Dynamics of a semi-flexible polar filament in Stokes flow

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In this work the dynamics and transport of a polarly driven filament is examined using a continuum slender-body model. Immersed in a viscous fluid, the filament gains polar propulsion from the motor proteins (anchored on the motility assay) while experiencing a viscous drag from the bottom wall. Results from the linear analysis on a straight polar filament illustrate the necessity of spatial inhomogeneity in the polar forcing for the buckling instability. The ensuing buckling leads to filament deformation, undulation, and change of its direction of motion in the numerical simulations. Repeated filament buckling in two types of motor protein concentration landscape results in diffusive transport of a polar filament on scales much larger than the mean-free-path and the average duration between filament buckling events.

I. INTRODUCTION

Many bio- and nano-fluidic systems involve conversion of chemical energy to mechanical work for transport at small scales. For example, nano-motors are bi-metallic catalytic nanowires that mobilize in a fluid environment in the presence of a \( \text{H}_2\text{O}_2 \) fuel [1, 2]. The average velocity of these chemically-powered nanowires can be controlled by switching the applied potential in a 5% (wt) \( \text{H}_2\text{O}_2 \) solution ([3] and references therein). In the “in vitro” motility assays, microtubules (or actins) are driven by kinesins (or myosins), which convert the chemical energy of ATP (adenosine triphosphate) hydrolysis into mechanical work [4–6]. In some of these in vitro studies the fluorescence microscopy is used for the analysis of actin filament motions at different temperatures and myosin coverage. The actin filaments lie in the plane of the motility assay and experience pulling forces from the myosins that are bound to them. Despite the thermal fluctuations and the randomness in the myosin pulling forces, the actin filaments move along straight lines until they encounter “defects” in the myosin concentration, around where the actin filaments deform, change direction of motion, and resume the straight line motion with a deflected angle. Depending on the temperature and myosin coverage, two types of actin filament motion are observed [5]: The first type is a homogeneous flow of actin filaments with well defined velocities at high myosin concentration and high temperature. The second type is actin filament motion with a wide velocity distribution at low myosin concentration and temperature. In addition the swirling of an actin filament around the defects in motility assays gives direct measurement of the polar force from the myosin-ATP cycle, and its duty ratio can be deduced by varying temperature and the myosin surface density [4].

The principal mechanism for transport of actins or microtubules in the motility assays has been utilized in emerging nanotechnology for directed transport of molecules and nanometer-sized cargoes in cellular-size synthetic devices [7–12]. Results from these studies are essential for direct molecular assembling, sorting and sensing [13–15]. By integrating motor proteins into synthetic devices, one can assemble a shuttle system where nanoscale cargo is transported between user-defined locations for specific nano-cargo delivery. Designing efficient tracks for such transport is a critical step in developing molecular shuttle systems, where tracks for motor proteins are derived from standard motility
assays. In addition, surface topography and coating of poly(methyl methacrylate) and polyurethan have also been used to help guide filaments on myosin- and kinesin-coated tracks, respectively. New technologies have been developed for guiding the filaments by aligning filaments parallel to the track patterns. For better guiding of the polar filaments in the tracks, the interaction between filaments and the sidewalls has been quantified in terms of track geometry (channel width), collision rate of filament with the sidewalls, and the filament approach angle [11]. Many of the derived relationships for guiding in polyurethane channels apply for other surface fabrication methods. Based on experimentally determined parameters (such as the trajectory persistence length of a polar filament in a channel), Monte-Carlo simulations have been conducted to aid the design of nanoscale transport systems that involve both actins and microtubules [16, 17].

Hydrodynamic flows [18] and electric fields [19] have also been used to actively guide microtubules on the kinesin-coated surface. Hydrodynamic shear flows align microtubules in the shear direction by the viscous drag. Electric fields steer microtubules to align with the electric field lines. Under these external forces, the microtubule bends like a loaded cantilever: Because the binding to motor proteins is weaker near the filament head, sufficiently strong drag force (due to shear flow) or electric force (due to electric field) can bend the microtubules, which then deflect and align with the forcing direction. Various combinations of shear flow strength and motor concentration have been used to study the effects of shear flow and electric fields on the microtubule transport.

