



Cite this: *Soft Matter*, 2025, 21, 5138

# Active-like dynamics of worm-like chains driven by an external traveling-wave force

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We present a simplified theory for semiflexible flagella under the action of a traveling-wave perturbation that emulates the organized active forces generated by molecular motors, capable of inducing beating patterns to the filament. By modeling the flagellum as a worm-like chain (WLC), we explore the interplay (competition) between the externally applied perturbation and the intrinsic bending rigidity of the filament. Our analysis aims to understand how this interplay can lead to a selection of conformations with the spatiotemporal behavior resembling the beating dynamics of axonemes such as those in sperm tails, in *Chlamydomonas* cilia, or eukaryotic flagella in general. Through a systematic analysis of the WLC's response to traveling-wave perturbations, we try to identify the key parameters that mostly influence the mechanical waveform profiles.

Received 13th February 2025,  
Accepted 20th May 2025

DOI: 10.1039/d5sm00153f

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## 1 Introduction

Flagella are relatively slender structures found in various living organisms playing a crucial role in motility and locomotion. While bacterial flagella are usually passive filaments actuated by motors located at their base,<sup>1</sup> eukaryotic flagella such as the cilia in organisms like *Chlamydomonas* or the tails of sperm cells are active filaments powered by numerous molecular motors distributed along their length.<sup>2</sup>

Flagella serve, in general, as the primary swimming apparatus that, by wiggling and rotating, enables microorganisms to move through fluid environments. Besides propulsion,<sup>3</sup> they perform, along with cilia and bio-filaments, a variety of other biological processes,<sup>4</sup> that include, for instance, movement of fluids and particles, pathogens removal, *e.g.* mucus clearance in lung tissue,<sup>5,6</sup> embryogenesis (cell signaling, tissue development and patterning),<sup>7–9</sup> mechanotransduction<sup>10</sup> and sensory reactions to environmental stimuli.<sup>11</sup>

The complex dynamics of flagella have attracted researchers for decades, inspiring investigations into the fundamental mechanical principles that govern their biological function. In recent years, interest has also grown for the theoretical and experimental study of dynamical fluctuations in the flagellum beating pattern, which is periodic only on average.<sup>12–15</sup>

This research is driven by the natural need for knowledge but also by the goal of emulating their working efficiency in engineered micro-scale devices and macroscopic biomimetic systems.<sup>10</sup> Several theoretical approaches have been developed or applied to address the wide range of flagella shapes and their complex dynamics,<sup>16</sup> as well as to explain and interpret a plethora of experimental evidence and observations.<sup>17,18</sup> Theory includes mechanical description based on the elasticity of flexible rod-like and slender bodies,<sup>19–23</sup> computational methods<sup>24–26</sup> and simple theoretical frameworks borrowed by active polymer physics,<sup>27–30</sup> each suited to account for the specific phenomenology of various types of flagella. In particular, the bending rigidity of long linear biomolecules, flagella, and biofilaments in general, is a crucial characteristic that significantly assists their biological functions, and such molecular stiffness is naturally assumed essential for the precise functional control of the beating dynamics. From this perspective, theoretical and computational models that accurately incorporate this bending rigidity are essential for capturing, mechanical, physical, and structural aspects of such functional dynamics.

Therefore, models of semiflexible polymers, which account for the stiffness of biopolymers like actin filaments, proteins, and DNA,<sup>31–33</sup> are also useful for describing flagella. This stiffness arises from the valence angles in their backbone structure.<sup>34</sup> However, these models are more difficult to handle theoretically, as they require additional constraints like preserving a fixed chain length.

A very popular approach resorts to employing the so-called “worm-like chain” (WLC) models representing a minimal yet meaningful physical approach to implementing bending rigidity, as they describe flexible elongated structures characterized

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by a certain persistence length.<sup>35,36</sup> This property has strongly motivated the modeling of flagella as active persistent polymers,<sup>28,29,37</sup> idealized as chains of units (molecular motors) that, through their organized or synchronized activity, determine the shape and the right collective dynamics to confer motility to the flagellum.<sup>30,38</sup>

From a hydrodynamical point of view, the locomotion is possible because the viscous friction of the fluid along slender bodies is anisotropic;<sup>39</sup> indeed, the hydrodynamic forces acting on slender bodies are predominantly anisotropic due to the different resistance encountered along and perpendicular to their length. This effect is embodied in the slender-body theory,<sup>40</sup> which simplifies the approach by focusing only on the body's centerline, especially when viscous forces dominate (low Reynolds number). The investigation of the complex interplay between hydrodynamics and elasticity in biofilament fluctuations has led to the elastohydrodynamic formulations of flagellar motion that inspired a series of interdisciplinary studies. Besides the seminal works by K. E. Machin<sup>41</sup> on the propagation of elastic waves along flagella, other interesting contributions include ref. 42 on the bending modulus measurement of microtubules and ref. 43 exploring the behavior of actin filaments under external oscillatory driving and viscous drag.

The implications of anisotropic hydrodynamic friction are essential to understanding biological propulsion and designing micro-scale devices. Although this issue is highly significant, it will not be addressed here because we are mainly interested in the dynamics of beating. Therefore, we only consider the situation in which the first monomer of the filament is anchored to a fixed point. Note that a similar condition has been realized experimentally,<sup>13</sup> in which sperm cells were confined within microscopic cages (Fig. 1). Since this setup forbids natation, tail conformations can be assumed to be weakly affected by the anisotropies of the hydrodynamic drag.

Therefore, we study through simulations and theory a simplified, yet not trivial, version of an anchored flagellum

depicted in Fig. 1 constrained to move in the 2D planar geometry and subject to the effects of a traveling-wave force representing an idealized version of the coherent activity of molecular motors during beating dynamics. In particular, we will analyze how spatially periodic conformational shapes of flagella can emerge from the interplay between its rigidity and the spatiotemporal periodicity of the driving.<sup>44,45</sup> To maintain the analysis as simple as possible, we consider a monochromatic traveling-wave force, as in ref. 46, characterized by a wavelength  $\lambda$  (*i.e.* wavevector  $k = 2\pi/\lambda$ ) and an oscillation frequency  $\omega$ . The study is performed at different  $\omega$  and  $k$  to show how these parameters affect the flagellum wave-form selection.

Our simple choice of the force  $h_n$  is due to the requirement that the continuum model, we will use to explain certain regimes of flagellum dynamics, be fully solvable. One might question whether such functional form and direction are compatible with the notion of active force, since: (i) the force is decoupled from the chain conformations; (ii) it always oscillates in a constant direction ( $y$ -axis). In its widest definition, an active force is an additional degree of freedom coupled to the system leading to out of equilibrium dynamics. In the literature, it is common practice to represent active forces as coloured noises independent of the conformation,<sup>30,46,47</sup> but any representation that breaks detailed-balance is legitimate.

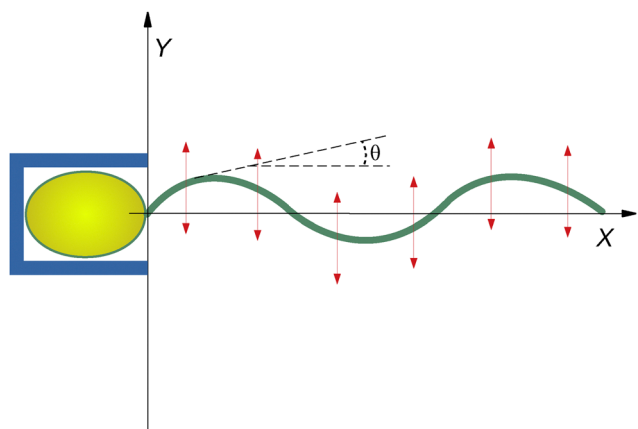
Additionally, it can be noted that in the approximation we will work with, weakly bending (small deformation from the straight conformation), the force directed along the  $y$ -axis is the relevant part of the force that is oriented as the normal to the flagellum. In this sense, it is reasonable to interpret  $h_n$  as the local average force exerted by molecular motors on a small segment of the filament. To further emphasize the concept, let us notice that molecular motors acting on a filament constitute additional degrees of freedom beyond those representing the filament. Moreover, each dynein exerts a shear force on a microtubule doublet, which is internal to the filament, such a shear force converts instantaneously into a bending (*i.e.* almost transversal) excitation inducing local curvature due to internal constraints.

The paper is structured as follows. In Section 2, we introduce the computational two-dimensional model of the flagellum, along with its continuum theoretical version, which provides a useful framework for interpreting the simulation results. Section 3 discusses the dynamics of the flagellum, analyzing the computational results in terms of parameters  $(\omega, k)$  that define the monochromatic active force. Finally, conclusions are drawn in Section 4.

## 2 Flagellum models

### 2.1 Computational model

In our approach, the flagellum is portrayed as a 2-dimensional chain of  $N + 1$  beads of mass  $m$  connected by stiff elastic springs of finite extension  $b$ . As the first bead is anchored to the origin,  $\mathbf{r}_0 = \mathbf{0}$ , the system cannot translate but can explore the full range of bending fluctuations. The bending energy



**Fig. 1** Sketch of the two-dimensional geometry setup that we consider in this work. The head of the bacterium is blocked in a cage device (blue box), thus the flagellum is practically hinged to the origin and constrained to move on the plane  $XY$ . The red arrows represent the amplitude and direction of the traveling-wave forces driving the beating dynamics.



introduces a penalty whenever three consecutive beads lose their alignment. The potential energy of the system is defined by the function<sup>48–50</sup>

$$V(\mathbf{r}_0, \dots, \mathbf{r}_N) = \frac{K}{2b^2} \sum_{n=1}^N (|\mathbf{r}_n - \mathbf{r}_{n-1}| - b)^2 + \frac{B}{2b^2} \sum_{n=1}^{N-1} |\mathbf{r}_{n+1} - 2\mathbf{r}_n + \mathbf{r}_{n-1}|^2. \quad (1)$$

In this notation, spring  $K$  and bending  $B$  constants have the dimension of energy ( $k_B T$ ); in the following, we will take  $b = 1$ ,  $K \gg B$  ( $K = 100$ ), as we assume to work in a regime as similar as possible to an inextensible polymer. Even though a moderate degree of extensibility of the chain cannot be excluded,<sup>51</sup> as small fluctuations of bond lengths  $|\mathbf{r}_n - \mathbf{r}_{n-1}|$  are still possible around their expected value  $b = 1$ .

