \quad (\text{A13})$$

The transverse terms in Eq. (A13) can be rewritten using Green's theorem as

$$\begin{aligned} \iint_{\Omega(z,t)} \partial_x P dx dy &= \oint_{\partial\Omega(z,t)} P(\vec{r}, \hat{e}, t) n_x d\ell, \\ \iint_{\Omega(z,t)} \partial_y P dx dy &= \oint_{\partial\Omega(z,t)} P(\vec{r}, \hat{e}, t) n_y d\ell. \end{aligned} \quad (\text{A14})$$

Due to the axisymmetry of the tube and the uniformity of $P(\vec{r}, \hat{e}, t)$ along the transverse direction (Assumption 3), these integrals evaluate to zero, i.e.,

$$\oint_{\partial\Omega(z,t)} P(\vec{r}, \hat{e}, t) n_x d\ell = 0, \quad (\text{A15})$$

$$\oint_{\partial\Omega(z,t)} P(\vec{r}, \hat{e}, t) n_y d\ell = 0. \quad (\text{A16})$$

The z -component in Eq. (A13) contains the self-propulsion along the tube axis. Using Leibniz's rule (at fixed t) gives

$$\begin{aligned} \iint_{\Omega(z,t)} \partial_z P dx dy &= \partial_z \left(\iint_{\Omega(z,t)} P dx dy \right) \\ &\quad - \oint_{\partial\Omega(z,t)} P(\vec{r}, \hat{e}, t) (\partial_z \vec{r} \cdot \hat{n}) d\ell \\ &= \partial_z P(z, \hat{e}, t) \\ &\quad - \oint_{\partial\Omega(z,t)} P(\vec{r}, \hat{e}, t) (\partial_z \vec{r} \cdot \hat{n}) d\ell. \end{aligned} \quad (\text{A17})$$

Differentiating $\vec{r}$ with respect to z yields

$$\partial_z \vec{r} = (\partial_z W(z, t) \cos \psi, \partial_z W(z, t) \sin \psi, 1). \quad (\text{A18})$$

Using the outward unit normal vector given in Eq. (A10), one finds that $\partial_z \vec{r} \cdot \hat{n} = 0$. Consequently, the boundary contribution vanishes,

$$\oint_{\partial\Omega(z,t)} P(\vec{r}, \hat{e}, t) (\partial_z \vec{r} \cdot \hat{n}) d\ell = 0. \quad (\text{A19})$$

The axial advection term becomes

$$-v_0 \cos \theta \iint_{\Omega(z,t)} \partial_z P(\vec{r}, \hat{e}, t) dx dy = -v_0 \cos \theta \partial_z P(z, \hat{e}, t). \quad (\text{A20})$$

The second term (translational diffusion) on the right-hand side of Eq. (A2) reads

$$\begin{aligned} D_0 \iint_{\Omega(z,t)} \nabla^2 P dx dy &= D_0 \left[\iint_{\Omega(z,t)} \nabla_{\perp}^2 P dx dy \right. \\ &\quad \left. + \iint_{\Omega(z,t)} \partial_z^2 P dx dy \right]. \end{aligned} \quad (\text{A21})$$

The transversal term in Eq. (A21) vanishes due to the no-flux condition (Assumption 4) at tube walls, i.e.,

$$\vec{J} \cdot \hat{n}|_{\partial\Omega(z,t)} = 0. \quad (\text{A22})$$

Using Leibniz's rule and Assumption 3, the axial contribution in Eq. (A21) becomes

$$D_0 \iint_{\Omega(z,t)} \partial_z^2 P dx dy = D_0 \partial_z \left[h(z, t) \partial_z \left(\frac{P(z, \hat{e}, t)}{h(z, t)} \right) \right]. \quad (\text{A23})$$