These developments in designing the integrated microdevices for guiding polar filament motion encourage more understanding of the detailed dynamics of a polar filament in a patterned forcing landscape without the external guiding force. Surprisingly very little quantitative knowledge can be found in the current literature to address the following questions: What is the underlying physical mechanism for deformation and deflection of a polar filament around defects in the assay? What is the consequence of such dynamics of polar filaments in terms of their transport across space? How important is the inhomogeneity in filament-protein binding to the filament dynamics and transport? These issues will be addressed in this study, and the results will help design better synthetic microdevices.

Buckling of an elastic filament is observed to affect the filament transport in an idealized cellular flow that consists of a doubly periodic array of stagnation points [20] where the filament experiences large compression from the fluid and the filament buckles and rotates. Such filament dynamics around the stagnation points is termed the “stretch-coil” transition. Repeated “stretch-coil” transitions lead to diffusive filament transport whose characteristic length and time are associated with the filament motion in the cellular flow [20]. One of the main goals of the present study is to examine if/how such filament buckling dynamics can be found for polar filaments in a patterned forcing landscape without any external guiding forces. If yes, how would the resultant filament deformation affect the filament transport? Our study shows that polar filament does buckle under a supercritical polar forcing, and the long-time transport of buckling polar filament in a given forcing landscape can be characterized by the “mean-free-path” (in the forcing landscape) of the polar filament between buckling events.

In this paper the dynamics of a polar filament (such as F-actin or microtubule) driven by a forcing landscape (concentration of molecular proteins) is modeled within the slender-body framework for the fluid-body interaction. The model formulation is given in § II, followed by a stability analysis in § III where we focus on how a polar filament may be susceptible to buckling instability due to (a) the spatial variation in the forcing landscape and (b) partial detachment between the filament and the motor proteins. Results from numerical simulations of filament buckling in both cases are presented in
§ IV. Quantification of the transport due to buckling polar filament is presented in § V, and conclusion is given in § VI.

II. FORMULATION

For the polar actin filaments in the motility assay filled with a viscous fluid, the typical aspect ratio $\epsilon \equiv R/L$ is in the range $1.5 \times 10^{-4} \leq \epsilon \leq 3 \times 10^{-3}$ and the Reynolds number $Re \equiv UL/\nu \sim 10^{-8}$ (with a typical radius $R \sim 3$ nm a typical contour length ($L$) ranging from $1 \mu$m to $20 \mu$m, a fluid viscosity $\nu \sim 1 \text{cm}^2/\text{s}$ and the filament speed $U \sim 1 \mu$m/s). Such small Reynolds number and small filament aspect ratio allow us to model the polar filament as a slender body in a Stokesian fluid that contains the anchored motor proteins in the assay \cite{4, 5, 21–23}. Free motor proteins (heavy meromyosin for actin filaments and kinesin for microtubules) bind to the polar filaments and can crawl along the polar filament as they make power strokes through cycles of ATP hydrolysis. In the motility assays, the motor protein molecules (myosin proteins are of length $\sim 100$ nm) are actuated on the assays (on a layer of the nitrocellulos for myosins), therefore the collective forces from the motor power strokes propel the filament to glide on the assay \cite{24, 25}. With the typical gliding speed in the range of $1 \sim 10 \mu$m/sec, the filament dynamics is governed by the balance between power strokes from the motor proteins, anti-bending force and hydrodynamic drag due to the strong viscous dissipation in Stokes flows. All three forces are much larger than the thermal fluctuations under normal conditions (i.e., the typical actin persistence length $l_p$ is comparable to their contour length $l_p \sim L$).

In our formulation the propelling force from the motor protein power strokes is modeled as a continuum polar force, pointing from filament tail to filament head. The amplitude of the continuum polar force is proportional to the local motor concentration. Ignoring other external forcing (such as gravity) and inertia effects (low-Reynolds number flows), the incompressible Stokes equations are appropriate to describe the dynamics of the polar filaments in the motility assays. In addition, the filaments are assumed to be gliding at a constant distance ($\leq 100$ nm for the actin-myosin system) above the assay bottom wall. In the experiments ($\cite{26}$ and references therein) the gliding filament motion is found to be almost two-dimensional, confined in the plane of motility assay with small fluctuations in the filament distance to the bottom wall. At this distance the interaction between the gliding polar filament and the bottom wall should be taken into account. Figure 1 is the schematic sketch that summarizes the configuration of in vitro experiments on the motility assay.