We consider the overdamped regime of the system when coupled to a weak thermal bath, so the equation of motion of each bead is

$$\gamma \dot{\mathbf{r}}_n = -\frac{\partial V}{\partial \mathbf{r}_n} + \mathbf{h}_n(t) + \sqrt{2\gamma T} \xi_n(t) \quad (2)$$

where  $\xi_n(t)$  is a Gaussian white noise of zero average and unitary variance,  $T$  is the solvent (bath) temperature, while  $\mathbf{h}_n(t) = (0, f_0 \sin(knb - \omega t))$  is a deterministic space-modulated and time-periodic perturbation (active-like force)<sup>52</sup> that, in our

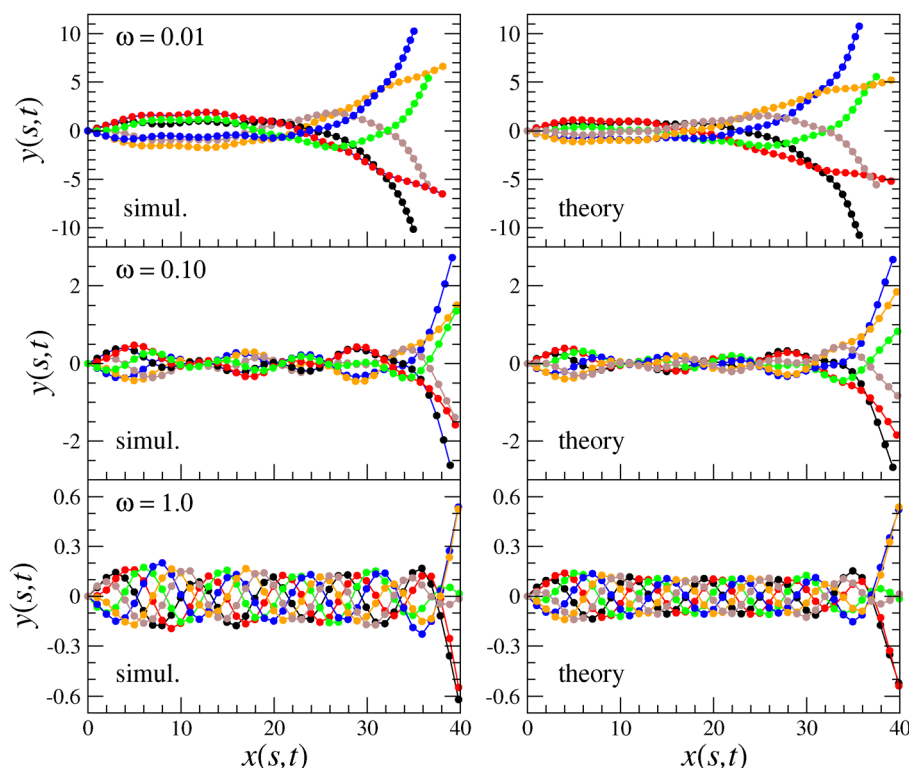
simplified scheme, confers to the flagellum a transversal beating dynamics. In the following, we set  $f_0 = B/20$  in all simulations and theoretical analysis to consider the active force as a relatively small perturbation with respect to bending and stretching interactions. The active force  $\mathbf{h}_n(t)$  competes with the bending rigidity in generating transversal undulatory fluctuations of the chain with a spatial modulation depending on the wave number  $k$ . We choose  $k = (2\pi/L)m$  where  $L = Nb$  is the length of the flagellum in terms of monomers and  $m$  is a positive integer defining the number of expected oscillations applied to the flagellum. This choice guarantees that the active force is spatially periodic over the polymer length  $L$  and implies

a zero net force as easily verified,  $f_0 \sum_{n=1}^N \sin[(2\pi m/N)n - \omega t] = 0$ .

In addition, we assume local isotropic dissipation with friction coefficient  $\gamma$  and neglect long-range hydrodynamic interactions.

As already mentioned in the introduction, a rigorous dynamical formulation would require anisotropic drag.<sup>32,53</sup> However, as we clearly show in Appendix D, the weakly bending regime we consider in simulation and theoretical analysis, where the motion is predominantly transverse, implies that only the normal drag enters the leading-order dynamics.

Here, the role of  $\gamma$  in the dynamics is to provide a time scale, *i.e.* the rate of energy dissipation due to the friction with the solvent, and then it can be set  $\gamma = 1$  in the simulations without loss of generality. Nevertheless, in the following theoretical



**Fig. 2** Snapshots of the flagellum stationary dynamics (left panels) compared with the corresponding conformations obtained from the approximated theory eqn (4) (right panels), for a chain of length  $L = Nb$  ( $N = 40$ ,  $b = 1$ ) and bending modulus  $B = 10$ . The different colors indicate six sampling times that are equally spaced within a force-cycle  $2\pi/\omega$ . The comparison is done for active perturbations of wavevector  $5(2\pi/L)$  and small, moderate, and high frequencies  $\omega = 0.01, 0.10, 1.0$ .



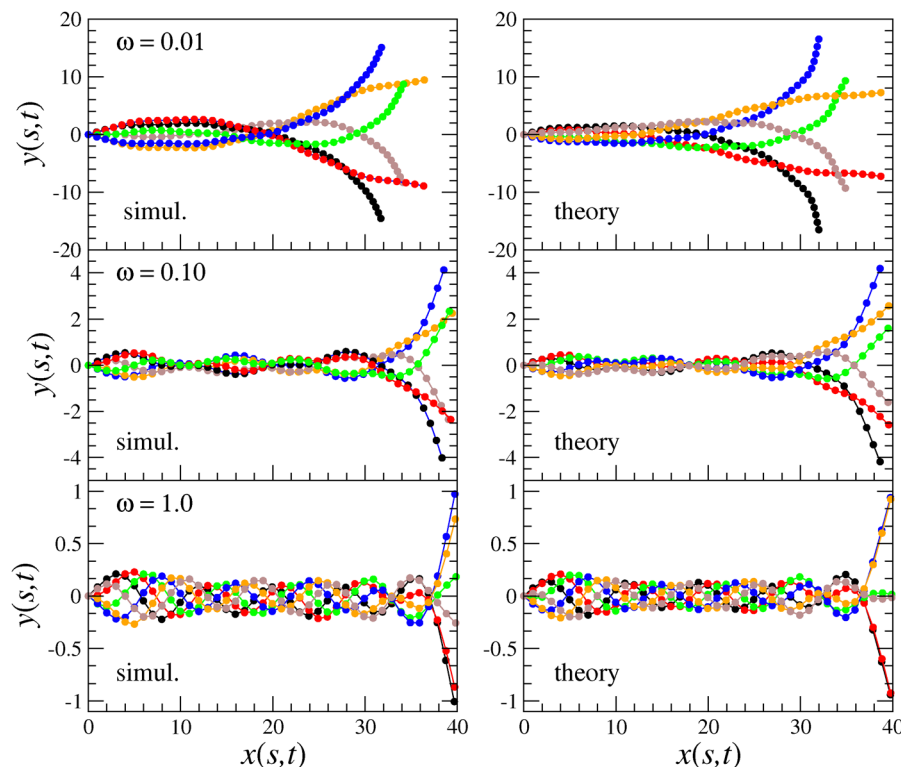


Fig. 3 Same conditions of Fig. 2, but higher bending stiffness,  $B = 20$ .

analysis, we leave it indicated to keep track of the correct physical units of the observables; we also anticipate that the theory will neglect the Gaussian noise.

This is because, in our simulations, the noise is completely overwhelmed by the forcing  $\mathbf{h}_n$ , i.e.  $f_0^2 \gg \gamma T$ . However, although small, its presence is necessary for running Brownian dynamics simulations.<sup>54</sup>

Along the same lines as the work by Machin,<sup>41</sup> we are interested in understanding how the interplay between bending rigidity and active forcing selects the resulting polymer conformations and in describing their relevant spatiotemporal patterns.<sup>55,56</sup> In the papers,<sup>32,53</sup> the same issue is studied under the effects of localized forces, applied to one of the endpoints of the flagellum, and under anisotropic hydrodynamic drag. Let us notice that, while hydrodynamics plays an important role in generating self-propulsion, it does not contribute significantly in the beating dynamics, which is instead mostly influenced by mechanical aspects (see Appendix D), especially when driven by an extended force like the one we consider.

For this reason, we first perform Brownian simulations<sup>54</sup> of the chain in an isotropic medium through the Langevin eqn (2). Then, to better clarify the role of the perturbation parameters  $(k, \omega)$ , we support the computational results with a theoretical analysis based on the continuous model discussed below. The left panels of Fig. 2 and 3 give the first qualitative idea about the beating phenomenology of the system by showing several conformations assumed by the flagellum sampled in simulations over one period,  $2\pi/\omega$ , of the forcing. When  $k = m(2\pi/L)$ , the flagellum can sustain undulations of wavelength  $\lambda = L/m$  as

one can see from the number of bumps along the conformations. The tail, instead, cannot follow the spatial periodicity due to the great moment of the external force on the free-end region making the tail perform considerable excursions.

Moreover, simulations indicate that at low frequencies,  $\omega \lesssim 10^{-2}$ , the flagellum oscillates over time but shows little undulation. In contrast, at high frequencies,  $\omega \gtrsim 1$ , it becomes more spatially modulated and undergoes a “stiffening” transition, assuming a more rod-like conformation. This occurs because its mechanical structure can no longer sustain and follow high-frequency modes. The transition is evident from the “cigar-like” shape seen in the final left panels of Fig. 2 and 3.

## 2.2 Continuum model

The continuum formulation of model (2) can be derived from the explicit expression of the internal forces obtained by direct differentiation of the potential (1)

$$\begin{aligned}
 -\frac{\partial V}{\partial \mathbf{r}_n} &= \frac{K}{b^2} [G(\mathbf{r}_{n+1} - \mathbf{r}_n) - G(\mathbf{r}_n - \mathbf{r}_{n-1})] \\
 &\quad - \frac{B}{b^2} (\mathbf{r}_{n+2} - 4\mathbf{r}_{n+1} + 6\mathbf{r}_n - 4\mathbf{r}_{n-1} + \mathbf{r}_{n-2})
 \end{aligned} \quad (3)$$

with  $\mathbf{G}(\mathbf{x}) = (1 - b/|\mathbf{x}|)\mathbf{x}$ . Since the head of the chain is fixed while the tail is free, eqn (3) holds for all the bulk monomers except the boundaries (precisely beads of number  $n = 0$ ,  $n = 1$ ,  $n = N - 1$ ,  $n = N$ ), we will discuss such conditions later. In the derivation of the continuum version of eqn (2), the flagellum is assimilated to a 2D-fluctuating string, hinged to the origin



$\mathbf{r}(0) = 0$ , with elongation  $2\nu = K/b$  and bending  $\varepsilon = Bb$  stiffness. The dimensional analysis suggests that  $\varepsilon/\nu$  has the dimension of a squared length, and more precisely, from ref. 57,  $\varepsilon/\nu = 2/\ell_p^2$ , being  $\ell_p$  the persistence length of the stiff polymer. As customary, we parameterize the curve with the arc length  $bn \rightarrow s$  measured from the origin coinciding with the hinged point (see Fig. 1).