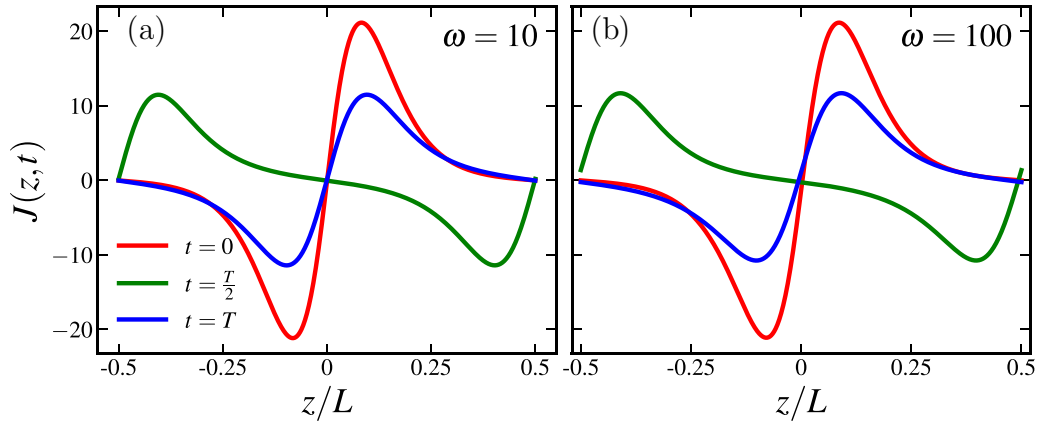


FIG. 6. Time evolution of the translational current $J(z, t)$ along the tube axis for (a) $\omega = 10$ and (b) $\omega = 100$, shown at identical time intervals within one oscillation period. The periodic deformation of the tube leads to a temporal symmetry of the current profiles, resulting in a reversal of the transport direction during the oscillation cycle. Parameters: $D_0 = D_r = 1$, $v_0 = 6$, $a = 1/(2\pi)$, $b = 2/(2\pi)$, and $L = 1$.

Rewriting the above equation using free energy $A(z, t) = -k_B \Phi \ln h(z, t)$, the axial diffusion term can be written as

$$\partial_t P(z, \hat{e}, t) = \partial_z \left[D_0 e^{-\frac{A(z, t)}{k_B \Phi}} \partial_z \left(e^{\frac{A(z, t)}{k_B \Phi}} P(z, \hat{e}, t) \right) \right]. \quad (\text{A24})$$

In the presence of confinement, the bulk diffusion coefficient D_0 can be replaced by a position- and time-dependent effective diffusion coefficient $D(z, t)$, which accounts for local geometric variations of the tube due to the dynamic boundaries [see Eq. (5)] [19,20]:

$$D(z, t) = D_0 (1 + (W'(z, t))^2)^{-\alpha}, \quad (\text{A25})$$

where $\alpha = 1/2$ and $d = 3$. The third term (rotational diffusion) on the right-hand side of Eq. (A2) becomes

$$\iint_{\Omega(z, t)} D_r \mathcal{L}P(\vec{r}, \hat{e}, t) dx dy = D_r \mathcal{L}P(z, \hat{e}, t). \quad (\text{A26})$$

Combining the above expressions, the Fick-Jacobs equation can be obtained as

$$\begin{aligned} \partial_t P(z, \hat{e}, t) = & -v_0 \cos \theta \partial_z P(z, \hat{e}, t) \\ & + \partial_z \left[D(z, t) e^{-\frac{A(z, t)}{k_B \Phi}} \partial_z \left(e^{\frac{A(z, t)}{k_B \Phi}} P(z, \hat{e}, t) \right) \right] \\ & + D_r \mathcal{L}P(z, \hat{e}, t), \end{aligned} \quad (\text{A27})$$

which describes the effective one-dimensional dynamics of active Brownian particles self-propelling inside an oscillating axisymmetric tube.