The velocity field around the slender ($\epsilon \ll 1$) filament immersed in the Stokesian fluid (no inertia effects) can be expressed in the boundary integral formulation. Expanding the velocity field in $\epsilon$ and applying the matched asymptotics to evaluate the velocity field on the filament surface, the equation of motion for the filament centerline is of order $O(\epsilon^2 \log(\epsilon))$. The complete slender-body equations are a system of nonlinear, non-local integro-differential equations similar to those in \cite{27}. The method of images \cite{28} is utilized to incorporate the interaction between the polar filament and the bottom wall. The slender-body equations are rendered dimensionless by using $L$ for the length unit, $8\pi\mu L^4/(-cE)$ for the time unit ($\mu$ is the fluid viscosity) and $E/L^2$ for the line tension (or force) unit. $x(s)$ is the center-line position of the filament parameterized by arclength $s \in [0, 1]$. The filament slenderness $\beta$ is defined as $\beta \equiv \frac{1}{\ln(\epsilon \cdot e)}$: $\beta = 0$ for infinitely slender filaments and $0.06 \leq \beta \leq 0.10$ for actin filaments. Throughout the paper the subscript $s$ denotes the derivative with respect to arclength. The dynamics
of the filament interacting with the bottom wall is given by the following dimensionless equations \[27\]
\[
\frac{\partial \mathbf{x}}{\partial t} = [(1 + 2\beta)\mathbf{I} + (1 - 2\beta)\mathbf{x}_s \otimes \mathbf{x}_s] \mathbf{f} - \beta \mathbf{K} + \beta I',
\]
with $\mathbf{I}$ the identity tensor and $\mathbf{x}_s \otimes \mathbf{x}_s$ a dyadic product. The term $I'$ is for the interaction with the bottom wall. The force-free boundary conditions give $\mathbf{x}_{ss} = \mathbf{x}_{sss} = 0$ at the filament end points. The line force density $\mathbf{f}$ consists of the polar forcing from motor proteins, a bending force and a tensile force that enforces filament inextensibility
\[
\mathbf{f}(s) = - (T(s)\mathbf{x}_s)_s + \mathbf{x}_{ssss} + \alpha \mathbf{F}(\mathbf{x})\mathbf{x}_s.
\]
$T(s)$ is the line tension, $\alpha \equiv \frac{F_a L_s^3}{E}$ is the polar forcing amplitude and $\mathbf{F}(\mathbf{x})$ is the polar forcing profile that may vary along the filament.

The self hydrodynamic interaction $K$ is given by the finite-part integral
\[
K = \int_0^1 \left( \frac{\mathbf{I} + \hat{\mathbf{R}}(s,s') \otimes \hat{\mathbf{R}}(s,s')}{|\mathbf{R}(s,s')|} \mathbf{f}(s') - \frac{\mathbf{I} + \mathbf{x}_s(s) \otimes \mathbf{x}_s(s)}{|s - s'|} \mathbf{f}(s) \right) ds'.
\]
The method of images gives the contribution from interaction with the filament image
\[
I' = - \int_0^1 \frac{\mathbf{I} + \hat{\mathbf{R}}'(s,s') \otimes \hat{\mathbf{R}}'(s,s')}{|\mathbf{R}'(s,s')|} \mathbf{f}'(s') ds' - 2h^2 \mathbf{PD}[\mathbf{g}] + 2h \mathbf{SD}[\hat{\mathbf{e}}_w, \mathbf{g}],
\]
where $\hat{\mathbf{e}}_w$ is the unit normal vector of the bottom wall as shown in figure 1. $\mathbf{PD}$ is the contribution from a potential dipole image with $\mathbf{g} = 2(\mathbf{f}' \cdot \hat{\mathbf{e}}_w)\hat{\mathbf{e}}_w - \mathbf{f}'$
\[
\mathbf{PD}[\mathbf{g}] = \int_0^1 \frac{\mathbf{g}}{|\mathbf{R}'(s,s')|^3} ds' - \int_0^1 \frac{(\mathbf{g} \cdot \hat{\mathbf{R}}'(s,s'))\hat{\mathbf{R}}'(s,s')}{|\mathbf{R}'(s,s')|^3} ds'.
\]
$\mathbf{SD}$ is the contribution from a Stokeslet doublet
\[
\mathbf{SD}[\hat{\mathbf{e}}_w, \mathbf{g}] = \int_0^1 ds' \frac{1}{|\mathbf{R}'(s,s')|^2} \left[ (\hat{\mathbf{e}}_w \cdot \mathbf{g})\hat{\mathbf{R}}'(s,s') + (\hat{\mathbf{e}}_w \cdot \hat{\mathbf{R}}'(s,s'))\mathbf{g} - (\mathbf{g} \cdot \hat{\mathbf{R}}'(s,s'))\hat{\mathbf{e}}_w 
- 3(\hat{\mathbf{e}}_w \cdot \hat{\mathbf{R}}'(s,s'))(\mathbf{g} \cdot \hat{\mathbf{R}}'(s,s'))\hat{\mathbf{R}}'(s,s') \right],
\]
In the above integrals $\mathbf{R}(s,s') = \mathbf{x}(s) - \mathbf{x}(s')$ and $\mathbf{R}'(s,s') = \mathbf{x}(s) - \mathbf{x}'(s')$ as sketched in Figure 1, $\hat{\mathbf{R}}(s,s') = \mathbf{R}(s,s')/|\mathbf{R}(s,s')|$ and $\hat{\mathbf{R}}'(s,s') = \mathbf{R}'(s,s')/|\mathbf{R}'(s,s')|$. The inextensibility condition of the filament $\mathbf{x}_s \cdot \mathbf{x}_s = 1$ gives the equation for the line tension
\[
2T_{ss} - (1 + 2\beta)(\mathbf{x}_{ss} \cdot \mathbf{x}_{ss})T = - \beta \mathbf{x}_s \cdot \frac{\partial}{\partial s} (-K + I') - (7 + 2\beta)(\mathbf{x}_{ss} \cdot \mathbf{x}_{ssss})
- 6(\mathbf{x}_{ssss} \cdot \mathbf{x}_{ssss}) - 2\alpha \mathbf{F}_s,
\]
subject to the force-free boundary condition $T(s = 0,1) = 0$.

