Motion of an active bent rod with an articulating hinge: exploring mechanical and chemical modes of swimming

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Swimming at the microscale typically involves two modes of motion: mechanical propulsion and propulsion due to field interactions. During mechanical propulsion, particles swim by reconfiguring their geometry. When propelled by field interactions, body forces such as phoretic interactions drive mobility. In this work, we employ slender-body theory to explore how a bent rod actuator propels due to a mechanical mode of swimming via hinge articulations and due to a chemical mode of swimming via diffusiophoretic interactions with a solute field. Although previous theoretical studies have examined mechanical and chemical modes of swimming in isolation, the simultaneous investigation of both modes has remained unexplored. For the mechanical mode of swimming, our calculations, both numerical and analytical, recover Purcell's scallop theorem and show that the bent rod actuator experiences zero net displacement during reciprocal motion. Additionally, we calculate the trajectories traced by a bent rod actuator under a non-reciprocal hinge articulation, revealing that these trajectories are influenced by the amplitude of the hinge articulation, geometric asymmetry, and the angular velocity distribution between the two arms of the bent rod actuator. We provide intuitive explanations for these effects using free-body diagrams. Furthermore, we explore the motion induced by simultaneous hinge articulations and self-diffusiophoresis. We observe that hinge articulations can modify the effective phoretic forces and torques acting on the bent rod actuator, either supporting or impeding propulsion. Additionally, during self-diffusiophoretic propulsion, reciprocal hinge articulations no longer result in zero net displacement. In summary, our findings chart a new direction for designing micron-sized objects that harness both mechanical and chemical modes of propulsion synchronously, offering a mechanism to enact control over trajectories.

1 Introduction

Microscale entities orchestrate physical and biological phenomena. Bacteria play a key role in the spread of infection [1], macrophages have the capacity to affect tumor malignancy [2], T cells can infiltrate solid tumors and kill tumor cells [3], and subsurface microparticles influence contaminant transport in groundwater [4]. Inspired by these natural systems, efforts have been made to create artificial micron-sized objects endowed with programmable actions to influence phenomena at the microscale. Commonly called microrobots, these micron-sized objects are capable of treating diseases [5–9], acting as biological sensors [10, 11], and removing microplastics [12], among others. A key factor that influences the efficacy of microrobots is how capable they are at swimming in fluid environments. Due to the small length scales, viscous forces dominate over inertial forces, such that the Reynolds number (Re) $Re = \frac{Inertial\ forces}{Viscous\ forces} \ll 1$. In the low Re regime, microrobots must adapt strategies for locomotion that differ when compared to their macroscopic counterparts [13–15].

The two modes of swimming commonly used to impart motility at the microscale are, taxonomically, mechanical propulsion and propulsion due to field interactions. In the mechanical swimming mode, motility is induced by continuous geometric reconfiguration [16–20]. In field-driven propulsion, the geometry typically remains unchanged, but body forces due to interactions with a field induce motility [21–24]. In this paper, we explore how chemical fields leading to self-diffusiophoretic propulsion, i.e., a chemical mode of swimming, can be employed in concert with a mechanical mode of swimming to alter the motion of a bent rod actuator.

We first focus on the mechanical mode of swimming. In the seminal paper "Life at low Reynolds number," Purcell outlined the scallop theorem and described the mechanical strategies that microscopic entities use to swim [15]. Purcell argued that any body with Re ≪ 1 experiences zero net displacement under reciprocal geometric reconfigurations, i.e., geometry changes that are identical when viewed forward or backward in time [15, 19]. Purcell illustrated this through the example of a microscopic scallop, whereupon opening and closing its shell, the scallop experienced zero net displacement [15]. More detailed mathematical works have confirmed the scallop theorem [25–27]. A consequence of the scallop theorem is that microscopic objects, both synthetic and biological, must use non-reciprocal swimming strokes to achieve non-zero net displacement. The simplest swimmer that Purcell described is a two-hinge swimmer that is able to achieve net displacement while still returning to the original configuration [15, 28]. In fact, microscopic biological organisms, such as *Escherichia coli* or spermatozoon, have developed strategies to swim by either rotating slender helical flagellar filaments or beating flexible flagella [29–33]. Advances in microfabrication and external field actuation techniques have enabled many of these biological swimming techniques to be replicated in synthetic systems [34–39].

In the field-driven mode of swimming, phoretic mechanisms, e.g., diffusiophoresis (the focus of this work) [40–52], thermophoresis [53–55], electrophoresis [56–64], and electrodiffusiophoresis [65, 66], are used to achieve directed motion at the microscale. Diffusiophoresis, the movement of particles in chemical gradients [67–80], has been a particularly rich area of research due to similarities with cell chemotaxis [81, 82]. Active diffusiophoretic particles use reactive patches on the particle surface, enabling the particle to generate local concentration gradients and achieve locomotion [40, 51, 83]. One key factor that influences self-diffusiophoretic particle motion is particle geometry [84–90]. Recently, Ganguly and Gupta have explored the effect of geometry on the diffusiophoretic motion of bent rod microparticles [42]. They found that bent rod particles with uniform or nonuniform surface activity, when constrained to move in two dimensions, have trajectories that are always circular, consistent with experimental reports [40, 55].

The aforementioned studies focus only on one mode of swimming. To the best of our knowledge, no study has explored low Re swimming due to a combination of a field-driven motion and mechanical reconfiguration. To this end, we extend the results from Ganguly and Gupta [42] by allowing the hinge connecting the self-propelling bent rod to articulate (Figure 1). We distinguish the articulating bent rod from the non-reconfigurable version by calling it a bent rod actuator. Here, hinge articulations facilitate the mechanical swimming mode, enabling the actuator to alter its geometry, whereas the surface reaction provides the field-driven mode via self-diffusiophoresis, herein called chemical swimming. The bent rod geometry is particularly useful because its configuration can be fully characterized by two dimensionless parameters, the length ratio of the two arms and the angle between the arms. In our framework, the mechanical mode is characterized by a normal surface velocity, whereas the chemical mode introduces a tangential surface velocity, see Figure 1, providing a convenient means to analyze the motion of the bent rod actuator.

First, in Section 2, we expand the theoretical framework developed by Roggeveen and Stone [91] and Ganguly and Gupta [42] to compute the motion of the actuator due to both self-diffusiophoresis as well as hinge articulations. In Section 3.1 and Section 3.2, we calculate the trajectories of the actuator moving due to reciprocal hinge articulations (Figure 4) and non-reciprocal hinge articulations (Figure 5). We present an intuitive understanding of the trajectories by considering free-body diagrams (Figure 6). Lastly, we study the motion due to self-diffusiophoresis with hinge articulations to determine particle trajectories that combine mechanical and chemical modes of swimming (Section 3.3; Figures 7, 8).

2 Methods

2.1 Problem setup

We adapt the hydrodynamic calculations outlined by Roggeveen and Stone [91] and Ganguly and Gupta [42] to study the motion of a bent rod actuator, Figure 1. We employ the non-dimensional particle geometry as described by Ganguly and Gupta [42]. The bent rod actuator is composed of two arms connected with a hinge that articulates, allowing for the angle θ between the two arms to be varied in time. The two arms have a combined length ℓ, with each arm having a length of $(\frac{1}{2} + q)\ell$ and $(\frac{1}{2} - q)\ell$, where q is a length asymmetry parameter. We consider the arms to have equal radius a and a small aspect ratio, i.e., $\epsilon = \frac{a}{\ell} \ll 1$. A non-dimensional schematic diagram of the particle geometry can be seen in Figure 1.