The equation of motion governing the evolution of the system's coordinate  $\mathbf{r}(s,t) = x(s,t)\mathbf{e}_x + y(s,t)\mathbf{e}_y$  is straightforwardly derived from the monomers's eqn (3) after performing the continuum limits  $\mathbf{r}_n - \mathbf{r}_{n-1} \rightarrow b \partial \mathbf{r}(s)/\partial s$ . In this way, the first term of eqn (3) formally represents the discrete first derivative of the function  $\mathbf{G}(\mathbf{x})$ , whereas the last term is the discrete 4-th derivative of  $\mathbf{r}(s)$  and neglecting the contribution of the Gaussian noise, this leads to

$$\gamma \dot{\mathbf{r}} = 2\nu \frac{\partial}{\partial s} \left[ g(|\partial_s \mathbf{r}|) \frac{\partial \mathbf{r}}{\partial s} \right] - \varepsilon \frac{\partial^4 \mathbf{r}}{\partial s^4} + \mathbf{h}(s, t) \quad (4)$$

where  $g(x) = 1 - 1/x$  and  $\mathbf{h}(s,t) = (0, f_0 \sin(ks - \omega t))$ . For consistency with the simulation setup, we have to assume:  $\mathbf{h}(0,t) \equiv \mathbf{0}$  because the external force on the hinged monomer is null. The boundary conditions for eqn (4) corresponding to a tethered-hinged polymer in the origin ( $s = 0$ ), and free at the other end ( $s = L$ ), can be derived from eqn (3) by adding the "virtual" monomers  $\mathbf{r}_{-1}$ ,  $\mathbf{r}_{N+1}$ ,  $\mathbf{r}_{N+2}$ , which must satisfy specific relations such that the equations of motion for the "actual" monomers  $\mathbf{r}_1$ ,  $\mathbf{r}_{N-1}$ ,  $\mathbf{r}_N$  can be treated as bulk eqn (3). This trick ensures the same description of the dynamics across the entire polymer chain, including the boundaries. Such conditions are, obviously,  $\mathbf{r}_0 = 0$  and

$$\mathbf{r}_1 - 2\mathbf{r}_0 + \mathbf{r}_{-1} = 0$$

$$\mathbf{r}_{N+1} - 2\mathbf{r}_N + \mathbf{r}_{N-1} = 0$$

$$2\nu g\left(\frac{|\mathbf{r}_{N+1} - \mathbf{r}_N|}{b}\right) \frac{\mathbf{r}_{N+1} - \mathbf{r}_N}{b} = \varepsilon \frac{\mathbf{r}_{N+2} - 3\mathbf{r}_{N+1} + 3\mathbf{r}_N - \mathbf{r}_{N-1}}{b^3}$$

which, to the continuum, leads to  $\mathbf{r}(0,t) = 0$  and

$$\begin{aligned} \frac{\partial^2 \mathbf{r}}{\partial s^2} \Big|_0 &= \frac{\partial^2 \mathbf{r}}{\partial s^2} \Big|_L = 0 \\ 2\nu g(|\partial_s \mathbf{r}|) \frac{\partial \mathbf{r}}{\partial s} \Big|_L &= \varepsilon \frac{\partial^3 \mathbf{r}}{\partial s^3} \Big|_L \end{aligned} \quad (5)$$

The vanishing of the second derivative at  $s = 0$  and  $s = L$  implies the absence of moments at the boundaries, while the last equation means no force at the free end  $s = L$ . In physical language,  $g(|\partial_s \mathbf{r}|)$  corresponds to a line tension that guarantees the chain connectivity and its small stretchability,<sup>28</sup> by introducing an energetic penalty paid to stretch (or contract) the filament beyond its rest length. Mathematically speaking this term emerges by a variational principle on the WLC energy by imposing the constraint that the total chain length is left unaltered by the dynamical fluctuations.<sup>28,58,59</sup> Therefore, in the literature,  $g$  is customarily introduced as a Lagrangian multiplier implementing the average inextensibility constraint

of the flagellum.<sup>57,60</sup> In our approach, the presence of a weak stretching contribution is simply justified by the simulation setup, for which the in-extensibility constraint is implemented only in a soft manner *via* stiff harmonic springs for the bonds.<sup>49,61</sup> This, of course, does not prevent tiny fluctuations of the bond lengths around their fixed values  $b = 1$ . Since our simulations are run under quasi-inextensible condition ( $K \gg B$ ) we have  $|r_n - r_{n-1}| \simeq b$  or, equivalently,  $|\partial_s \mathbf{r}| \simeq 1$ .<sup>51</sup> It means that the factor  $g(|\partial_s \mathbf{r}|)$  should be considered, if not vanishing, small. Moreover, the external force  $\mathbf{h}$  that we implemented in our simulations tends to increase the distance between the beads; this slight but distributed stretching of the chain ( $|\partial_s \mathbf{r}| \gtrsim 1$ ) implies that the small value assumed by  $g(|\partial_s \mathbf{r}|)$  is generally positive and weakly dependent on  $s$ . Nevertheless, trying to linearize directly eqn (4) by assuming a small and constant value of  $\nu g(|\partial_s \mathbf{r}|) \rightarrow \nu_{\text{eff}}$ , leads to several inconsistencies, the worst of which is the collapse of the entire chain at the origin.<sup>62,63</sup>

### 2.3 Weakly bending approximation

The weakly bending approximation (WBA)<sup>59,64</sup> is a convenient approach to recovering extensibility; it assumes the flagellum undergoes only small deviations from a straight or rod-like conformation, likewise, the active force is considered small enough to remain consistent with the weakly bending regime. In our case, we see that WBA provides a satisfactory scheme for interpreting computational results. As customary in WBA, a convenient parameterization of the flagellum centerline is  $\mathbf{r}(s,t) = (s + u(s,t), y(s,t))$ , where  $u$  is a small longitudinal deviation from  $x = s$ , with a small derivative as well,  $\partial_s u(s) \ll 1$ .

Such a parameterization is required to satisfy the inextensibility constraint

$$|\partial_s \mathbf{r}|^2 = [1 + \partial_s u(s,t)]^2 + [\partial_s y(s,t)]^2 = 1, \quad (6)$$

that, to the leading order, implies

$$\partial_s u(s,t) \simeq -\frac{1}{2} [\partial_s y(s,t)]^2, \quad (7)$$

from which  $u(s,t)$  is obtained by a direct integration, yielding

$$x(s,t) = s - \frac{1}{2} \int_0^s d\xi \left[ \frac{\partial y(\xi,t)}{\partial \xi} \right]^2. \quad (8)$$

In the WBA, the fluctuations  $y(s,t)$  completely determines the shape of the flagellum, as the variable  $u(s,t)$ , describing small longitudinal deformations, is enslaved to  $y(s,t)$  through eqn (7). To be consistent with the constraint,  $g(|\partial_s \mathbf{r}| = 1) = 0$ , the equation that the transversal component  $y(s,t)$  satisfies is

$$\gamma \dot{y} = -\varepsilon \frac{\partial^4 y}{\partial s^4} + f_0 \sin(ks - \omega t). \quad (9)$$

Unfortunately, it provides solutions that deviate from numerical results, especially for the tail region, as discussed in the section results, see Fig. 6. A decidedly better affinity is instead obtained by including a "small" stretching term leading to the





effective equation

$$\gamma \dot{y} = 2\nu_{\text{eff}} \frac{\partial^2 y}{\partial s^2} - \varepsilon \frac{\partial^4 y}{\partial s^4} + f_0 \sin(ks - \omega t) \quad (10)$$

$$y(0, t) = 0, \quad \left. \frac{\partial^2 y}{\partial s^2} \right|_0 = \left. \frac{\partial^2 y}{\partial s^2} \right|_L = 0$$

$$2\nu_{\text{eff}} \frac{\partial y}{\partial s} - \varepsilon \frac{\partial^3 y}{\partial s^3} \Big|_L = 0$$

with  $\nu_{\text{eff}}$  small and positive parameter that has to be determined. As already mentioned,  $\nu_{\text{eff}}$  could be considered as a Lagrangian multiplier (within the approximation  $g$  constant) which implements inextensibility constraint of the flagellum. However, since we are already working within the WBA framework, which approximates this constraint, we need only to determine a reasonable value of  $\nu$  from the simulation data (see next section). As a consequence,  $\nu$  naturally turns out to be a function of the  $\omega$  and  $k$ ,  $\nu_{\text{eff}} = \nu_{\text{eff}}(k, \omega)$  of the active force, like it always happens when a stiff polymer undergoes the action of an external driving (shear flow, pulling, or active random force).<sup>37,65,66</sup>

In the rest of the paper, for simplicity, we use  $\nu$  instead of  $\nu_{\text{eff}}$ .

Besides the need to reproduce numerical simulations, another guess for the presence of the stretching term stems from the observation that by plugging the condition (7) into eqn (6) implies that  $|\partial_s \mathbf{r}|^2 \simeq 1 + (\partial_s y)^4/4$ , thus  $|\partial_s \mathbf{r}|$  is allowed to take on values slightly larger than 1. This is consistent with our expectation regarding the role of the term  $g(|\partial_s \mathbf{r}|)$  in eqn (4).

Definitely, our analytical estimate of the flagellum conformations in the WBA is given by eqn (10) together with eqn (8). The solution to eqn (10) can be obtained by an expansion<sup>37,58</sup>

$$y(s, t) = \sum_{n=1}^{\infty} y_n(t) \psi_n(s) \quad (11)$$

in the orthogonal eigenmodes

$$\psi_n(s) = \frac{1}{\sqrt{W_n}} \left[ \frac{1}{\alpha_n^2} \frac{\sin(\alpha_n s)}{\sin(\alpha_n L)} + \frac{1}{\beta_n^2} \frac{\sinh(\beta_n s)}{\sinh(\beta_n L)} \right], \quad (12)$$

of the differential operator appearing in eqn (10), *i.e.*,

$$\varepsilon \frac{d^4 \psi_n(s)}{ds^4} - 2\nu \frac{d^2 \psi_n(s)}{ds^2} = \lambda_n \psi_n(s), \quad (13)$$

consistent with boundary conditions (5), where  $\lambda_n$  are the corresponding eigenvalues. Appendix A reports the derivation of the eigenmodes and eigenvalues  $\lambda_n$ , including the definition of  $\alpha_n$  and  $\beta_n$ , along with the formula of the normalization constants  $W_n$ . With a little abuse of language  $\alpha_n$  or  $\beta_n$  can be referred to as “quantum numbers” of the eigenmodes.