The collective magnitude of all the polar forces from the motor proteins is $\alpha = f \tilde{r} \sigma$, where $f$ is the force from a single motor between the average distance $\tilde{r}$, and $\sigma$ is the surface density of the motor proteins [5]. $f \sim 3$ pN for myosin-actin interaction over the distance 1 nm $< \tilde{r} < 1.5$ nm, and 1 $\mu$m$^{-2} \leq \sigma \leq 1000$ $\mu$m$^{-2}$. The rigidity for semi-flexible bio-filaments (such as actins and microtubules) is in the range 1 $\leq E \leq 30 \times 10^{-24}$ N$\cdot$m$^2$ [29]. For filament of length 1 $\mu$m $\leq L \leq 10$ $\mu$m the dimensionless parameter $\alpha$ is in the range $10^{-4} < \alpha < 10^4$. The typical shape parameter is in the range 0.03 $\leq \beta \leq 0.27$ for bio-polymers. Small values of $\beta$ correspond to very slender filaments, for which the hydrodynamic interactions are weak. For the following simulation results we set $\beta \leq 0.1$ as we focus on the effects of HIs for slender filaments suitably described by the slender-body theory.
FIG. 1: Schematic sketch of the \textit{in vitro} experiment of actin filaments in the motility assay. The filament \( x(s) \) is driven by the myosins motor proteins anchored on the assay. \( \hat{e}_w \) is the unit normal vector on the motility assay plane, and \( h \) is the distance between the actin and the wall. \( \mathbf{x}'(s) \) (dashed line) is the image of the filament on the other side of the assay.

III. DYNAMICS AND STABILITY OF A STRAIGHT POLAR FILAMENT

In this section we focus on the dynamics of a straight, infinitely slender filament \((\epsilon \to 0)\). In this limit \( \beta \to 0 \) and the interaction with the bottom wall can be ignored. We investigate how a straight polar filament moves in a spatially varying forcing landscape, and the condition for it to undergo the buckling stability. For a straight filament the centerline position is

\[
x(s, t) = \mathbf{x}_c(t) + \left( s - \frac{1}{2} \right) \hat{e} = \mathbf{x}_c(t) + \left( s - \frac{1}{2} \right) (\cos(\theta(t)), \sin(\theta(t)), 0),
\]

where \( \mathbf{x}_c \) is the position of the filament center, \( \hat{e} \) is the unit tangent of the straight filament, \( s \in [0, 1] \) is the arclength, and \( \theta(t) \) is the filament angle with respect to the horizontal axis. Substituting equation 8 into equation 1 gives

\[
\dot{\mathbf{x}}_c + \left( s - \frac{1}{2} \right) \dot{\theta}(- \sin \theta, \cos \theta, 0) = 2(T_s + \alpha F)(\cos \theta, \sin \theta, 0),
\]

\[
(T_s + \alpha F)_{x_3} = 0.
\]