The position along the center-line of the bent rod actuator is described by the non-dimensional arc-length s (scaled by ℓ), where
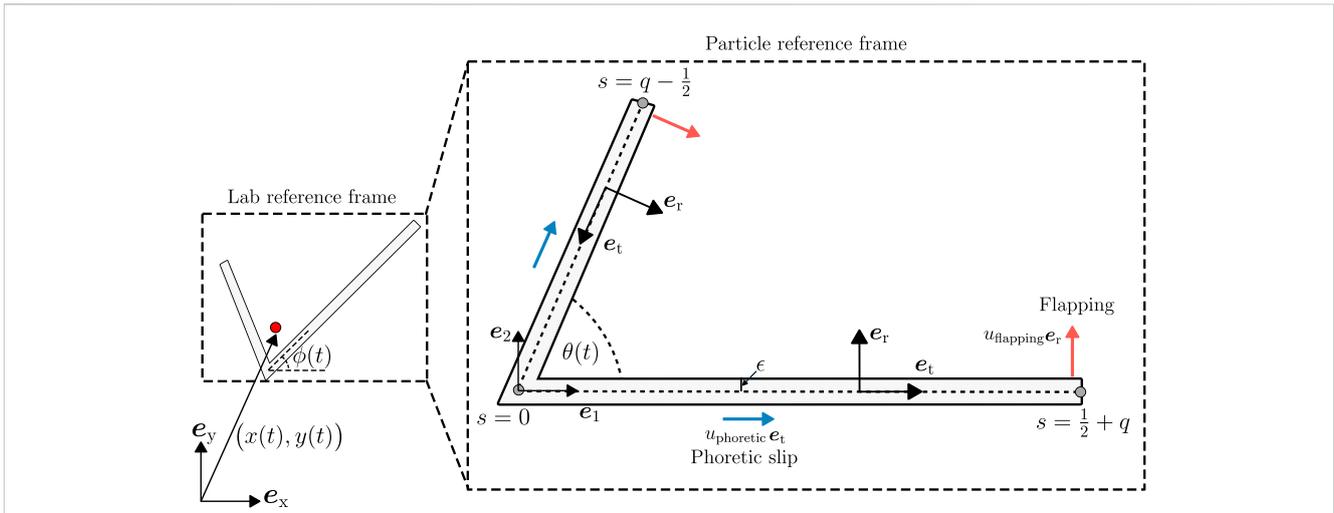
FIGURE 1
Non-dimensional geometry of a bent rod actuator. We consider the motion of a bent rod actuator with an angle $\theta(t)$ between the positive ($s > 0$) and negative ($s < 0$) arms. The angle $\theta(t)$ is allowed to vary in time via an articulating hinge at $s = 0$ that connects the positive and negative arms. Hinge articulations induce a normal velocity $u_{\text{flapping}}e_{\text{r}}$ on the surface of the actuator arms. We also consider the motion of the bent rod actuator due to a self-diffusiophoretic slip velocity $u_{\text{phoretic}}e_{\text{t}}$ in the direction tangential to the arms. The diffusiophoretic velocity is caused by a solute flux $j(s)$ into the fluid surrounding the bent rod actuator imposing concentration gradients in the solution. We determine the velocity $\boldsymbol{U}$ and angular velocity $\boldsymbol{\Omega}$ of the bent rod actuator in the particle frame of reference, as described with the $e_1 - e_2$ unit basis vectors. After calculating $\boldsymbol{U}$ and $\boldsymbol{\Omega}$, we integrate Eq. 14 to find the trajectory and orientation of the bent rod actuator in the laboratory frame of reference.

$s \in [q - \frac{1}{2}, q + \frac{1}{2}]$. $s = 0$ describes the location of the hinge connecting the two actuator arms that is allowed to articulate. We call the arm with $s < 0$ the negative arm and the arm with $s \geq 0$ the positive arm. When $q = 0$, both arms have the same length; when $q < 0$, the negative arm is longer; and when $q > 0$, the positive arm is longer. We define a coordinate system with unit basis vectors $e_1 - e_2$ in the particle frame of reference and assume the bent rod actuator propels in the $e_1 - e_2$ plane and rotates about the $e_1 \times e_2$ axis. We also define local normal e_{r} and tangential e_{t} unit vectors to the surface of the bent rod actuator. In terms of $e_1 - e_2$, $e_{\text{t}} - e_{\text{r}}$ are defined as

$$e_{\text{t}} = \begin{cases} -\cos(\theta)e_1 - \sin(\theta)e_2 & s < 0 \\ e_1 & s \geq 0 \end{cases}, \quad (1\text{a})$$

$$e_{\text{r}} = \begin{cases} \sin(\theta)e_1 - \cos(\theta)e_2 & s < 0 \\ e_2 & s \geq 0 \end{cases}. \quad (1\text{b})$$

We extend the results of Ganguly and Gupta [42] to determine the dimensionless velocity $\boldsymbol{U}$ (scaled by $U_{\text{ref}} = \frac{k_{\text{b}}Ta J_{\text{ref}}\lambda^2}{\mu D \ell}$) and angular velocity $\boldsymbol{\Omega}$ (scaled by $\frac{U_{\text{ref}}}{\ell}$) in response to both self-diffusiophoresis [42, 90, 92–94] and hinge articulations. In our non-dimensionalization, k_{b} is the Boltzmann constant, T is the ambient fluid temperature, J_{ref} is the reference solute surface flux, λ is the phoretic interaction length scale, D is the solute diffusivity, and μ is the fluid viscosity. The self-diffusiophoretic motion is caused by a surface flux $j(s)$ (scaled by J_{ref}) on the surface of the bent rod actuator. The surface activity creates a concentration field $c(s, r)$ (scaled by $\frac{a J_{\text{ref}}}{D}$) in the surrounding solution. Gradients along the length of the rod in the solute concentration field cause the bent rod actuator to move by inducing a diffusiophoretic slip velocity $u_{\text{phoretic}}e_{\text{t}}$ on the surface of the rod. In addition to the self-diffusiophoretic motion, we also consider bent rod actuator motion due to the hinge altering the angle θ between both arms, denoted as hinge articulations or flapping. As the hinge articulates, the arms move with

an angular velocity, ω_{n} for the negative arm and ω_{p} for the positive arm, which induces a normal fluid velocity $u_{\text{flapping}}e_{\text{r}}$ on the surface of the bent rod actuator.

2.2 Slender-body theory

The velocity $\boldsymbol{U}$ and angular velocity $\boldsymbol{\Omega}$ of the bent rod actuator, in the particle frame of reference, can be determined via the mobility relation,

$$\begin{bmatrix} \boldsymbol{U} \\ \boldsymbol{\Omega} \end{bmatrix} = \underline{\underline{\boldsymbol{R}}}^{-1} \cdot \begin{bmatrix} \boldsymbol{F}_{\text{eff}} \\ \boldsymbol{T}_{\text{eff}} \end{bmatrix}, \quad (2)$$

where $\underline{\underline{\boldsymbol{R}}}^{-1}$ is the 6 × 6 mobility matrix and $\boldsymbol{F}_{\text{eff}}$ and $\boldsymbol{T}_{\text{eff}}$ are the effective force and torque acting on the center of mass of the bent rod actuator due to self-diffusiophoresis and hinge articulations. Assuming that the bent rod actuator is only able to translate in the $e_1 - e_2$ plane and rotate about the $e_1 \times e_2$ axis, we write Eq. 2 as

$$\begin{bmatrix} U_1 \\ U_2 \\ \Omega_3 \end{bmatrix} = \underline{\underline{\boldsymbol{M}}} \cdot \begin{bmatrix} F_1 \\ F_2 \\ T_3 \end{bmatrix}. \quad (3)$$