The amplitudes of each mode are independent and evolve according to the following equation

$$\gamma \frac{dy_n}{dt} = -\lambda_n y_n + b_n \cos(\omega t) - a_n \sin(\omega t) \quad (14)$$

where

$$a_n = f_0 \langle \cos(ks), \psi_n(s) \rangle, \quad b_n = f_0 \langle \sin(ks), \psi_n(s) \rangle, \quad (15)$$

are the coefficients representing the projection of the external force  $f_0[\sin(ks)\cos(\omega t) - \cos(ks)\sin(\omega t)]$  on the eigenmodes; having defined the scalar product

$$\langle g(s), \psi_n(s) \rangle = \int_0^L ds g(s) \psi_n(s).$$

Their explicit expression is

$$a_n = \frac{f_0}{\sqrt{W_n}} \left[ \frac{\alpha_n \tan(\alpha_n L/2)}{\alpha_n^2 (\alpha_n^2 - k^2)} + \frac{\beta_n \tanh(\beta_n L/2)}{\beta_n^2 (\beta_n^2 + k^2)} \right] \quad (16)$$

$$b_n = \frac{f_0}{\sqrt{W_n}} \left[ \frac{k}{\alpha_n^2 (\alpha_n^2 - k^2)} - \frac{k}{\beta_n^2 (\beta_n^2 + k^2)} \right]. \quad (17)$$

In Appendix B, we show that eqn (14) is solved by the following (stationary) periodic solution:

$$y_n(t) = \frac{b_n \lambda_n + a_n (\gamma \omega)}{\lambda_n^2 + (\gamma \omega)^2} \cos(\omega t) + \frac{b_n (\gamma \omega) - a_n \lambda_n}{\lambda_n^2 + (\gamma \omega)^2} \sin(\omega t). \quad (18)$$

We note that all coefficients appearing above, *e.g.*  $a_n$ ,  $b_n$  depend on the forcing parameters ( $k, \omega$ ), but – to make the notation less burdensome, we have omitted such dependencies.

After putting all the terms together and using the  $\psi_n(s)$ , we obtain the full solution of the  $y$ -profile of the flagellum that can be rearranged into the very simple expression

$$y(s, t) = \mathcal{A}_{k, \omega}(s) \cos(\omega t) + \mathcal{B}_{k, \omega}(s) \sin(\omega t) \quad (19)$$

upon defining, for the sake of shorthand notation,

$$\begin{aligned} \mathcal{A}_{k, \omega}(s) &= \sum_{n=1}^{\infty} \psi_n(s) \left[ \frac{b_n \lambda_n + a_n (\gamma \omega)}{\lambda_n^2 + (\gamma \omega)^2} \right] \\ \mathcal{B}_{k, \omega}(s) &= \sum_{n=1}^{\infty} \psi_n(s) \left[ \frac{a_n (\gamma \omega) - b_n \lambda_n}{\lambda_n^2 + (\gamma \omega)^2} \right]. \end{aligned} \quad (20)$$

Here the indexes “ $k, \omega$ ” recall the parametric dependence on the active force numbers.

The amplitudes  $\mathcal{A}_{k, \omega}(s)$  and  $\mathcal{B}_{k, \omega}(s)$  play the role of a response of the system to a given forcing with spatiotemporal periodicity  $k, \omega$ : high or low values of those amplitudes indicate if the traveling-wave perturbation is consistent with or is attenuated by the bending rigidity of the flagellum. Such amplitudes seem to be suppressed by increasing  $\omega$ , therefore in large  $\omega$  regimes, the dynamics of the flagellum is expected to become noise-dominated and it loses the periodic behavior. In other terms, the flagellum response to high-frequency active forces resembles a low-pass filter for which high-frequency perturbations are strongly attenuated, or in a more structural sense, this corresponds to a “straightening” crossover.

It is also interesting to remark that the flagellum acts as a sort of “spectral device” which decomposes a “monochromatic” perturbation of parameters ( $k, \omega$ ) into a superposition of responses characterized by a set of numbers  $\{\alpha_n, \lambda_n\}_{n=1}^{\infty}$  where  $\alpha_n$  (and  $\beta_n$  that is strictly connected to it) plays the role of a generalized wave vector and  $\lambda_n$  is the corresponding “vibration” frequency.

For visualizing the impact of the wave number,  $k$ , on the flagellum properties we plot, in Fig. 4, the coefficients (16) and



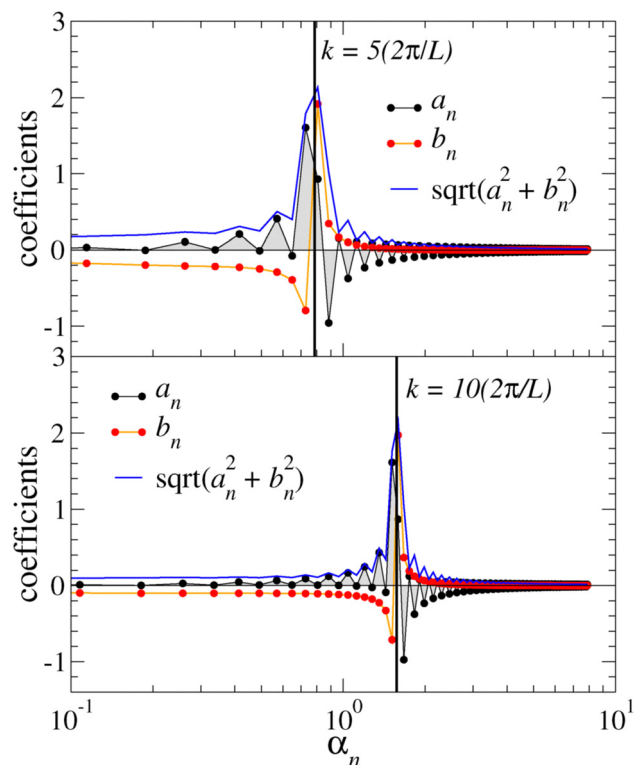


Fig. 4 Coefficients, eqn (16) and (17) plotted versus  $\alpha_n$ , of the perturbation  $f_0 \sin(ks - \omega t)$  expanded into the orthonormal eigenfunctions  $\psi_n(s)$ . The thick black vertical line marks the wave-number  $k$  of the spatiotemporal forcing,  $k = 5(2\pi/L)$  and  $k = 10(2\pi/L)$ . The blue line indicates the amplitude  $\sqrt{a_n^2 + b_n^2}$  of the  $n$ -th eigenmode. The picture resembles a “spatial-resonance” scenario because the maximal variation of coefficients occurs around  $k$ , even if the other contributions can not be considered negligible.

(17) of the active-force expansion in eigenmodes as a function of  $\alpha_n$ .

The coefficient  $a_n$  (black dots) displays oscillations that intensify as  $\alpha_n$  approaches  $k$  (marked by the thick vertical line), whereas  $b_n$  (red dots) exhibits a growth towards  $k$  without oscillations, undergoing a sign change when crossing  $k$ . The behavior of  $\sqrt{a_n^2 + b_n^2}$ , which is a sort of composite envelope of  $a_n$  and  $b_n$ , distinctly reveals a pronounced peak at  $k$ .

These plots closely resemble a “spatial resonance” scenario, because the maximal variation of  $a_n$  and  $b_n$  occurs around a neighborhood of  $k$ , even though the remaining contributions are not negligible. This suggests that the flagellum modes with  $\alpha_n \simeq k$  are the most sensible to the perturbation.

In the following section, we discuss the simulation results on the flagellum beating behavior by using the above continuum string theory as a reference and interpretative basis.

### 3 Results

We run simulations of a flagellum according to eqn (2) for  $N + 1 = 41$  monomers (beads), the first of which is anchored to the origin, forming a hinged restrain, by numerically integrating eqn (2) for each monomer forming the flagellum. We select

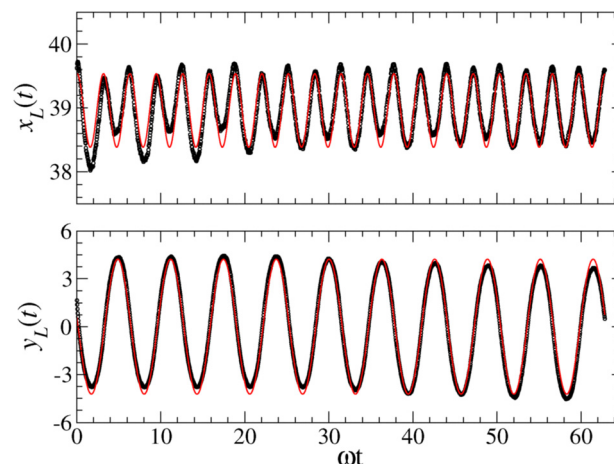


Fig. 5 Trajectory of the tail position  $x_L(t), y_L(t)$  of a flagellum of  $N + 1 = 41$  beads (length  $L = Nb$ ), bending rigidity  $B = 20$  and under a active perturbation with  $k = 5$ ,  $\omega = 0.10$ . Black dots are the simulated data and the red curves represent the fit with eqn (21) and (22).

$K = 100$ , as a reasonable choice for granting inextensibility, and consider different bending modulus  $B$  and active cycles,  $2\pi/\omega$ . The time step is chosen to be of the order of  $h \simeq 10^{-4}$  to avoid instabilities of the Brownian dynamics code (Euler scheme) within the whole explored range of parameters. The flagellum is initialized by aligning all the monomers to the  $x$ -axis in their relaxed configuration:  $x_n = nb$ , ( $n = 0, \dots, N$ ). Main observables needed to characterize the flagellum dynamics were sampled and eventually averaged over a time  $10(2\pi/\omega)$ , *i.e.* for ten forcing cycles, after discarding a transient of about  $10^6$  time steps to allow the system's relaxation onto a robust stationary regime.