Combining equations 9-10 we find that for a straight filament (1) the angle remains constant \( \dot{\theta} = 0 \), and (2) the velocity \( \dot{\mathbf{x}}_c \) for any forcing landscape \( \alpha F \). In addition, the line tension for a straight polar filament in any given forcing landscape \( \alpha F \) is computed by the integral

\[
T(s) = - \int_0^s \alpha F \left( \mathbf{x}_c(t) + s' \hat{e} \right) ds' + \frac{1}{2} Us,
\]

where the filament speed \( U \equiv \dot{\mathbf{x}}_c(t) \cdot \hat{e} \) can be computed from the force-free boundary condition \( T(s = 1) = 0 \) as

\[
U = 2 \int_0^1 \alpha F \left( \mathbf{x}_c(t) + s' \hat{e} \right) ds'.
\]
Equation 12 is the force-velocity relationship for a straight polar filament in a forcing landscape specified by the local motor protein concentration $\alpha F$. For a uniform motor concentration $F(x) = 1$, a straight polar filament travels along its tangent direction at a constant speed $U = 2\alpha \int_0^1 ds' = 2\alpha$, and the line tension $T = 0$ from equation 11. From this we conclude that a straight filament in a spatially uniform polar forcing landscape is always stable, and travels at a constant speed along its polar direction.

We perturb the straight filament by $\varepsilon \hat{x}$ with the small parameter $\varepsilon \ll 1$, and $\varepsilon \hat{T}$ and $\varepsilon \hat{F} = (\nabla F) \cdot \varepsilon \hat{x}$ are the corresponding disturbances in tension and polar forcing:

$$\mathbf{x} = \mathbf{x}_c + s \hat{e} + \varepsilon \hat{x}, \quad T \to T + \varepsilon \hat{T}, \quad F \to F + \varepsilon \hat{F}. \tag{13}$$

Linearizing equations 1 and 7 with respect to the disturbances, we obtain the linear equations for disturbances $\hat{x}$ and $\hat{T}$

$$\begin{align*}
\hat{x}_t &= 2(T_s + \alpha F) \hat{x}_s + T \hat{x}_{ss} - \hat{x}_{ssss} + 2 \left( \hat{T}_s + \alpha \hat{F} \right) \hat{e}, \tag{14} \\
\hat{T}_{ss} &= -\alpha \hat{F}_s. \tag{15}
\end{align*}$$

Enforcing the inextensibility at the linear order, we obtain $\hat{e} \cdot \hat{x}_{st} = 0$ and $\hat{e} \cdot \hat{x}_s = \hat{e} \cdot \hat{x}_{ss} = \hat{e} \cdot \hat{x}_{ssss} = 0$. Projecting equation 14 against $\hat{e}$ we find

$$\hat{e} \cdot \hat{x}_t = 2 \left( \hat{T}_s + \alpha \hat{F} \right). \tag{16}$$

Combining equations 15 and 16 gives $\hat{e} \cdot \hat{x}_t = \text{constant}$ in time and space. This implies that $\hat{T}_s + \alpha \hat{F} = 0$ for non-trivial disturbance $\hat{x}(s,t)$, and equation 14 can be simplified to

$$\begin{align*}
\hat{x}_t &= 2(T_s + \alpha F) \hat{x}_s + T \hat{x}_{ss} - \hat{x}_{ssss} = U \hat{x}_s + T \hat{x}_{ss} - \hat{x}_{ssss}, \tag{17}
\end{align*}$$

where $T$ and $2(T_s + \alpha F) = U$ are given in equations 11 and 12, respectively. In a nonuniform forcing landscape, both $U$ and $T$ vary with time (via $\mathbf{x}_c(t)$) and the linear equation 17 is nonautonomous, thus cannot be solved as an eigen system for the linear stability. Further progress for the linear stability analysis can be made for the following two cases: (1) A spatially periodic forcing landscape, and (2) a partially detached filament in a uniform forcing landscape. For the spatially periodic forcing landscape, the linear system can be studied using the Floquet theory for multi-dimensional systems. For the partially detached filament in a uniform forcing landscape, $U$ and $T$ no longer depend on time, and equation 17 reduces to an autonomous eigen system where eigenvalues can be computed for the linear stability/instability.