The bent rod actuator can move with a velocity U_1 in the e_1 direction, U_2 in the e_2 direction, and angular velocity Ω_3 about the $e_1 \times e_2$ axis. The motion is caused by an effective force F_1 in the e_1 direction, F_2 in the e_2 direction, or an effective torque T_3 about the $e_1 \times e_2$ axis. The mobility coefficients $\underline{\underline{\boldsymbol{M}}}$ are determined by numerically inverting the resistance coefficients (multiplied by a minus sign) determined by Roggeveen and Stone (Eq. 3.5 in their work) [91] using the Python module *Scipy* with the *linalg.inv* function. Using the results from Ganguly and Gupta [42], calculated with the reciprocal theorem, we express the effective force and torque in terms of a velocity on the surface of the bent rod actuator,
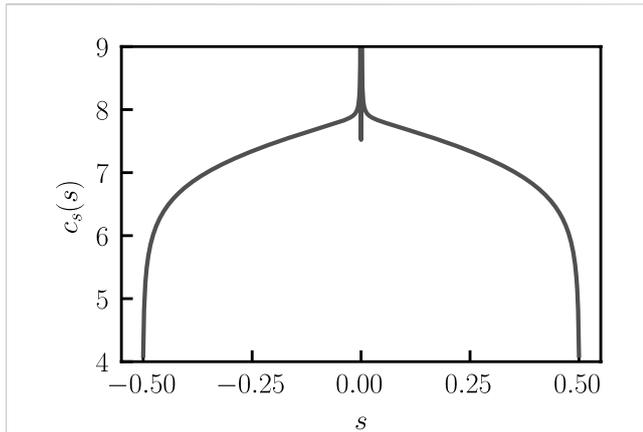
FIGURE 2
Concentration profile across the bent rod actuator.
Concentration profile across the bent rod actuator for $q = 0$, $\theta = \pi/4$, and $j(s) = 1$, as determined by solving Eq. 8 with Eq. 1 using the *Scipy.integrate.quad* function.

$$\begin{bmatrix} U_1 \\ U_2 \\ \Omega_3 \end{bmatrix} = \underline{\underline{M}} \cdot \begin{bmatrix} \int u_{\text{surf}} \cdot \left(I - \frac{1}{2} e_t e_t \right) \cdot e_1 ds \\ \int u_{\text{surf}} \cdot \left(I - \frac{1}{2} e_t e_t \right) \cdot e_2 ds \\ \int u_{\text{surf}} \cdot \left(I - \frac{1}{2} e_t e_t \right) \cdot e_3 \times (x_h(s) - r_{\text{com}}) ds \end{bmatrix}, \quad (4)$$

where $x_h(s) = s e_t$ is the position of a point along the center-line of the bent rod and $r_{\text{com}} = \int_{q-1/2}^{q+1/2} s e_t ds = (\frac{1}{2} \cos \theta (q - \frac{1}{2})^2 + \frac{1}{2}(q + \frac{1}{2})^2) e_1 + \frac{1}{2} \sin \theta (q - \frac{1}{2})^2 e_2$ is the center of mass of the bent rod. We consider the surface velocity to be composed of a tangential component due to self-diffusiophoresis and a normal component due to hinge articulations,

$$u_{\text{surf}} = u_{\text{phoretic}} e_t + u_{\text{flapping}} e_r. \quad (5)$$

Following similar treatments in the literature [42, 90, 94], we model the velocity induced by solute concentration gradients with

$$u_{\text{phoretic}} = \Gamma(s) \frac{dc_s(s)}{ds}, \quad (6)$$

where $\Gamma(s)$ is a lumped phoretic mobility parameter, $c_s(s) = c(s, \epsilon)$, and $\frac{dc_s(s)}{ds}$ is the surface concentration gradient. For simplicity, we consider $\Gamma(s) = \pm 1$, a value representative for diffusiophoretic systems [72]. Considering the slip velocity to be composed of only a phoretic component, Eq. 4 can be integrated and written as

$$\begin{bmatrix} U_{1,\text{phoretic}} \\ U_{2,\text{phoretic}} \\ \Omega_{3,\text{phoretic}} \end{bmatrix} = \text{sign}(\Gamma) \, \underline{\underline{M}}$$

$$\cdot \begin{bmatrix} \frac{1}{2} \Delta c_0^{q+\frac{1}{2}} - \frac{\cos \theta}{2} \Delta c_{q-\frac{1}{2}}^0 \\ -\frac{\sin \theta}{2} \Delta c_{q-\frac{1}{2}}^0 \\ \frac{\sin \theta}{4} \left(\left(q - \frac{1}{2} \right)^2 \Delta c_0^{q+\frac{1}{2}} + \left(q + \frac{1}{2} \right)^2 \Delta c_{q-\frac{1}{2}}^0 \right) \end{bmatrix}, \quad (7)$$

where $\Delta c_0^{q+\frac{1}{2}} = c_s(q + \frac{1}{2}) - c_s(0)$ and $\Delta c_{q-\frac{1}{2}}^0 = c_s(0) - c_s(q - \frac{1}{2})$ [42]. The phoretic motion is driven by the concentration difference between the hinge and ends of the bent rod actuator arms. As we are considering bent rod actuators with a small aspect ratio $\epsilon \ll 1$, we use boundary layer theory [42, 95] to determine the concentration profile along the bent rod actuator by numerically solving

$$c_s(s) = \frac{1}{2} \int_{q-\frac{1}{2}}^{q+\frac{1}{2}} \frac{j(s')}{\left| x_h(s') + \epsilon e_r(s) - x_h(s) \right|} \, ds'. \quad (8)$$

We note that all results shown are calculated with $\epsilon = 10^{-3}$. The framework is agnostic to the flux profile used; however, we use a uniform flux profile $j(s) = 1$ for simplicity. The concentration profile is derived for the case of small Péclet number, i.e., $\text{Pe} = \frac{U_{\text{ref}} \ell}{D} \sim \mathcal{O}(10^{-3})$ [42]. The numerical solution of Eq. 8 is difficult to resolve near $s = 0$ due to a singularity in the concentration profile at $s = 0$ (Figure 2) caused by the sharp turn in the bent rod actuator at the hinge, see Figure 3A.

To achieve a numerical solution, we approximate the entire bent rod actuator center-line with the smooth continuous function $x_h(s) = \mathcal{X}(s) e_1 + \mathcal{Y}(s) e_2$, where

$$\mathcal{X}(s) = -s \cos \theta + \frac{1 + \cos \theta}{k} \ln \left(\frac{1 + e^{ks}}{2} \right), \quad (9a)$$

$$\mathcal{Y}(s) = -s \sin \theta + \frac{\sin \theta}{k} \ln \left(\frac{1 + e^{ks}}{2} \right), \quad (9b)$$

and k is a smoothness parameter that controls the curvature of the approximate bent rod actuator near $s = 0$. A larger k corresponds to a corner with higher curvature and a better approximated bent rod actuator, while a smaller k corresponds to a corner with lower curvature and a worse approximation of the bent rod actuator, see Figure 3A. To approximate the concentration profile near the hinge, we use Eq. 9 to calculate Eq. 8 with $k = 100$ and $k = 1,000$ (Figure 3B). We determine the values of s for $s < 0$ and $s > 0$, where the value of concentration profiles differs by 5% and fit the concentration profile for $k = 1,000$ with a fourth-order spline using the *Scipy. interpolate.UnivariateSpline* function (Figure 3B) between the two s values.