APPENDIX B: TIME EVOLUTION OF CURRENT

We solve the time-dependent Fick-Jacobs equation to obtain the translational current $J(z, \theta, \phi, t)$, and the longitudinal current is computed as

$$J(z, t) = \int_0^{2\pi} \int_0^\pi J(z, \theta, \phi, t) \sin \theta d\theta d\phi. \quad (\text{B1})$$

Due to the periodic modulation of the tube's geometry, the translational current $J(z, t)$ exhibits time dependency over each oscillation cycle. Importantly, the boundary shape evolves symmetrically over time, such that the configuration at $t = T/2$ is a mirror reversal of that at $t = 0$, and the system

returns to its initial shape at $t = T$. As a result, the current profiles exhibit a temporal symmetry: The current at $t = T/2$ is the exact negative of that at $t = 0$, and the profile at $t = T$ is identical to the one at $t = 0$, as seen in Fig. 6. This dynamic symmetry results in the periodic reversal of particle transport along the tube. In the first half of the cycle, particles tend to move toward specific regions of the tube, resulting in a net current flowing in one direction. In the second half, the boundary deformation reverses, and particles redistribute in the opposite direction, reversing the current. These alternating transport results in peaks and dips in the current profiles $J(z, t)$, which are spatially symmetric with respect to the tube center ($z = 0$).

APPENDIX C: EFFECT OF BOTTLENECK ON FREE ENERGY AND CURRENT

The free energy of the system is given by Eq. (6). In the absence of an external bias, the free energy entering the Fick-Jacobs description is purely entropic. As the tube amplitude a increases, the free-energy barrier at the bottleneck increases. Since the tube radius $W(z, t)$ and the corresponding cross-sectional area $h(z, t)$ attain their minimum values at the bottleneck, the quantity $-\ln h(z, t)$ becomes maximal, and therefore the entropic free energy $A(z, t)$ also reaches its maximum [Figs. 7(a) and 7(b)]. Correspondingly, the current $J(z, t)$ exhibits pronounced extrema at the same locations [Figs. 7(c) and 7(d)]. In the limiting case where the bottleneck closes completely, the accessible phase-space volume vanishes, leading to an infinite entropic barrier, $A(z, t) \rightarrow \infty$, which suppresses particle transport through the pinch region. The entropic free energy is given by

$$\begin{aligned} A(z, t) = & -k_B \Phi \ln h(z, t) \\ = & -k_B \Phi \left[\ln \pi + 2 \ln \left(\frac{W(z, t)}{L} \right) \right], \end{aligned} \quad (\text{C1})$$

where $h(z, t) = \pi [W(z, t)/L]^2$. When $a = b$, the bottleneck radius vanishes, $W_{\min} = 0$, and the free-energy term $\ln (W_{\min}/L)$ diverges, rendering the pinch region inaccessible to particle transport. In the reduced 1D description, this

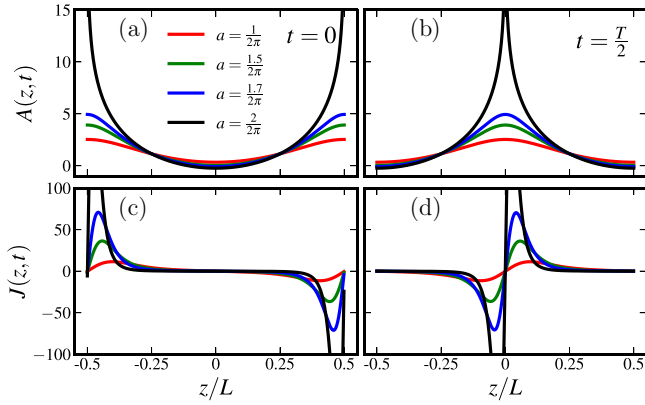


FIG. 7. Dynamics of the free energy and particle current along the tube axis for different amplitudes. Panels (a) and (b) show $A(z, t)$ at $t = 0$ and $t = T/2$, respectively. Panels (c) and (d) show the translational current $J(z, t)$ corresponding to the parameters $v_0 = 6$ and $D_0 = D_r = 1$ at the same times. Tube parameters are $b = 2/(2\pi)$, $L = 1$, and $\omega = 10$.

boundary shows up as a steep slope when $a = b$ and the free energy term in the drift makes the current $J(z, t) \rightarrow \infty$. Note that the divergence of the current is not physical. It is a result of a mathematical singularity (which is shown below) in the reduced FJ equation when the bottleneck radius of the tube becomes zero. The FJ approximation does not apply in this case since there is no transverse domain. The corresponding current is given by

$$J(z, \theta, \phi, t) = v_0 \cos \theta P(z, \theta, \phi, t) - D(z, t) \partial_z P(z, \theta, \phi, t) + 2k_B \Phi D(z, t) \frac{W'(z, t)}{W(z, t)} P(z, \theta, \phi, t). \quad (\text{C2})$$