**A. Periodic Spatial Variation in Motor-Protein Concentration**

In the experiments actins are found to deform around the defects (large concentration variation) in the motility assay. The deformed actins change their direction of motion, and sometimes get trapped and swirl around the defects. To better design the motility assays for efficient filament transport, it is important to elucidate the effects of spatial variation in the polar forcing on the filament dynamics in order to avoid trapping or stalling of filaments. For this purpose we consider an idealized case where
the forcing landscape has a sinusoidal fluctuation with an amplitude $\delta$ and a characteristic length $W/L = 2\pi/k$

$$F(x) = 1 + \delta \cos(kx).$$

(18)

This forcing landscape varies along $\nabla F/|\nabla F| = (1, 0, 0)$, and the filament angle is defined as $\theta = \cos^{-1}(e \cdot \nabla F/|\nabla F|)$. For $\theta \neq \pi/2$, a straight polar filament (equation 8) moves with the following speed $U$ and line tension $T$

$$\dot{x}_c = U(t) = 2\alpha \left(1 + \frac{\delta}{k \cos \theta} g(1)\right),$$

(19)

$$T(s) = -\frac{\alpha \delta}{k \cos \theta} (g(s) - sg(1)),$$

(20)

$$g(s) = \sin(k(x_c(t) + \left(s - \frac{1}{2}\right) \cos \theta)) - \sin(k(x_c(t) - \frac{\cos \theta}{2})), $$

(21)

where $x_c(t)$ is $x$-coordinate of the filament center.

For a straight filament orthogonal to the forcing gradient ($\theta = \pi/2$), the filament moves along the $y$-axis at a constant speed $U = 2\alpha \left(1 + \delta \cos(kx_c)\right)$ and the line tension $T = 0$, as expected for a constant polar forcing. For a straight filament parallel to the forcing gradient ($\theta = 0$) the filament speed versus filament center positions is shown in figure 2(a), and figure 2(b) shows the line tension at four different filament center positions. The forcing amplitude $\alpha = 1000$ and variation magnitude $\delta = 0.1$. At $x_c = \pi/2$ the line tension (equation 20) is negative as shown in figure 2(b). This illustrates that the spatial variation in the forcing is essential to the buckling instability of a straight polar filament.

For the periodic forcing landscape in equation 18, the filament speed $U$ and tension $T$ (equations 19-20) are periodic in time: $U(t + p) = U(t)$ and $T(s, t + p) = T(s, t)$, where the periodicity $P$ is determined from the condition $x_c(t + P) - x_c(t) = 2\pi/k$. In this case equation 17 is a periodic partial differential equation that can be cast to a linear system of periodic ordinary differential equations for the amplitude $a_i(t)$ in the expansion $\dot{\mathbf{x}} = \sum_i a_i(t) \phi_i(s)$: Substituting this expansion into equation 14 and projecting it against the orthonormal base functions we obtain a system of linear, nonautonomous periodic differential equations

$$\frac{da_i}{dt} = \sum_j A_{ij}(t)a_j = \sum_j A_{ij}(t + P)a_j.$$  

(22)

The base functions $\phi_i$ satisfy

$$\phi_{i\text{ssss}} - \lambda_i^4 \phi_i = 0,$$

(23)

with boundary conditions $\phi_{i\text{ss}} = \phi_{i\text{sss}} = 0$ at $s = 0$ and $s = 1$. $\lambda_i$ are roots of the equation

$$\cos(\lambda_i) \cosh(\lambda_i) - 1 = 0.$$  

(24)

Explicitly $\phi_i$ is the linear combination

$$\phi_i(s) = \alpha_i (\cos(\lambda_i s) + \cosh(\lambda_i s)) + \beta_i (\sin(\lambda_i s) + \sinh(\lambda_i s)),$$

(25)

with $\alpha_i$ and $\beta_i$ satisfying

$$\frac{\alpha_i}{\beta_i} = -\frac{\sin(\lambda_i) + \sinh(\lambda_i)}{\cos(\lambda_i) - \cosh(\lambda_i)} \quad \text{and} \quad \int_0^1 \phi_i^2 ds = 1.$$  