In addition to the phoretic contribution, we consider the motion of the bent rod actuator due to hinge articulations, $\theta \rightarrow \theta(t)$. The articulation of the hinge induces an angular velocity ω_n for the negative arm and ω_p for the positive arm. The angular velocity of each arm is related to the hinge articulation via

$$\frac{d\theta}{dt} = -(\omega_n + \omega_p) = -\omega. \quad (10)$$

We write the flapping velocity as

$$u_{\text{flapping}} = \begin{cases} -\omega_n s & s < 0, \\ \omega_p s & s \geq 0. \end{cases} \quad (11)$$

Inserting Eq. 11 into Eq. 4 and integrating yields

FIGURE 3
Determination of the concentration profile with approximated bent rod actuator geometry. **(A)** Comparison between bent rod actuator geometry, as approximated by Eq. 9 for $k = 100$ and $k = 1,000$ and Eq. 1. **(B)** Concentration profiles ($q = 0$, $\theta_0 = \pi/4$, and $j(s) = 1$) for the approximated bent rod actuator with $k = 100$ and $k = 1,000$ as well as the spline interpolated concentration profile near $s = 0$.
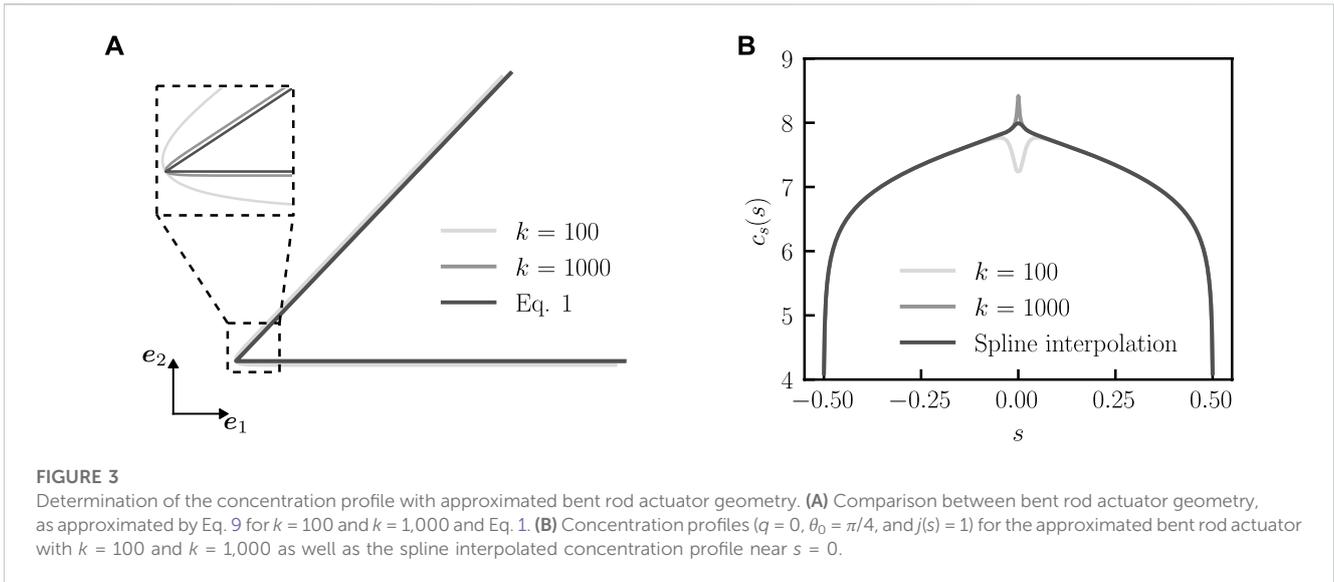
$$\begin{bmatrix} U_{1,\text{flapping}} \\ U_{2,\text{flapping}} \\ \Omega_{3,\text{flapping}} \end{bmatrix} = \underline{\underline{M}}.$$

$$\cdot \begin{bmatrix} \frac{1}{2}\omega_n \sin\theta\left(q - \frac{1}{2}\right)^2 \\ -\frac{1}{2}\omega_n \cos\theta\left(q - \frac{1}{2}\right)^2 + \frac{1}{2}\omega_p\left(q + \frac{1}{2}\right)^2 \\ \frac{1}{192}\left\{(2q-1)^3(6q+5)\omega_n - (2q+1)^3(6q-5)\omega_p + 3\cos\theta(\omega_n - \omega_p)(1 - 4q^2)^2\right\} \end{bmatrix}. \tag{12}$$

The total velocity and angular velocity of the bent rod actuator is determined by a linear combination of Eqs. 7, 12:

$$\begin{bmatrix} U_1 \\ U_2 \\ \Omega_3 \end{bmatrix} = \begin{bmatrix} U_{1,\text{phoretic}} \\ U_{2,\text{phoretic}} \\ \Omega_{3,\text{phoretic}} \end{bmatrix} + \begin{bmatrix} U_{1,\text{flapping}} \\ U_{2,\text{flapping}} \\ \Omega_{3,\text{flapping}} \end{bmatrix}. \tag{13}$$

We note that in order to use the combined phoretic and flapping contributions to the bent rod actuator motion, the Péclet number due to flapping must also be small. To justify, we briefly restore dimensions and note that $\text{Pe}_{\text{flapping}} = \frac{\omega\ell\frac{U_{\text{Ref}}}{\ell}\ell}{D} = \frac{\omega U_{\text{ref}}\ell}{D}$. In our simulations, $\omega \sim \frac{\theta_a}{T}$, where $\theta_a \in [0, 2\pi]$ is the amplitude of an articulation and T is a typical period for a given articulation. By constraining our results to $T \sim \mathcal{O}(1)$, we ensure that $\text{Pe}_{\text{flapping}} \sim \mathcal{O}(10^{-3}) \ll 1$. In addition to the dependence of Eq. 13 on geometric parameters, the phoretic velocities and flapping velocities also linearly depend on $j(s)$ and ω, respectively. Therefore, the relative contribution of each velocity can be tuned by either changing $j(s)$ or by changing ω through θ_a or T.

2.3 Numerical procedure

To calculate the bent rod actuator trajectory, we convert from the particle ($e_1 - e_2$) to the laboratory ($e_x - e_y$) frame of reference by employing the rotation matrix

$$\frac{d}{dt}\begin{bmatrix} x(t) \\ y(t) \\ \phi(t) \end{bmatrix} = \begin{bmatrix} \cos\phi(t) & -\sin\phi(t) & 0 \\ \sin\phi(t) & \cos\phi(t) & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} U_1 \\ U_2 \\ \Omega_3 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \omega_p \end{bmatrix}, \tag{14}$$

where $\phi(t)$ is the angle between e_1 and e_x and t is the dimensionless timescale (scaled by $\frac{\ell}{U_{\text{Ref}}}$). Additionally, as e_1 in the particle frame of reference aligns with the tangential direction of the positive arm, we need to account for changes in $\phi(t)$ due to the angular velocity ω_p of the positive arm about the hinge at $s = 0$. To do so, we add ω_p to $\frac{d\phi(t)}{dt}$. Eq. 14 is evaluated use an eighth-order Runge–Kutta integration scheme (DOP853) as implemented in the Python *Scipy* package via the *Solve-IVP* function. We use initial conditions $x(0) = y(0) = \phi(0) = 0$. We note that $x(t)$ and $y(t)$ correspond to the center of mass of the bent rod actuator in the laboratory reference frame. To determine the coordinates of the hinge and end points of the bent rod actuator at each time point in the laboratory reference frame, we first determine the position of the hinge point $\boldsymbol{r}_{\text{hinge}}(t)$ and two end points, $\boldsymbol{r}_{s=q-\frac{1}{2}}(t)$ and $\boldsymbol{r}_{s=q+\frac{1}{2}}(t)$, relative to the center of mass of the bent rod actuator in the particle frame of reference.