Since $W(z, t) \rightarrow 0$ when the bottleneck is closed while $W'(z, t)$ remains finite, $W'(z, t)/W(z, t) \rightarrow \pm\infty$, and therefore from Eq. (B1), $J(z, t) \rightarrow \pm\infty$. Note that in the latter case, the Fick-Jacobs approximation fails, as shown by divergences in free energy and current in Figs. 7(a)–7(d). We terminate the semianalytical calculation in Fig. 5 at tube closure, as the FJ approximation is no longer appropriate for describing particle dynamics beyond this limit.

APPENDIX D: THE MEAN SQUARE DISPLACEMENT

To investigate the diffusive behavior of the particles, we analyze the mean squared displacement, which is numerically computed from the variance of the particle positions along the

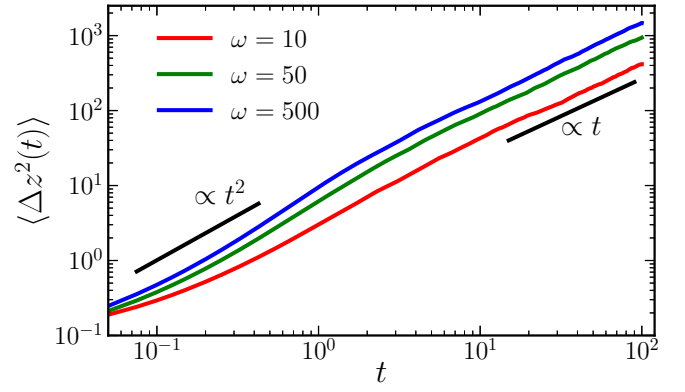


FIG. 8. Numerically computed mean squared displacement $\langle \Delta z^2(t) \rangle$ as a function of time t for different oscillation frequencies ω . The MSD is computed using Eq. (D1). At long times, the MSD exhibits a linear growth, i.e., $\langle \Delta z^2(t) \rangle \propto t$, indicating normal diffusive behavior. The other parameters are chosen as $v_0 = 6$ and $D_0 = D_r = 1$ and tube parameters $a = 1/(2\pi)$, $b = 2/(2\pi)$, and $L = 1$.

tube axis (z) as [48]

$$\langle \Delta z^2(t) \rangle = \langle z^2(t) \rangle - \langle z(t) \rangle^2, \quad (\text{D1})$$

where $z(t)$ denotes the particle position along the axial direction at time t and $\langle \cdot \rangle$ denotes the ensemble average. The diffusive behavior of the particles can be characterized from the scaling relation of the MSD,

$$\langle \Delta z^2(t) \rangle \propto t^\alpha, \quad (\text{D2})$$

where the exponent α determines the nature of the diffusion process. In particular, $\alpha = 1$ corresponds to normal diffusion and $\alpha < 1$ indicates subdiffusion, while $\alpha > 1$ represents superdiffusive behavior. The instantaneous scaling exponent $\alpha(t)$ is defined as [48,63,64]

$$\alpha(t) = \frac{d \ln \langle \Delta z^2(t) \rangle}{d \ln t}. \quad (\text{D3})$$

The exponent α therefore provides a convenient way to identify the diffusion regime of the system. Figure 8 indicates that for short times, particles move persistently due to their self-propulsion, leading to the ballistic regime, which is characterized by $\langle \Delta z^2(t) \rangle \propto t^2$. For sufficiently long times, the MSD exhibits a linear growth with time, $\langle \Delta z^2(t) \rangle \propto t$, corresponding to normal diffusion. These results hold for both low and high oscillation frequencies of the tube boundaries. Although the magnitude of the MSD depends on the driving frequency ω [see Fig. 2(b)], the diffusive nature is unaffected by ω . As usual, the effective diffusion coefficient (D_{eff}) can be obtained from the slope of the MSD in the long-time limit as described in Eq. (15).

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