(26)
For the nonautonomous system in equation 22, the corresponding initial value problem for the fundamental matrix is

$$\frac{d}{dt} \Phi = A(t) \Phi, \quad \Phi(t_0, t_0) = I,$$

where $I$ is the identity matrix, and the two indexes in $\Phi(t, t_0)$ mean that the solution of the original system with initial value $x(t_0) = x_0$ is simply given by $x(t) = \Phi(t, t_0)x_0$. The periodic system is absolutely unstable if the largest eigenvalue of the matrix $\Phi(t_0 + P, t_0)$ is greater than unity. The $i$-th column of the matrix $\Phi(P, 0)$ is the solution of the equation 22 integrated from $t = 0$ to $t = P$ with initial value $a_j(t = 0) = \delta_{ij}$. Figure 3(a) shows the typical solution after integration over one period. The perturbation magnitude grows initially until the forcing gradient turns positive in the second half of the period, when the perturbation magnitude decays. Absolute instability is possible when $a(P)/a(0) > 1$, which corresponds to at least one eigenvalue (of $\Phi(P, 0)$) larger than unity. Figure 3(b) shows the critical forcing amplitude $\alpha_c$ for the onset of the absolute instability in the periodic forcing profile with $k = 1$ in equation 18 and filament angle $\theta = 0$ in equations 19-20.

The oscillation of $a_{10}(t)/a_{10}(0)$ in the example of figure 3(a) is found for all other values of $\delta$ in figure 3(b). The amplitude amplification reaches maximum when $x_c \sim \pi/2$, the location where the line tension is most negative. Despite the large amplitude amplification in figure 3(a), the filament angle remains constant at all time at the linear order in our model which does not include any external torque exerted from the motors. This is because (1) the inextensibility is enforced at the linear order, and (2) the small parameter $\varepsilon$ can be rendered as small as needed for the validity of equation 17. The polar filament can change its angle $\theta$ (or its direction of motion) only through nonlinear interactions (such as the term $\dot{\mathbf{x}}_s \cdot \dot{\mathbf{x}}_s$) in our model. Furthermore, we also note that the amplitude amplification in figure 3(a) is fast compared to the periodicity: The initial growth rate is $\sim 35(1/P)^{-1}$ which means the e-folding time is about $0.029P$, much shorter than a period in figure 3(a). Such fast amplitude amplification implies that the time variation in $\mathbf{x}_c(t)$, $U$ and $T$ may be ignored, and equation 17 can be solved as an eigenvalue problem for $\dot{\mathbf{x}}(s, t)$ at a fixed filament center location $\mathbf{x}_c$ with the corresponding $U$ and $T$. Then each component of $\dot{\mathbf{x}}(s, t)$ takes the form $y(s)e^{\lambda t}$, with $y(s)$ satisfying the boundary conditions $y_{ss} = y_{sss} = 0$ at the end points.

The “quasi-steady” eigen equation for $y$ is solved numerically for the simple forcing landscape (equation 18) characterized by $\delta$ and $k$: $\delta$ quantifies the forcing fluctuation, and $2\pi/k = W/L$ is the ratio of forcing length scale to filament contour length. Figure 2(b) shows that the filament experiences most compression from the forcing gradient at $x_c = \pi/2$. Figure 4(a) shows the dependence of the critical forcing amplitude $\alpha_c$ on $\delta$ with $\theta = 0$, $k = 1$ and $x_c = \pi/2$. For a value of forcing fluctuation $0 \leq \delta \leq 1$, the straight filament undergoes buckling instability for $\alpha \geq \alpha_c$. The straight filament remains stable for $\alpha < \alpha_c$. The filament is more susceptible to buckling instability for larger concentration fluctuation $\delta$. The inset shows the $\theta$-dependence of $\alpha_c$ with $\delta = 0.5$. $\alpha_c$ increases with $\theta$ and approaches infinity $\alpha_c \to \infty$ as $\theta \to \pi/2$: The straight polar filament is absolutely stable when it is orthogonal to the forcing gradient. The critical forcing amplitudes in figure 4(a) are much smaller than those for the absolute instability in figure 3(b). This is because the initial growth in the quasi-steady analysis does not guarantee $a(P)/a(0) > 1$ for the absolute instability. In the experiments or simulations, the initial perturbation amplitudes are always finite. Therefore the linear assumption in the Floquet analysis is no longer valid when the perturbation grows to $\sim 1/\varepsilon$, where $\varepsilon$ is the initial perturbation amplitude. As will be shown in § IV, buckling leads to large filament deformation within one period, and the filament angle changes as a result of the nonlinear interactions.
FIG. 2: (a) Speed of a straight filament as a function of filament center $x_c$ with $\alpha = 1000$, $\delta = 0.1$, $k = 1$ and filament angle $\theta = 0$. (b) The corresponding line tension as a function of $s$ at different filament positions with $\alpha = 1000$ and $\delta = 0.1$.