$$\boldsymbol{r}_{\text{hinge}}(t) = -\boldsymbol{r}_{\text{com}}, \tag{15a}$$

$$\boldsymbol{r}_{s=q-\frac{1}{2}}(t) = -\left(q - \frac{1}{2}\right)\cos\theta(t)e_1 - \left(q - \frac{1}{2}\right)\sin\theta(t)e_2 - \boldsymbol{r}_{\text{com}}, \tag{15b}$$

$$\boldsymbol{r}_{s=q+\frac{1}{2}}(t) = \left(q + \frac{1}{2}\right)e_1 - \boldsymbol{r}_{\text{com}}. \tag{15c}$$

We apply the rotation matrix and translate the hinge and end points to determine the coordinates of the hinge and end points of the bent rod actuator in the laboratory frame of reference at each instant of time.

$$\boldsymbol{r}'_{\text{hinge}}(t) = \begin{bmatrix} \cos\phi(t) & -\sin\phi(t) \\ \sin\phi(t) & \cos\phi(t) \end{bmatrix} \cdot \boldsymbol{r}_{\text{hinge}}(t) + \begin{bmatrix} x(t) \\ y(t) \end{bmatrix}, \tag{16a}$$

$$\boldsymbol{r}'_{s=q-\frac{1}{2}}(t) = \begin{bmatrix} \cos\phi(t) & -\sin\phi(t) \\ \sin\phi(t) & \cos\phi(t) \end{bmatrix} \cdot \boldsymbol{r}_{s=q-\frac{1}{2}}(t) + \begin{bmatrix} x(t) \\ y(t) \end{bmatrix}, \tag{16b}$$

$$\boldsymbol{r}'_{s=q+\frac{1}{2}}(t) = \begin{bmatrix} \cos\phi(t) & -\sin\phi(t) \\ \sin\phi(t) & \cos\phi(t) \end{bmatrix} \cdot \boldsymbol{r}_{s=q+\frac{1}{2}}(t) + \begin{bmatrix} x(t) \\ y(t) \end{bmatrix}. \tag{16c}$$

We then sequentially solve 14 and 16 to determine the trajectories of the bent rod actuator. Trajectories shown in Figure 4, Figure 5,

FIGURE 4
Motion of a bent rod actuator due to reciprocal hinge articulations. **(A)** $\theta(t)$ used for a bent rod actuator with reciprocal hinge articulations. $\theta(t)$ is characterized by an initial angle θ_0, flapping amplitude θ_a, and period T. **(B)** Schematic illustration of flapping distribution between arms, as characterized by n. $n = 1$ describes a bent rod actuator where all changes in $\theta(t)$ are ascribed to the negative arm. $n = 0.5$ describes a bent rod actuator where the positive and negative arms are equally responsible for changes in $\theta(t)$. $n = 0$ describes a bent rod actuator where the positive arm is responsible for all changes in $\theta(t)$. Trajectory plots of r_{hinge} over one half period for **(C)** $\theta_0 \in [\pi/4, \pi/2, \pi]$, $\theta_a = \pi/2$, $T = 1$, $q = 0$, and $n = 0.5$. **(D)** $\theta_0 = \pi$, $\theta_a = \pi/2$, $T = 1$, $q \in [0, 0.15, 0.3]$, and $n = 0.5$. **(E)** $\theta_0 = \pi$, $\theta_a = \pi/2$, $T = 1$, $q = 0$, and $n \in [0, 1/2, 1]$.

Figure 6, and Figure 7 are ascertained from Eq. 16a, with the coordinates of the hinge and end points of the bent rod actuator drawn according to Eqs. 16b, 16c.

3 Results and discussion

3.1 Reciprocal motion

We first show that the bent rod actuator experiences zero net displacement while undergoing reciprocal hinge articulations without the contribution of diffusiophoresis

(see Figure 4A). At $t = 0$, the hinge initiates articulation, changing $\theta(t)$ from an initial angle of θ_0 to a final angle of $\theta_0 + \theta_a$ over a time $\frac{T}{4}$. The hinge then changes θ from $\theta_0 + \theta_a$ back to θ_0 over a time $\frac{T}{4}$. Therefore, by $\frac{T}{2}$, the bent rod actuator has reciprocally articulated the hinge. To determine the angular velocity of the positive and negative arms (ω_p and ω_n), we use Eq. 10. First, we note that $\theta(t)$ is piece-wise defined as

$$\theta(t) = \begin{cases} \theta_0 + \theta_a \sin\left(2\pi\dfrac{t}{T}\right)\mathcal{H}(t) & t \leq \dfrac{T}{2} \\ 0 & t > \dfrac{T}{2} \end{cases}, \qquad (17)$$
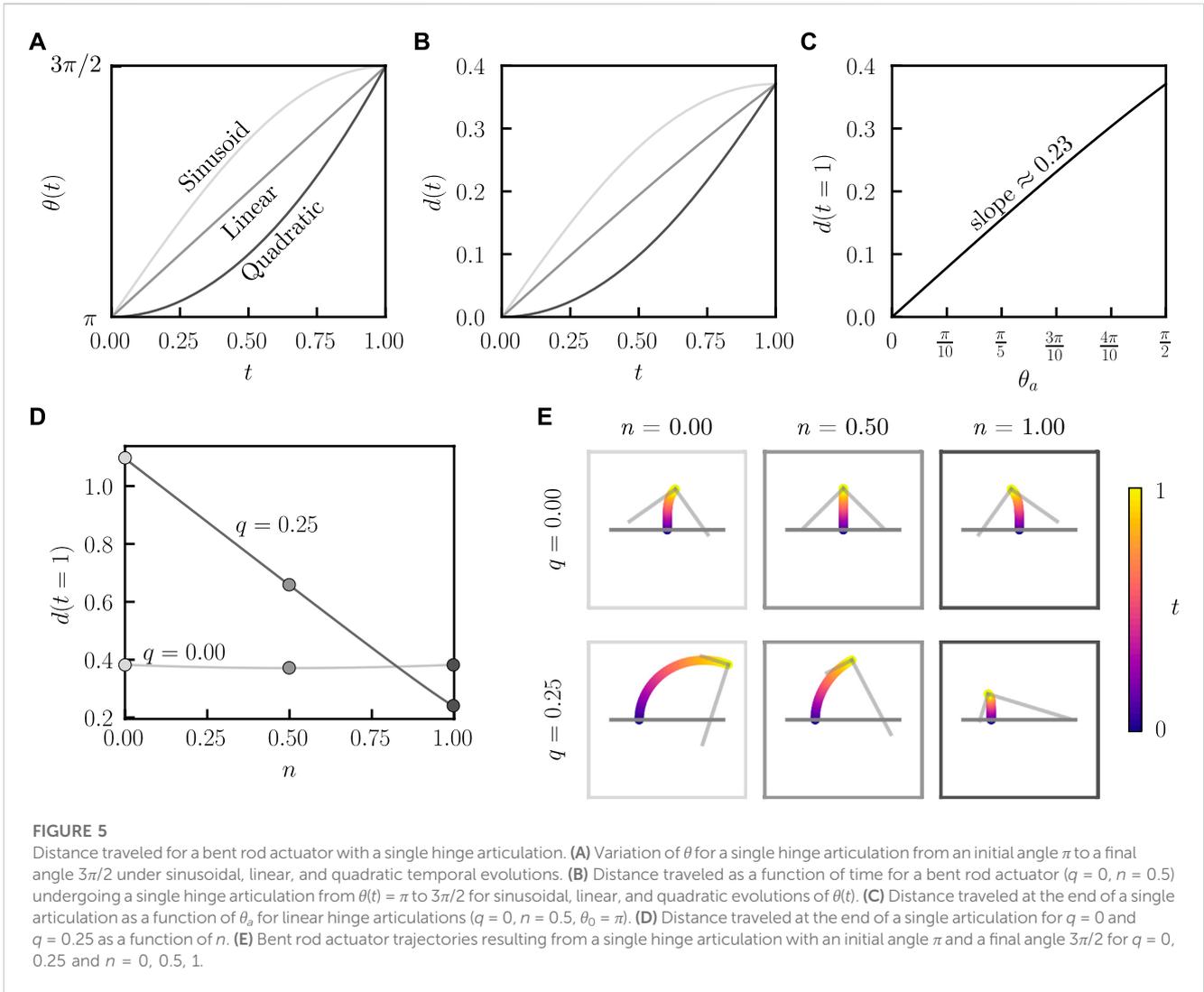
FIGURE 5
Distance traveled for a bent rod actuator with a single hinge articulation. **(A)** Variation of θ for a single hinge articulation from an initial angle π to a final angle $3\pi/2$ under sinusoidal, linear, and quadratic temporal evolutions. **(B)** Distance traveled as a function of time for a bent rod actuator ($q = 0$, $n = 0.5$) undergoing a single hinge articulation from $\theta(t) = \pi$ to $3\pi/2$ for sinusoidal, linear, and quadratic evolutions of $\theta(t)$. **(C)** Distance traveled at the end of a single articulation as a function of θ_a for linear hinge articulations ($q = 0$, $n = 0.5$, $\theta_0 = \pi$). **(D)** Distance traveled at the end of a single articulation for $q = 0$ and $q = 0.25$ as a function of n. **(E)** Bent rod actuator trajectories resulting from a single hinge articulation with an initial angle π and a final angle $3\pi/2$ for $q = 0$, 0.25 and $n = 0$, 0.5, 1.