The left panels of Fig. 2 and 3 show snapshots of flagellum conformations from simulations for three values of  $\omega$ , with  $B = 10$  and  $B = 20$  respectively, while the right panels report the corresponding theoretical flagellum conformations obtained by solving eqn (10) and using eqn (8) to reconstruct the  $x$ -coordinate in the WBA. The reasonable agreement between simulation and theory has been possible by adjusting the coefficient  $\nu$  of the stretching term. For calibrating  $\nu$ , we compared the motion of the flagellum tail (last monomer) with its theoretical prediction from eqn (10). The beating oscillations of the tail observed in the simulations and displayed in Fig. 5 (black dots), can be described by the following simple evolutionary laws

$$x(t) = x_0 + a_x \cos(2\omega t) + b_x \sin(2\omega t) \quad (21)$$

$$y(t) = a_y \cos(\omega t) + b_y \sin(\omega t). \quad (22)$$

As we will see in the following, the frequency doubling of the  $x$  coordinate is a natural consequence of the quasi-inextensibility of the flagellum. This phenomenon has also been observed in simulations of wall-anchored semiflexible polymers under oscillatory shear flow.<sup>56</sup>

The amplitude of the  $y(t)$  signal is  $F = \sqrt{a_y^2 + b_y^2}$  whose numerical value can be obtained by a fitting procedure to the simulation time series, see Fig. 5. The effective value of  $\nu$  is



**Table 1** Table reporting the values of the estimated  $\nu$  obtained by comparing the amplitudes  $F^2 = a_y^2 + b_y^2$  of the fitting eqn (22) with the expected amplitudes  $\mathcal{A}(L)^2 + \mathcal{B}(L)^2$  from the semiflexible flagellum theory

$\omega$	0.01	0.10	1.0
$B = 10$	$\nu = 0.1696$	$\nu = 0.1950$	$\nu = 0.5632$
$B = 20$	$\nu = 0.3375$	$\nu = 0.3710$	$\nu = 0.7150$

such that  $F^2 \simeq \mathcal{A}^2(L) + \mathcal{B}^2(L)$ , where

$$\begin{aligned}\mathcal{A}(L) &= \sum_{n=1}^{\infty} \frac{1}{\sqrt{W_n}} \left( \frac{1}{\alpha_n^2} + \frac{1}{\beta_n^2} \right) \frac{b_n \lambda_n + a_n (\gamma \omega)}{\lambda_n^2 + (\gamma \omega)^2}, \\ \mathcal{B}(L) &= \sum_{n=1}^{\infty} \frac{1}{\sqrt{W_n}} \left( \frac{1}{\alpha_n^2} + \frac{1}{\beta_n^2} \right) \frac{b_n (\gamma \omega) - a_n \lambda_n}{\lambda_n^2 + (\gamma \omega)^2}.\end{aligned}\quad (23)$$

are the amplitudes predicted by eqn (20), for shorthand notation we dropped the indexes  $\omega, k$ . The satisfactory numerical values of  $\nu$  are reported in Table 1. Once we set an “optimal” value for  $\nu$ , we can compare the simulated trajectory of the flagellum tail (last monomer), describing a Lissajous-like figure in Fig. 6 with the corresponding result obtained by using eqn (8) and (19) at various values of  $\omega$  and stiffness  $B$

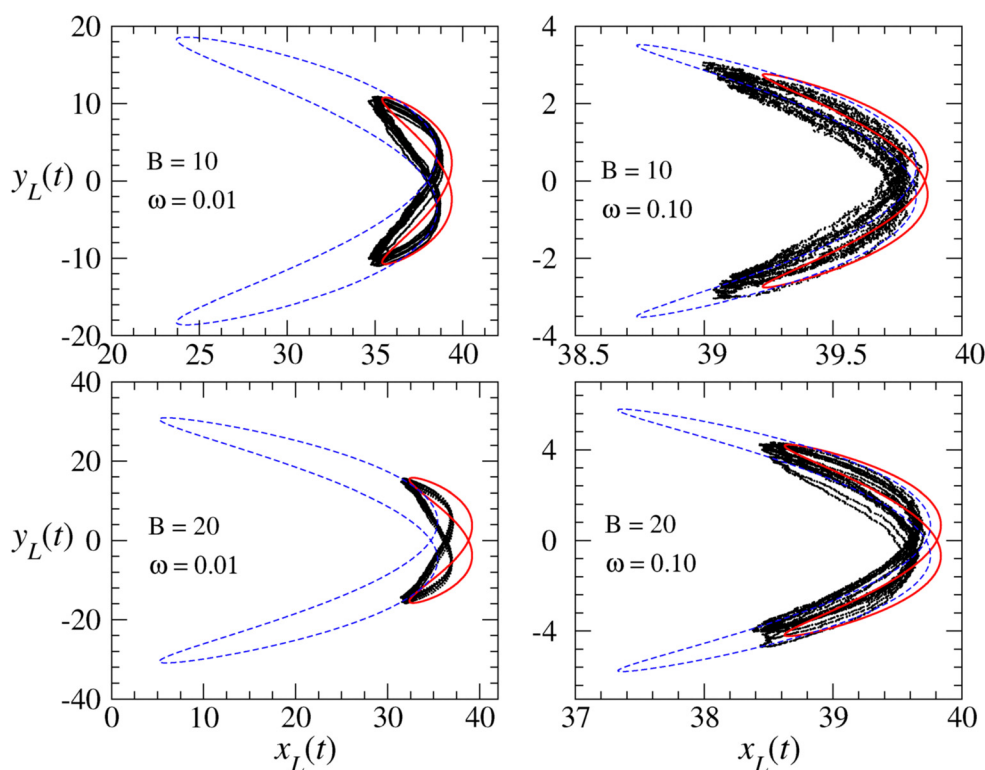
$$\frac{x_L(t)}{L} = 1 - \frac{1}{2L} \int_0^L ds [\partial_s y(s, t)]^2 \quad (24)$$

$$N_x \omega_x = N_y \omega_y,$$

The dashed lines in Fig. 6 represent the theoretical Lissajous plots that by tuning  $\nu$  converge and overlap with the simulation data.

The scattering (spread) observed in the simulation data is presumably due to the interplay of chaos and thermal noise which we do not investigate here. The reader can refer to ref. 67 for a discussion of possible chaotic behaviors in anchored polymers driven by a localized oscillating force. It is, however, clear that on passing from  $\omega = 0.01$  to  $\omega = 0.10$ , the positions of the tail turn out to be more scattered, even if the thermal noise in the simulation is the same. This is an intriguing role of the active forcing at high frequencies, which introduces a sort of “stochastization effect” that dominates over the small thermal noise, as shown in eqn (19).

It is interesting to discuss how the bi-lobed Lissajous-like behavior of the tail emerges in terms of the continuum theory from eqn (24) and (25). Fig. 6 shows that such Lissajous figures are characterized by a frequency ratio 2:1, corresponding to a frequency doubling of the  $x$ -motion:  $\omega_x = 2\omega_y$ . Indeed, the frequencies of a Lissajous' figure are known to satisfy the relationship



**Fig. 6** Trajectory described during the beating process by the position of the tail (last-monomer) of a flagellum with  $N = 40$  monomers of length  $b = 1$ , for two bending constants and two frequencies as indicated in the panels. The motion recalls a bi-lobed Lissajous figure, the points are the simulation results, whereas the curves are the predicted trajectory described by eqn (26a) and (26b). The red-thick Lissajous figures correspond to the optimal  $\nu$  reported in Table 1. For comparison, we also plot the dashed blue lines corresponding to the flagellum with  $\nu = 0$  to underscore the important role of the stretching contribution.





with  $N_x$  and  $N_y$  being the number of intersections of the curve with generic horizontal and vertical lines respectively and in our specific case  $N_x = 2$  and  $N_y = 4$ , thus  $\omega_x = 2\omega_y$ .

This ratio is expected as a straightforward consequence of the quasi-inextensibility of the chain, in fact by substituting eqn (25) into eqn (24), and expressing formally the integrals as  $L\langle \cdot \cdot \rangle$ , we get

$$\frac{x_L(t)}{L} = S + \frac{Q-P}{4}\cos(2\omega t) - \frac{R}{2}\sin(2\omega t)$$

$$\frac{y_L(t)}{L} = \frac{\mathcal{A}(L)}{L}\cos(\omega t) + \frac{\mathcal{B}(L)}{L}\sin(\omega t),$$

where we have defined

$$P = \langle [\mathcal{A}'(s)]^2 \rangle, \quad Q = \langle [\mathcal{B}'(s)]^2 \rangle, \quad R = \langle \mathcal{A}'(s)\mathcal{B}'(s) \rangle,$$

with  $S = 1 - (P + Q)/4$ , and used the following trigonometric identities

$$\cos^2(\omega t) = [1 + \cos(2\omega t)]/2$$

$$\sin^2(\omega t) = [1 - \cos(2\omega t)]/2$$

to make explicit the frequency doubling of the  $x$ -motion. The above equations, after simple manipulation, can be recast in the traditional form of Lissajous figures

$$x_L(t)/L = S + S_x \cos(2\omega t + \Delta_x) \quad (26a)$$

$$y_L(t)/L = S_y \cos(\omega t + \Delta_y), \quad (26b)$$

upon setting  $S_x \cos(\Delta_x) = (Q - P)/4$ ,  $S_x \sin(\Delta_x) = R/2$  and  $S_y \cos(\Delta_y) = \mathcal{A}(L)/L$ ,  $S_y \sin(\Delta_y) = \mathcal{B}(L)/L$ . In conclusion, the tail's behavior can be mathematically explained by considering that the solution (8) and (19) evaluated at  $s = L$  results in a combination of  $\sin(\omega t)$  and  $\cos(\omega t)$  which can be rearranged in the form (26a) and (26b). Moreover, the shape figure depends not only on the frequency (2 : 1) and amplitude ratio ( $S_x : S_y$ ) but also on the phase shift,  $\Delta = \Delta_y - \Delta_x$ .

It's worth noting that each internal monomer of the flagellum also undergoes a similar type of Lissajous motion, albeit the greatest amplification is observed in the free tail.

Another quantity often used to characterize the dynamical response of the flagellum and its conformational properties is the end-to-end distance, which for the hinged system to the origin simply reads

$$R_{ee}^2(t) = x^2(L, t) + y^2(L, t).$$

Fig. 7 reports the time behavior of  $R_{ee}(t)$  obtained from the simulations of a flagellum of 41 beads (black curve) and compares it with the theoretical prediction (red curve) derived by squaring eqn (26a) and (26b). The observable  $R_{ee}(t)$  exhibits a cyclical behavior with the active-force period  $2\pi/\omega$  which is well reproduced by the theoretical curve (red) once the free parameter  $\nu$  in eqn (4) is properly set, as reported in Table 1.