where $\mathcal{H}(t)$ is the Heaviside function. By using Eq. 17 and Eq. 10, we write the angular velocities as

$$
\omega_\mathrm{p} = \begin{cases} -(1-n)\dfrac{2\pi\theta_a}{T}\cos\left(2\pi\dfrac{t}{T}\right)\mathcal{H}(t) & t \leq \dfrac{T}{2} \\[3mm] 0 & t > \dfrac{T}{2} \end{cases}, \qquad (18a)
$$

$$
\omega_\mathrm{n} = \begin{cases} -n\dfrac{2\pi\theta_a}{T}\cos\left(2\pi\dfrac{t}{T}\right)\mathcal{H}(t) & t \leq \dfrac{T}{2} \\[3mm] 0 & t > \dfrac{T}{2} \end{cases}, \qquad (18b)
$$

where $n \in [0, 1]$ describes the distribution of angular velocities between the positive and negative arms, Figure 4B. When $n = 1$, only the articulation of the negative arm contributes to the changes in θ. When $n = 0$, only the positive arm articulates. When $n = 0.5$, both arms equally articulate. Thus, $n = 0.5$ distinguishes symmetric flapping, where both arms have the same angular velocity, and $n \neq 0.5$ describes asymmetric flapping, where one arm has a larger angular velocity than the other. We solve Eq. 14, including no phoretic contributions, using Eq. 18. Figure 4C shows the trajectories of the hinge as well as the orientation of the bent rod

actuator with an asymmetry parameter $q = 0$, flapping distribution $n = 0.5$, flapping amplitude $\theta_a = \frac{\pi}{2}$, flapping period $T = 1$, and initial angles $\theta_0 \in [\frac{\pi}{4}, \frac{\pi}{2}, \frac{3\pi}{4}, \pi]$. For a symmetric bent rod with symmetric flapping ($q = 0$, $n = 0.5$), the trajectory makes an angle of $\frac{\theta_0}{2}$ with $\boldsymbol{e}_\mathrm{x}$. This is a consequence of Ω_3 identically going to 0 for a bent rod actuator with symmetric flapping and geometry. In contrast, rotation and curved trajectories can be induced by either introducing geometric asymmetry via q (Figure 4D) or flapping asymmetry via n (Figure 4E). As geometric asymmetry is introduced, the bent rod actuator moves in the positive $\boldsymbol{e}_\mathrm{x}$ direction, toward the longer arm, and rotates counter-clockwise up to $t = \frac{T}{4}$ before retracing the same trajectory in reverse to attain the original position and orientation of the bent rod actuator. See Supplementary Video S1 for a movie of a bent rod actuator moving due to sinusoidal hinge articulations, described by $\theta(t) = \theta_0 + \theta_a \sin\left(2\pi\frac{t}{T}\right)$, with $q = 0.3$, $n = 0.5$, $\theta_0 = \frac{\pi}{2}$, $\theta_a = \frac{\pi}{4}$, and $T = 1$. A similar behavior is observed when the flapping asymmetry is introduced (Figure 4E). Both the direction of rotation, clockwise or counter-clockwise, and the direction of translation depend on which arm has a larger angular velocity. When $n > 0.5$, the negative arm has a larger angular velocity and the entire bent rod actuator rotates
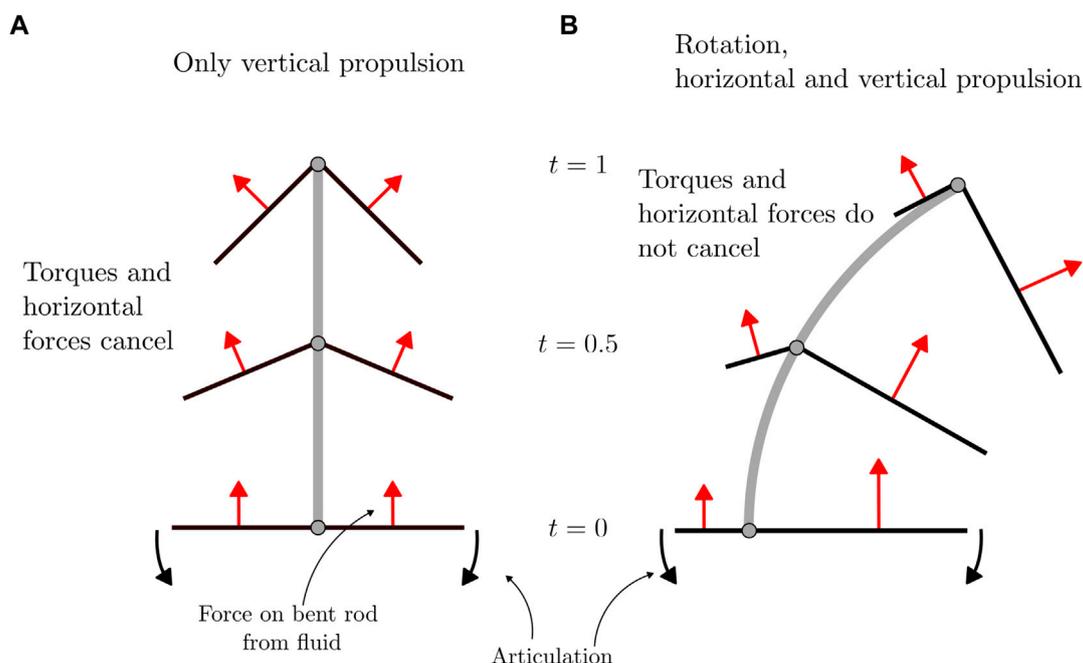
FIGURE 6
Free-body diagram of forces applied to a bent rod actuator due to hinge articulations. **(A)** Forces acting on a bent rod with geometric and flapping symmetry. **(B)** Forces acting on a bent rod with geometric asymmetry and flapping symmetry. *The trajectories and bent rod are not to scale.*

clockwise and translates in the negative e_x direction during the first half of the articulation. Inversely, when $n < 0.5$, the positive arm has a larger angular velocity and the entire bent rod actuator rotates counter-clockwise and translates in the positive e_x direction during the first half of the articulation. An intuitive understanding of this motion based on free-body diagrams will be explored in Sec. 3.2.

We also note that the bent rod actuator does return to its original position after undergoing a reciprocal hinge articulation. While known mathematically, to our knowledge, this is the first time where the trajectories of the bent rod actuator have been calculated numerically. It can be shown analytically via our framework that the bent rod actuator must return to its original location, as given in Eq. 14 and 12. We note that Eq. 12 can be expressed as

$$\begin{bmatrix} U_{1,\text{flapping}} \\ U_{2,\text{flapping}} \\ \Omega_{3,\text{flapping}} \end{bmatrix} = \begin{bmatrix} \mathcal{A}(q,n,\theta) \\ \mathcal{B}(q,n,\theta) \\ \mathcal{C}(q,n,\theta) \end{bmatrix} \frac{d\theta}{dt}, \quad (19)$$

where $\mathcal{A}, \mathcal{B}$ & $\mathcal{C}$ are functions of q, n, and θ only. Upon inserting into Eq. (14), we write

$$\frac{d}{dt}\begin{bmatrix} x(t) \\ y(t) \\ \phi(t) \end{bmatrix} = \begin{bmatrix} \cos\phi(t)\mathcal{A}(q,n,\theta) - \sin\phi(t)\mathcal{B}(q,n,\theta) \\ \sin\phi(t)\mathcal{A}(q,n,\theta) + \cos\phi(t)\mathcal{B}(q,n,\theta) \\ \mathcal{C}(q,n,\theta) + n - 1 \end{bmatrix} \frac{d\theta}{dt}. \quad (20)$$

By integrating Eq. 20, we see that ϕ is a unique function of θ only (up to an arbitrary choice of $\phi(0)$, q, and n). Therefore, any trajectory characterized by a reciprocal choice of θ, i.e., $\theta(t=0) = \theta(t_{\text{final}})$, implies that $x(t=0) = x(t=t_{\text{final}})$, $y(t=0) = y(t=t_{\text{final}})$, and $\phi(t=0) = \phi(t=t_{\text{final}})$.

In summary, our framework using slender-body theory is able to recapitulate Purcell's scallop theorem both numerically and

analytically. In addition, we are able to numerically determine the trajectories taken by the bent rod actuator due to reciprocal hinge articulations. Either geometric or flapping asymmetry can be used to introduce rotation and motion along a curved trajectory.

3.2 Non-reciprocal articulation

To further understand the relationship between geometric and flapping asymmetry, we calculate the trajectories and cumulative distance traveled $d(t)$ by a bent rod undergoing non-reciprocal hinge articulations, Figure 5A. In these simulations, the bent rod actuator starts with an initial angle of $\theta = \pi$ and the hinge articulates to a final angle of $\theta = \frac{3\pi}{2}$, representing a total increase in the angle of $\frac{\pi}{2}$ over a time period $t = 1$. We vary the time rate of change of $\theta(t)$ using a sinusoidal, linear, and quadratic function, Figure 5A. Figure 5B shows that the total distance traveled remains equal among the three temporal variations by $t = 1$. Additionally, Figure 5C shows that the total distance traveled is linearly dependent on the amplitude of the hinge articulation. We also determine the total distance traveled by the bent rod actuator when both geometric and flapping asymmetries are introduced. Figure 5D shows the total distance traveled by a bent rod actuator undergoing displacements from an initial angle π to a final angle $\frac{3\pi}{2}$ as a function of n for $q = 0$ and $q = 0.25$. When $q = 0$, the variation in total distance traveled is weakly dependent on n. Interestingly, we find a minimum at $n = 0.5$. To better understand why a minimum exists at $n = 0.5$, we plot the trajectories that the bent rod actuators undergo, Figure 5D. When $n = 0$ and $n = 1$, we see that the bent rod actuator turns during the trajectory, while the bent rod actuator with $n = 0.5$ moves in a straight line. In this way, the projected surface area along the

direction of the trajectory is smaller for $n = 0$ and $n = 1$, allowing these bent rod actuators to travel slightly further. The relationship between $d(t = 1)$ and n is more distinct for the $q = 0.25$ case. In these cases, $d(t = 1)$ decreases with n. This shows that for a bent rod actuator with geometric asymmetry, articulating the longer arm leads to a larger distance traveled. In addition to traveling further, the bent rod actuator also traces a circular trajectory.

An intuition for the motion of the bent rod actuator under non-reciprocal articulations can be understood by considering how forces are distributed across the bent rod arms as a function of geometric and flapping asymmetry, Figure 6. In the case of a bent rod actuator with both geometric ($q = 0$) as well as flapping ($n = 0.5$) symmetry, as the hinge articulates, the force applied to the bent rod actuator arms from the fluid is distributed across both arms, see Figure 6A. This leads to a net effective force in the e_y direction. While the force does have a component in the e_x direction, the contributions from the positive and negative arms cancel, leading to no net force in the e_x direction. The same is true for the effective torque about the $e_1 \times e_2$ axis applied to the center of mass of the bent rod actuator. As the arms are of the same length and flapping is symmetric, the torque produced by both arms is equal and opposite, leading to a net zero effective torque. When geometric (or similarly flapping) asymmetry is introduced ($q > 0.5$, Figure 6B), the effective force applied to the bent rod actuator due to hinge articulations is biased toward the longer arm. In this case, the effective force in the e_y direction remains non-zero; however, the contributions to effective force in the e_x direction as well as the effective torque about the $e_1 \times e_2$ axis no longer cancels between the two arms.

In summary, an intuitive picture of bent rod actuator motion can be built by considering how forces acting on the bent rod from the fluid are distributed at each instant of time. In the case of flapping, this is done by considering normal force components distributed across the arms and decomposing the forces into their constitutive laboratory frame of reference components.

3.3 Phoretic motion with hinge articulations

To investigate interactions between the chemical mode of swimming from self-diffusiophoresis and the mechanical mode of swimming due to hinge articulations, we begin by comparing trajectories and the change in total distance traveled due to either a positive or negative $\Gamma(s)$ when the arms open and close, Figure 7A. We notice that the bent rod actuator always moves further when closing its arms, independent of whether the phoretic mobility is positive or negative. This is due to two effects. First, as the angle between the arms decreases, the concentration difference between the hinge and end points increases [42]. As the effective phoretic forces, see Eq. 7, are proportional to the concentration differences, this leads to a larger effective force and, thus, a larger velocity. The inverse is true for the scenario when the arms are opening. As the arms open, the concentration difference between the hinge and end points decreases, leading to a smaller effective phoretic force and a shorter distance traveled. Second, as the arms close, the projected surface area along the direction of motion decreases, decreasing the drag and leading to a larger distance traveled over a given period of time.