### 3.1 Spatial modulation

So far, we have analyzed the influence of the force cycle, defined by  $\omega$ , on the flagellum beating dynamics, now, we would like to

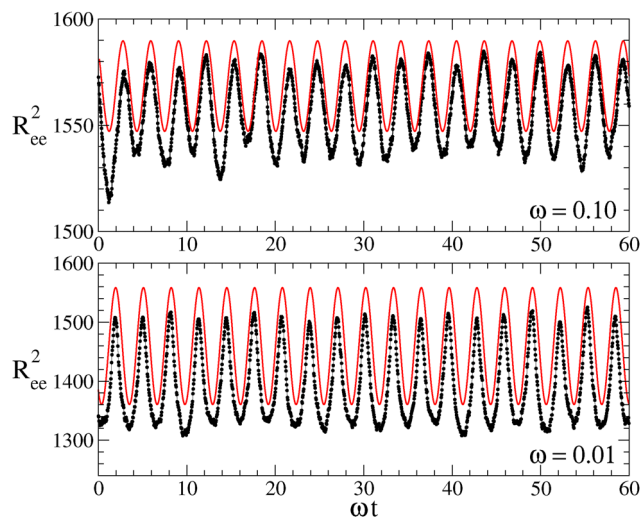


Fig. 7 Simulated time course (black) of the squared end-to-end distance  $R_{ee}^2$  of a flagellum with  $N + 1 = 41$  beads each of diameter  $b = 1$ , corresponding to a length  $L = Nb$ . The chain has a bending rigidity strength  $B = 10$  and perturbation  $k = 5$ ,  $\omega = 0.01$  and  $\omega = 0.10$ . The simulations show a periodic behavior with a main frequency  $\omega$  that is double the forcing frequency. The red curve represents the expected  $R_{ee}^2$  obtained by the solution (8) and (19).

focus on the role of  $k$  in shaping the spatial conformation of the flagellum. To check if the spatial modulation induced by the perturbation is sustained by the filament dynamics, we computed the bond-bond correlation starting from the hinged point,  $x_0 = 0$ ,  $y_0 = 0$ ,

$$C_b(n) = \overline{\mathbf{u}_1 \cdot \mathbf{u}_n} \quad n = 1, \dots, N, \quad (27)$$

with  $\mathbf{u}_n = \mathbf{r}_{n+1} - \mathbf{r}_n$  being the bond vector connecting the positions of two consecutive beads. The notation  $\overline{f(t)}$  indicates

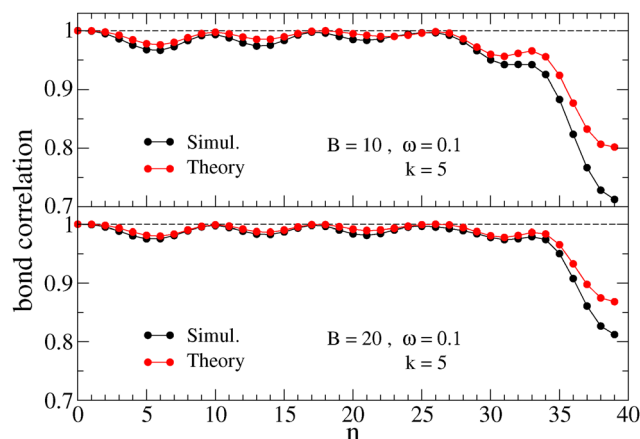


Fig. 8 Bond-bond correlation  $C(n)$  for filaments of  $N = 40$  monomers, with bending stiffness  $B = 10$  and  $B = 20$ , both having the same  $\omega = 0.10$ . Black dots represent simulation data, while red dots represent theoretical predictions. Both the simulation and theoretical plots reveal spatial modulation with five peaks, consistent with the active-force wave number  $k = 5(2\pi/L)$ , where  $L = Nb$ . The average is taken over a long equilibrium simulation run at temperature  $T = 0.001$ . The red plots, drawn from eqn (29), show a pattern of peaks similar to the simulation data.



the time average, which in our case, coincides with the average over a period,  $2\pi/\omega$ , of the active force. Fig. 8 presents the simulated data for  $C_b(n)$  (black points) averaged over a long equilibrium run at low temperature  $T = 0.001$ , corresponding to a flagellum of bending stiffness  $B = 10$ , (upper panel) and  $B = 20$  (lower panel) both perturbed with frequency  $\omega = 0.10$ .  $C_b(n)$  exhibits five peaks, consistent with the oscillations imposed by the active-force wave number,  $k = 5(2\pi/L)$ , indicating that the chain's stiffness can support the external modulation.

Simulations also show that the bond orientation becomes more correlated as the bending stiffness increases, this is expected since the persistence length is higher for  $B = 20$ . The faster decay of the correlation for  $B = 10$  is also indicative of weaker persistence, and a “visual estimate” of the persistence length of the flagellum can be obtained from the onset of a large deviation of the tail region from the horizontal dashed line.

A theoretical prediction of bond–bond correlation behavior can be obtained from the continuum model by using the following formula

$$C_b(s) = b^2 \overline{\frac{\partial \mathbf{r}(s, t)}{\partial s} \cdot \frac{\partial \mathbf{r}(0, t)}{\partial s}} \quad (28)$$

in which  $b \partial_s \mathbf{r}(s, t)$  is the continuum analogue of a bond vector in eqn (27). The overbar denotes the time average over a force cycle ( $2\pi/\omega$ ) and we recall that, throughout the text, we set  $b = 1$  to eliminate inessential parameters. Fig. 8 presents the simulated data for  $C_b(n)$  (black points) averaged over a long equilibrium run at low temperature  $T = 0.001$ , corresponding to a flagellum of bending stiffness  $B = 10$ , (upper panel) and  $B = 20$  (lower panel) both perturbed with frequency  $\omega = 0.10$ .  $C_b(n)$  exhibits five peaks, consistent with the oscillations imposed by the active-force wave number,  $k = 5(2\pi/L)$ , indicating that the chain's stiffness can support the external modulation.

In the WBA, the bond vector can be written as

$$\frac{\partial \mathbf{r}}{\partial s} = \left( 1 - \frac{1}{2} \left( \frac{\partial y}{\partial s} \right)^2, \frac{\partial y}{\partial s} \right)$$

therefore,  $C_b(s)$  to the leading order becomes

$$C_b(s) \simeq 1 - \frac{1}{2} \left[ \overline{\left( \frac{\partial y(s, t)}{\partial s} \right)^2} - \frac{1}{2} \overline{\left( \frac{\partial y(0, t)}{\partial s} \right)^2} + \overline{\frac{\partial y(s, t) \partial y(0, t)}{\partial s}} \right]$$

By using eqn (19) and the average properties of trigonometric functions over a period, after simple algebraic manipulations,  $C(s)$  can be recast to the form

$$C_b(s) = 1 - \frac{1}{4} [\mathcal{A}'(s) - \mathcal{A}'(0)]^2 + [\mathcal{B}'(s) - \mathcal{B}'(0)]^2 \quad (29)$$

where  $\mathcal{A}$  and  $\mathcal{B}$  are the expressions in eqn (23). Notice that correctly  $C_b(s = 0) = b^2 = 1$ , as expected from the “quasi-inextensibility” of the flagellum bonds.

For a comparison, Fig. 8 also displays the corresponding quantity  $C_b(s)$  derived from the continuum model, eqn (29) (red

points). Although a precise quantitative agreement between  $C_b(n)$  and  $C_b(s)$  is lacking especially in the tail region where the application of WBA is questionable, it is noteworthy that they exhibit five similar oscillations driven by the active forcing modulation,  $k = 5(2\pi/L)$ .

This suggests that the qualitative structure of the beating dynamics remains consistent when passing from the discrete to the continuum models.

## 4 Conclusions

The main purpose of this study was to investigate the selection of flagella conformations arising from the bending resistance of a slender semi-flexible structure to an extended force (mimicking the activity of molecular motors) and driving its evolution across different spatiotemporal patterns characterized by  $\omega, k$ .

In particular, we developed an effective mechanical theory, that upon “tuning” the longitudinal stretching term, can explain (at least qualitatively) some important features of the beating dynamics observed in the simulation, such as the bond–bond spatial correlation and temporal oscillation of the flagellum tail which, in a certain frequency range of the active force, describes Lissajous' figures of 2:1 frequency ratio. The theory clearly explains that such a 2:1 frequency ratio arises from a frequency doubling of the  $x$ -oscillation, which in turn, is a natural consequence of the chain inextensibility.

Furthermore, our theoretical analysis sheds light on the ranges of  $\omega$  and  $k$  of the active force required to confer a prescribed spatial modulation to the flagellum and produce a significant effect on its beating dynamics. Indeed, as explained in Section 2.2, for high-frequencies forcing ( $\omega \gg 1$ ) the amplitude of periodic modulations of transversal profile  $y(s, t)$  is largely suppressed, and thermal fluctuations dominate the flagellum dynamics.

Additionally, the wavelength,  $2\pi/k$ , of the active forcing must be consistent with the persistence length,  $l_p$ , of the flagellum, as high levels of spatial modulation cannot be energetically sustained by a system with a given bending stiffness, see Appendix C for a less qualitative argument. Such a result could play a key role in designing bio-inspired self-propelled engines.

We also provided evidence (see Appendix D) that, as long as WBA holds, anisotropies in hydrodynamical interaction, which are crucial for self-propulsion, play a little role in the selection of conformations of flagella.

Although the modeling of active-like dynamics is not fully realistic from a biological point of view, we expect that the theory could be generalized to describe different scenarios, including cases where the active force has true “internal” origin by modeling the action of molecular motors distributed along the flagella. Thus, this work constitutes a first step towards more realistic description of active bio-filaments giving insight into the mechanism that arises from the interplay between mechanical and active forces, which is responsible for their conformation dynamics.



## Data availability

The source files for Fig. 2–8 of the manuscript are available at <https://github.com/cecconif/flagellum-wlc-data>. Each file can be opened using the graphical software Grace, which can be found and downloaded from the site <https://plasma-gate.weizmann.ac.il/Grace/>. Such files also contain, at the end, the raw data used to generate the figures.

## Conflicts of interest

There are no conflicts to declare.

## Appendices

### A Derivation of the eigenmodes

In this appendix, we derive the eigenmodes which are solutions of the equation

$$\varepsilon \frac{d^4 \psi_n(s)}{ds^4} - 2\nu \frac{d^2 \psi_n(s)}{ds^2} = \lambda_n \psi_n(s) \quad (30)$$

satisfying the boundary conditions:

$$\begin{aligned} \psi_n(0) = 0, \quad \frac{\partial^2 \psi_n(s)}{\partial s^2} \Big|_0 = 0 \\ \frac{\partial^2 \psi_n(s)}{\partial s^2} \Big|_L = 0, \quad 2\nu \frac{\partial \psi_n(s)}{\partial s} \Big|_L = \varepsilon \frac{\partial^3 \psi_n(s)}{\partial s^3} \Big|_L \end{aligned}$$

Since eqn (30) is linear, its solution requires solving the associated characteristic polynomial

$$\varepsilon \mu^4 - 2\nu \mu^2 - \lambda_n = 0,$$

the roots of which are, complex  $\mu = \pm i\alpha$  and real  $\mu = \pm\beta$ , where

$$\alpha^2 = \sqrt{\left(\frac{\nu}{\varepsilon}\right)^2 + \frac{\lambda}{\varepsilon}} - \frac{\nu}{\varepsilon}, \quad \beta^2 = \sqrt{\left(\frac{\nu}{\varepsilon}\right)^2 + \frac{\lambda}{\varepsilon}} + \frac{\nu}{\varepsilon},$$

then, it is straightforward to obtain the following algebraic identities

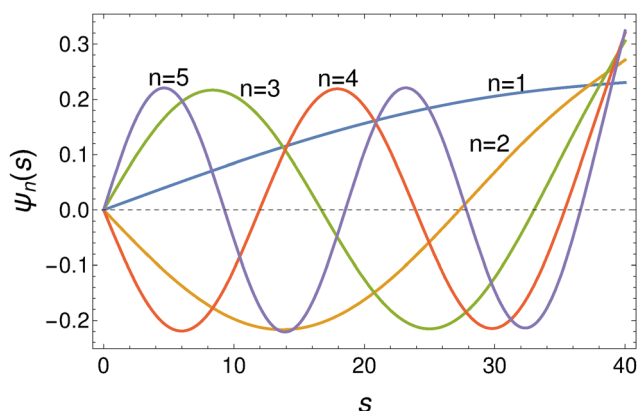


Fig. 9 First five eigenfunctions  $\psi_n(s)$  as a function of the arclength coordinate,  $s$ . Oscillations are associated with the generalized wavenumber  $\alpha_n$ , which must be compared with the wavenumber  $k$  of the active force modulation.

$$\beta^2 - \alpha^2 = 2\nu/\varepsilon \quad (31)$$

$$\lambda = \varepsilon \alpha^4 + 2\nu \alpha^2 = \varepsilon \beta^4 - 2\nu \beta^2. \quad (32)$$

Then the general solution of eqn (30) can be written as

$$\psi(s) = A \sin(\alpha s) + B \sinh(\beta s) + C \cos(\alpha s) + D \cosh(\beta s); \quad (33)$$

the coefficients  $A, B, C, D$  and the eigenvalues  $\lambda$  are determined by imposing the four boundary conditions plus the normalization. The condition at  $s = 0$  obviously implies that  $C = D = 0$ , while the condition in  $s = L$  implies

$$\alpha^2 \sin(\alpha L) A - \beta \sinh(\beta L) B = 0$$

$$\beta \cos(\alpha L) A - \alpha \cosh(\beta L) B = 0,$$

to simplify, we used the identity  $\varepsilon(\beta^2 - \alpha^2) = 2\nu$ . In matrix form, the boundary conditions lead to the following linear systems

$$\begin{bmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & -\alpha^2 & \beta^2 \\ \alpha^2 \sin(\alpha L) & -\beta^2 \sinh(\beta L) & 0 & 0 \\ \beta \cos(\alpha L) & -\alpha \cosh(\beta L) & 0 & 0 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

To exclude the nontrivial solution  $A = B = D = 0$ , the determinant of the coefficient matrix should be zero, therefore we have the condition  $\alpha^3 \sin(\alpha L) \cosh(\beta L) = \beta^3 \cos(\alpha L) \sinh(\beta L)$  that can be recast to

$$\alpha^3 \tan(\alpha L) = \beta^3 \tanh(\beta L) \quad (34)$$

After simple algebraic manipulations, we obtain from eqn (33) the final expression of the eigenfunctions (Fig. 9),

$$\psi_n(s) = W_n \left[ \frac{1}{\alpha_n^2} \frac{\sin(\alpha_n s)}{\sin(\alpha_n L)} + \frac{1}{\beta_n^2} \frac{\sinh(\beta_n s)}{\sinh(\beta_n L)} \right], \quad (35)$$

$W_n$  being a normalization constant such that

$$\int_0^L ds \psi_n^2(s) = 1,$$

then using the trigonometric identities,  $\sin^{-2}(p) = \cot^2(p) + 1$ ,  $\sinh^{-2}(p) = \coth^2(p) - 1$ , and eqn (34), this can be expressed as

$$\begin{aligned} W_n^{-2} = L \frac{2\nu^2 + \varepsilon \lambda_n}{\lambda_n^2} \\ + \frac{\coth(\beta_n L)}{\beta_n^3} \left( \frac{3\nu}{\lambda_n} - \frac{L\nu \coth(\beta_n L)}{\varepsilon \beta_n^3} \right) \end{aligned} \quad (36)$$

### B Solution of the mode amplitude equation

We derive the evolution of the  $n$ -th mode amplitude,  $y_n(t)$ , that obeys the equation

$$\gamma \frac{dy_n}{dt} + \lambda_n y_n = a_n \cos(\omega t) + b_n \sin(\omega t) \quad (37)$$

The solution of this first-order equation in the stationary



regime is

$$y_n(t) = \frac{e^{-\lambda t/\gamma}}{\gamma} \int_{-\infty}^t dz e^{\lambda z/\gamma} [a_n \cos(\omega z) + b_n \sin(\omega z)]$$

after a change of variable  $t - z \rightarrow z$

$$y_n(t) = \int_0^\infty dz \frac{e^{-\lambda z/\gamma}}{\gamma} \{a_n \cos[\omega(t - z)] + b_n \sin[\omega(t - z)]\}$$

and expanding  $\cos[\omega(t - z)]$  and  $\sin[\omega(t - z)]$ , we obtain

$$y_n(t) = (a_n Z_1 - b_n Z_2) \cos(\omega t) + (a_n Z_2 + b_n Z_1) \sin(\omega t)$$

where

$$Z_1 = \frac{1}{\gamma} \int_0^\infty dt e^{-\lambda t/\gamma} \cos(\omega t) = \frac{\lambda}{\lambda^2 + (\gamma\omega)^2}$$

$$Z_2 = \frac{1}{\gamma} \int_0^\infty dt e^{-\lambda t/\gamma} \sin(\omega t) = \frac{\gamma\omega}{\lambda^2 + (\gamma\omega)^2}.$$

Thus re-arranging, we can write

$$y_n(t) = \frac{a_n \lambda - b_n (\gamma\omega)}{\lambda^2 + (\gamma\omega)^2} \cos(\omega t) + \frac{a_n (\gamma\omega) + b_n \lambda}{\lambda^2 + (\gamma\omega)^2} \sin(\omega t),$$

which is the searched solution, eqn (18) of the main text.

The same expression could have been obtained, by substituting the test function (similar to the known term)  $y_n(t) = C_1 \cos(\omega t) + C_2 \sin(\omega t)$  into eqn (37) and choosing the coefficients  $C_1, C_2$  to make both members equal.

### C A simple criterion

In this appendix, we discuss a simple energetic argument that justifies the physical limits of the flagellum response.

The argument compares the energy of a perturbation mode and the energy of the flagellum solution (11), using the continuum energy formula<sup>59</sup>

$$E = \int_0^L ds \left[ \frac{\varepsilon}{2} \left( \frac{\partial^2 \mathbf{r}}{\partial s^2} \right)^2 + \nu \left( \frac{\partial \mathbf{r}}{\partial s} \right)^2 \right] \quad (38)$$

The active perturbation reads

$$F(s, t) = 2 \frac{f_0}{L} \sin(ks - \omega t)$$

where, the pre-factor  $2f_0/L$  is the necessary scale to make the amplitude of  $F(s, t)$  and the flagellum longitudinal oscillation  $y(s, t)$  of the same order. When substituted into eqn (38),  $F(s, t)$  requires an energetic cost

$$E(k) = \frac{f_0^2}{4} (ek^4 + 2\nu k^2).$$

This cost has to be compared with the energy of the flagellum solution, which can be computed using its expansion in eigenmodes, which due to their orthogonality, yields (11)

$$E_f = \frac{f_0^2}{4} \sum_{n=1}^{\infty} \frac{\bar{a}_n^2 + \bar{b}_n^2}{\lambda_n^2 + (\gamma\omega)^2} \lambda_n,$$

note that, with respect to the expressions (16) and (17), the

forcing amplitude,  $f_0$ , has been factored out, thus we obtain

$$ek^4 + 2\nu k^2 \simeq \sum_{n=1}^{\infty} \frac{\bar{a}_n^2 + \bar{b}_n^2}{\lambda_n^2 + (\gamma\omega)^2}. \quad (39)$$

This equation suggests a criterion that determines the range of  $k$  and  $\omega$ . Specifically, once  $k$  is chosen, the equation determines a range of feasible  $\omega$  values around the solution of the equation. Conversely, if  $\omega$  is assigned, a range of feasible  $k$  values can be derived from the equation.

In other words, if  $E(k)$  is too large due to a high value of  $k$ , we introduce too much energy into the system, which must be balanced by choosing a small  $\omega$ , and *vice versa*, if  $k$  is too small, it requires a very large  $\omega$ .

This situation is also critical because, at high frequencies, the system dynamics are significantly attenuated, leading to a decoupling between the flagellum's dynamics and the fast oscillating perturbation: in this regime, the flagellum perceives this rapid oscillation as additional "noise".