While changes to phoretic motion are the primary reason for changes in the total distance traveled, a subtle effect involving the competition between mechanical and chemical swimming can also be noticed. When the arms open, the bent rod with a positive phoretic mobility experiences a smaller decrease in the total distance traveled when compared to the bent rod with a negative phoretic mobility. This is because the effective force

FIGURE 7
Trajectories of an active bent rod actuator undergoing hinge articulations. **(A)** Comparison between bent rod actuator motion due to a uniform surface activity ($j(s) = 1$) with a phoretic mobility $\Gamma(s) = \pm 1$, $\theta_0 = \pi/2$, $q = 0$, $n = 0.5$ and arms either opening or closing by $\theta_a = \pm\pi/4$ over $t = 1$ of linear temporal variation. **(B)** Trajectories for an active bent rod actuator undergoing sinusoidal hinge articulations, $\Gamma(s) = 1$, $T = 1$, $\theta_a = \frac{\pi}{4}$, and $n = 0.5$ for $q \in [0.15, 0.30]$ and $\theta_0 \in [\pi/2, \pi]$.

FIGURE 8
Trajectories of an active bent rod actuator undergoing sinusoidal hinge articulations with $\theta_a = \frac{\pi}{4}$, $q = 0.3$, $n = 0.5$, $T = 1$, and $\theta_0 = \frac{\pi}{2}$ for **(A–D)** $j(s) \in [0.5, 1, 2, 4]$.

acting on the bent rod actuator due to a positive phoretic mobility and the arms opening are in the same direction. Similarly, the bent rod actuator with a negative phoretic mobility and arms that close experiences a larger increase in the total distance traveled.

We also investigate how θ_0 and q affect the motion of a self-diffusiophoretic bent rod actuator undergoing sinusoidal hinge articulations described by $\theta(t) = \theta_0 + \theta_a \sin\left(2\pi \frac{t}{T}\right)$, Figure 7B. First, we notice that when $\theta_0 = \pi/2$, the bent rod actuator travels in a circular trajectory (see Supplementary Video S3), while the bent rod actuator with $\theta_0 = \pi$ travels in trajectories that map circular arcs. Additionally, we notice that the bent rod actuator no longer experiences zero net displacement upon reciprocal articulations. This is due to the fact that the effective phoretic forces, Eq. 7, do not depend on $\frac{d\theta}{dt}$ and instead are functions of θ (as well as q and $j(s)$). Therefore, upon integrating, the time dependence of θ matters. This leads to trajectories that do not end and start at the same location.

We briefly discuss how the relative contributions of hinge articulations and diffusiophoresis impact the trajectory of the bent rod actuator. By increasing $j(s)$, the contribution of diffusiophoresis relative to hinge articulations increases. Conversely, by increasing the articulation amplitude θ_a, the contribution of diffusiophoresis relative to hinge articulations decreases. Figure 8 shows the trajectories of a bent rod actuator moving due to both hinge articulations and diffusiophoresis, with $j(s)$ increasing while keeping θ_a constant. As $j(s)$ increases, the bent rod actuator traces a larger distance (though not necessarily displacement) during a given time period. This is attributed to the increase in the effective force and torque acting on the bent rod caused by the increasing $j(s)$. Additionally, increasing $j(s)$ causes the trajectories to become more circular and approach the trajectory of a self-diffusiophoretic bent rod without hinge articulations (refer to Supplementary Video S2) [42].

4 Applications to biomedical microrobots

An improved understanding of the motion of a bent rod actuator with both mechanical and chemical swimming modes has direct applicability to the growing field of biomedical

microrobots. Biomedical microrobots have found use in the delivery of small-molecule drugs, living cells, and contrast agents through complex biological media for precision medicine [8]. Primarily, the ability to enact real-time geometric changes and predict the resultant motion can have implications for the design of biomedical microrobots. First, real-time changes to microrobot geometry may allow the robot to switch between characteristic trajectories. In one sense, the ability to switch between straight-line trajectories and circular trajectories could enable enhanced motion through porous media [61]. In a similar manner, the direction of the microrobot for a given propulsion mechanism can be changed through flapping asymmetry and geometry alterations, for instance, by flapping a single arm to induce rotation that alters the direction of propulsion (Figure 5). This may be particularly useful for microrobots traversing through complex environments with multiple barriers, wherein real-time changes to trajectories may allow the swimmer to move around barriers and potentially escape confinement [96]. We note that the proposed hydrodynamic model of the bent rod actuator would need to be significantly modified to account for the presence of boundaries and is currently limited to two-dimensional motion. This warrants further studies that expand motion to three dimensions and include the effects of boundaries.

Experimental realizations of microrobots with similar geometries to the bent rod actuators exist [97–100]. These systems use polymeric cubes, typically fabricated at the micron scale with photolithography, coated with a ferromagnetic patch, that assemble into linear chains with hinges in a constant uniform magnetic field [97–99]. Systems could also be fabricated at the nanoscale using electron-beam lithography [101]. Upon turning the external magnetic field on and off, the assemblies open and close, allowing them to propel in non-Newtonian fluids, such as xanthan gum solutions for shear thinning fluids or fumed silica suspensions for shear thickening fluids, by using time asymmetric hinge articulations [97, 100]. Endowing such microrobots with a chemical mode of propulsion could be enabled by conjugating enzymes, such as urease, to the particles, allowing the microrobot to generate propulsion by converting urea, a chemical commonly found in the human body, to CO_2 and NH_3 [102]. In summary, our results will encourage scientists and engineers aiming to design microrobots with multiple swimming modalities for biomedical applications.

5 Conclusion

In this article, we have developed a mobility framework to calculate the trajectories taken by a bent rod actuator under chemical and mechanical modes of swimming. In the mechanical mode, where propulsion is induced by hinge articulations, we show numerically and analytically that Purcell's Scallop theorem holds. To better understand the role of geometry on the bent rod actuator motion, we calculate the trajectories traced under non-reciprocal hinge articulations. Rotation and curved trajectories can be induced either through geometric or flapping asymmetry. This is explained through free-body diagrams that consider how forces are distributed across the bent rod actuator's arms. To further explore the bent rod actuator's motion, we also include self-diffusiophoresis to study the interplay between chemical and mechanical modes of swimming. We find that hinge articulations either aid or hinder self-diffusiophoretic motion. These effects are caused by changes to mobility, increasing or decreasing the effective phoretic force, and by the interference between the effective phoretic and flapping forces. Our work invites future studies to expand to swimmers with more than one hinge [28, 98, 99], to study swimmers in non-Newtonian fluids [48, 97, 103, 104], and to incorporate optimization schemes to control microrobot trajectories via hinge articulations. One intriguing direction is to extend the analysis to non-Newtonian fluids by scaling the applied forces in response to a viscosity that depends on the hinge articulation rate [100]. Another interesting possibility is to explore simultaneous mechanical reconfiguration with other methods of field-driven propulsion, such as electrochemical reactions [105], where the time dependence of the reactive flux [65, 66, 106] is known to impact the directed assembly of particles [107]. This may further influence the ability of swimmers to transport through confined porous media [108, 109], where it is known that both motion [110, 111] and the distribution of electrochemical species are altered [112, 113].

Data availability statement

The raw data supporting the conclusion of this article will be made available by the authors, without undue reservation.

Author contributions

RR: writing–original draft and writing–review and editing. ArG: writing–review and editing. CB: writing–review and editing. CS: writing–review and editing. AnG: writing–original draft and writing–review and editing.

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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Supplementary material

The Supplementary Material for this article can be found online at: https://www.frontiersin.org/articles/10.3389/fphy.2023.1307691/full#supplementary-material

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