### D Anisotropic hydrodynamic drag

In this appendix, we justify neglecting anisotropic effects of the drag coefficient used in our model of flagellar dynamics. The overdamped anisotropic dynamics of the  $i$ -th bead of the flagellum is governed by the stochastic differential equation,

$$\Gamma_i \dot{\mathbf{r}}_i = -\frac{\partial V}{\partial \mathbf{r}_i} + \mathbf{h}_i(t) + \sqrt{2D} \xi_i(t), \quad (40)$$

where the diffusion coefficient  $D$  is proportional to the temperature  $T$ , while  $\Gamma_i$  is the drag tensor projecting the velocity  $\dot{\mathbf{r}}_i$  into components parallel and perpendicular to the local filament axis:

$$\Gamma_i \dot{\mathbf{r}}_i = \gamma_{\parallel} (\dot{\mathbf{r}}_i \cdot \mathbf{t}_i) \mathbf{t}_i + \gamma_{\perp} (\dot{\mathbf{r}}_i \cdot \mathbf{n}_i) \mathbf{n}_i. \quad (41)$$

The coefficients  $\gamma_{\parallel}$  and  $\gamma_{\perp}$  are the drags along the tangent and normal directions, respectively. The vectors  $\mathbf{t}_i$  and  $\mathbf{n}_i$  denote the unit tangent

$$\mathbf{t}_i = \frac{\mathbf{r}_{i+1} - \mathbf{r}_i}{|\mathbf{r}_{i+1} - \mathbf{r}_i|}$$

and normal vector  $\mathbf{n}_i \cdot \mathbf{t}_i = 0$  referred to bead  $i$ , with the boundary condition on the last bead  $\mathbf{t}_{N+1} = \mathbf{t}_N$ .

By inverting  $\Gamma_i$ , or equivalently projecting eqn (40) along  $\mathbf{t}_i$  and  $\mathbf{n}_i$ , we obtain the Brownian dynamics in the anisotropic drag

$$\dot{\mathbf{r}}_i = \left( \frac{1}{\gamma_{\parallel}} - \frac{1}{\gamma_{\perp}} \right) (\mathbf{F}_i \cdot \mathbf{t}_i) \mathbf{t}_i + \frac{\mathbf{F}_i}{\gamma_{\perp}}, \quad (42)$$

where

$$\mathbf{F}_i = -\nabla_i V + \mathbf{h}_i(t) + \sqrt{2D} \xi_i(t)$$

is the total effective force.

Eqn (42) was integrated using the same Euler scheme to obtain the flagellum conformations presented in Fig. 10. The comparison shows that the conformations are weakly affected by drag anisotropy. This observation is further supported by looking at the trajectories of the terminal monomer, which





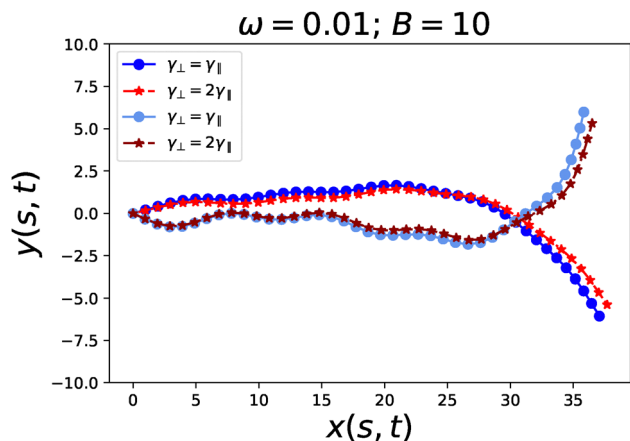


Fig. 10 Snapshots of the flagellum stationary dynamics for isotropic ( $\gamma_{\parallel} = \gamma_{\perp} = 1.5$ ) and anisotropic ( $\gamma_{\parallel} = 1$ ,  $\gamma_{\perp} = 2\gamma_{\parallel}$ ) drag (blue solid lines with circles and red dashed lines with stars, respectively), for a chain of length  $L = Nb$  ( $N = 40$ ,  $b = 1$ ) and bending modulus  $B = 10$ .

form Lissajous figures that remain essentially unchanged, apart from a slight adjustment in their aspect ratio (see Fig. 11).

A similar conclusion could have been derived from the theoretical side by using the WBA. Indeed, let us consider the continuum model, eqn (4),

$$\Gamma \dot{\mathbf{r}} = 2\nu \frac{\partial}{\partial s} \left[ g(|\partial_s \mathbf{r}|) \frac{\partial \mathbf{r}}{\partial s} \right] - \varepsilon \frac{\partial^4 \mathbf{r}}{\partial s^4} + \mathbf{h}(s, t), \quad (43)$$

now, the drag matrix  $\Gamma$  takes the form

$$\Gamma = \gamma_{\parallel} \mathbf{t} \mathbf{t}^T + \gamma_{\perp} \mathbf{n} \mathbf{n}^T \quad (44)$$

denoting, as above by  $\mathbf{t}$  and  $\mathbf{n}$ , the unitary vectors along the tangential and orthogonal directions of the flagellum, respectively.

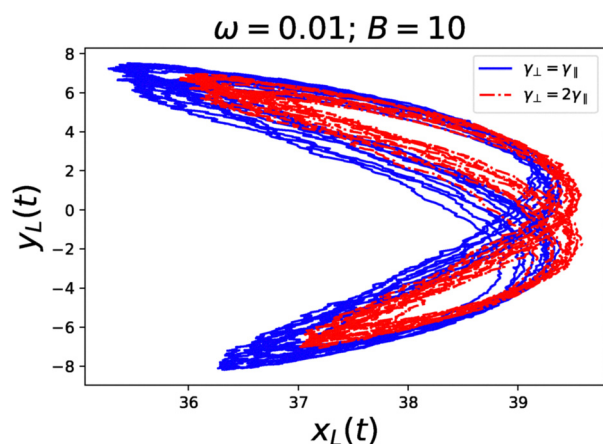


Fig. 11 Trajectory described during the beating process by the position of the tail (last-monomer) of a flagellum with  $N = 40$  monomers of length  $b = 1$ , for isotropic and anisotropic drag ( $p = 0$  blue solid line and  $p = 1$  red dashed line, respectively).

According to eqn (7), when the weakly bending approximation holds,  $\mathbf{t}$  and  $\mathbf{n}$  can be parametrized as

$$\mathbf{t} = \frac{1}{\sqrt{1 + \frac{1}{4}(\partial_s y)^4}} \begin{pmatrix} 1 - \frac{1}{2}(\partial_s y)^2 \\ \partial_s y \end{pmatrix} \quad (45)$$

$$\mathbf{n} = \frac{1}{\sqrt{1 + \frac{1}{4}(\partial_s y)^4}} \begin{pmatrix} -\partial_s y \\ 1 - \frac{1}{2}(\partial_s y)^2 \end{pmatrix}.$$

Inserting these expressions into eqn (44) leads to

$$\Gamma = \begin{pmatrix} \gamma_{\parallel} + p \frac{(\partial_s y)^2}{1 + (\partial_s y)^4/4} & -p \frac{(\partial_s y) [1 - (\partial_s y)^2/2]}{1 + (\partial_s y)^4/4} \\ -p \frac{(\partial_s y) [1 - (\partial_s y)^2/2]}{1 + (\partial_s y)^4/4} & \gamma_{\perp} - p \frac{(\partial_s y)^2}{1 + (\partial_s y)^4/4} \end{pmatrix} \quad (46)$$

thus

$$\Gamma = \begin{pmatrix} \gamma_{\parallel} & 0 \\ 0 & \gamma_{\perp} \end{pmatrix} + \delta \Gamma, \quad (47)$$

where,  $p = \gamma_{\perp} - \gamma_{\parallel}$  and the elements of  $\delta \Gamma$  are at least  $O(\partial_s y)$ . Let us notice that, from eqn (44),  $\Gamma^{-1}$  is easily obtained by substituting  $\gamma_{\parallel}$  and  $\gamma_{\perp}$  with  $1/\gamma_{\parallel}$  and  $1/\gamma_{\perp}$ , arriving at

$$\Gamma^{-1} = \begin{pmatrix} 1/\gamma_{\parallel} & 0 \\ 0 & 1/\gamma_{\perp} \end{pmatrix} + \frac{\gamma_{\perp}^{-1} - \gamma_{\parallel}^{-1}}{1 + \frac{1}{4}(\partial_s y)^4} \times \begin{pmatrix} (\partial_s y)^2 & -(\partial_s y) \left( 1 - \frac{1}{2}(\partial_s y)^2 \right) \\ -(\partial_s y) \left( 1 - \frac{1}{2}(\partial_s y)^2 \right) & -(\partial_s y)^2 \end{pmatrix}. \quad (48)$$

Retaining only terms up to the first order in  $\partial_s y$ ,  $\Gamma^{-1}$  takes the form

$$\Gamma^{-1} = \begin{pmatrix} \frac{1}{\gamma_{\parallel}} & 0 \\ 0 & \frac{1}{\gamma_{\perp}} \end{pmatrix} - \left( \frac{1}{\gamma_{\perp}} - \frac{1}{\gamma_{\parallel}} \right) (\partial_s y) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (49)$$

By applying this tensor to the external force  $\mathbf{h}(s, t)$  we get

$$\Gamma^{-1} \begin{pmatrix} 0 \\ f_0 \sin(ks - \omega t) \end{pmatrix} = \begin{pmatrix} (\gamma_{\parallel}^{-1} - \gamma_{\perp}^{-1}) (\partial_s y) f_0 \sin(ks - \omega t) \\ f_0 / \gamma_{\perp} \sin(ks - \omega t) \end{pmatrix}. \quad (50)$$

Showing that the anisotropic drag leaves unaltered the force along  $y$ . Therefore, the time evolution of  $y(s, t)$  from eqn (4) and (43) are identical at leading order in  $\partial_s y$ , being equal to eqn (9) with  $\gamma$  or  $\gamma_{\perp}$  as drag coefficient. Moreover, since within the weakly bending approximation  $x$  is enslaved to  $y$ , we can



conclude that the overall dynamics is weakly affected by drag anisotropies.

The above theoretical considerations are also confirmed by numerical simulation, as shown in Fig. 10 and 11.

In conclusion, both simulation results and theoretical analysis indicate that drag anisotropy plays a minor role when the system is anchored and unable to swim. In this constrained scenario, the absence of net translation suppresses the influence of anisotropic drag on the flagellum's dynamics and conformations.

## Acknowledgements

The authors are grateful to A. Cavagna for stimulating discussions and his precious remarks and suggestions, we also thank L. Caprini for a critical reading of the manuscript. F. C., A. P., M. V. acknowledge funding from the Italian Ministero dell'Università e della Ricerca under the programme PRIN 2022 ("re-ranking of the final lists"), number 2022KWTEB7, cup B53C24006470006.

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