FIG. 3: (a) $a_{10}(t)/a_{10}(0)$ as a function of time for $\theta = 0$, $\delta = 0.2$, $\alpha = 10^5$ and $k = 1$. $a_{10}(0) = 1$ and $P$ is the periodicity of $A(t)$. (b) The critical forcing amplitude $\alpha_c$ versus $\delta$ for the absolute instability in equation 22 with $\theta = 0$ and $k = 1$ in equations 18,19 and 20.

Figure 4(b) shows the variation of $\alpha_c$ with filament location in the forcing landscape: The filament is most unstable at $x_c = \pi/2$ where the compression and the line tension are most negative (dotted line in Figure 2(b)) and the corresponding $\alpha_c$ is minimum. At $x_c = 0$ the line tension oscillates between positive and negative values (solid line in Figure 2(b)), and thus a larger critical forcing amplitude at this location. The inset shows the dependence of $\alpha_c$ on the length ratio $W/L$: The filament is most unstable (minimum $\alpha_c$) when $W/L \approx 1.5$. For smaller forcing length scales, the filament becomes more stable (larger $\alpha_c$) because the polar forcing cancels over multiple periods. For large forcing length scales ($W/L \gg 1$) the critical forcing amplitude is proportional to the length ratio: $\alpha_c \propto W/L = \phi(\delta)W/L$, where $\phi(\delta)$ is the prefactor that depends on $\delta$ and filament angle $\theta$ only. This scaling relation implies that the straight filament is susceptible to buckling instability if the filament...
length is sufficiently large

\[ L > \sqrt[3]{\frac{\alpha E L \delta}{F_0}} \]

(28)

for a given filament rigidity \( E \), line density of forcing \( F_0 \) and constant length ratio \( W/L \). The above scaling for buckling instability is similar to that obtained in Karpeev [23] if \( F_0 \) is substituted.

Alternatively, equation 28 also implies a critical filament length \( L_c \) above which the straight polar filament is linearly unstable:

\[ L > L_c \equiv \sqrt[4]{\frac{\phi(\delta) E W}{F_0}}. \]  

(29)

B. Effects of Partial Detachment of Motor Proteins

Results in § IIIA show that the spatial gradient in the polar forcing is essential for the buckling instability of a straight filament. Such spatial variation can also be caused by the non-homogeneous motor binding to the filament. In experiments where microtubule transport is directed by an electric field or a shear flow [18, 19], the microtubules are often found to detach from the kinesin motors near the filament heads. For example, when the direction of electric field is changed, the microtubule head is found to detach from the kinesin proteins so it can bend to align with the electric field. This implies that the binding to the motor proteins is not homogeneous, and the microtubule head can be completely detached from the proteins. In our model, such inhomogeneous binding with the motor proteins leads to a gradient in polar forcing profile along the filament as shown in figure 5(a), where the polar forcing profile \( F(s) \) (or degree of attachment) is modeled as

\[ F(s) = \frac{1}{2} \left[ 1 + \tanh(\gamma(1 - \delta L - s)) \right], \]  

(30)
FIG. 5: (a) Schematics of the detached filament head. $\delta L$ is the length of detachment: $F = 1$ for complete attachment while $F = 0$ for detachment of the motor proteins from the filament. (b) Critical forcing amplitude $\alpha_c$ as a function of $\delta L$.

with $\delta L$ the detachment length (see figure 5(a)), and $1/\gamma$ the length of the transition layer between bound and unbound segments.

The line tension and filament speed can be computed from equation 11 as

$$U = \alpha \left[ 1 - \frac{1}{\gamma} \ln \left( \frac{\cosh (\gamma \delta L)}{\cosh (\gamma (1 - \delta L))} \right) \right],$$

$$T(s) = -\frac{\alpha}{2\gamma} s \ln \left( \frac{\cosh (\gamma \delta L)}{\cosh (\gamma (1 - \delta L))} \right) + \frac{\alpha}{2\gamma} \ln \left( \frac{\cosh (\gamma (1 - \delta L - s))}{\cosh (\gamma (1 - \delta L))} \right).$$

Equation 32 shows that the partial detachment near the filament head always leads to negative line tension. For large $\delta L$ we can reasonably expect the line tension to be sufficiently negative for the buckling instability. The linear analysis in § IIIA is repeated for the partially detached polar filament with the forcing profile in equation 30. Figure 5(b) shows the critical forcing amplitude as a function of $\delta L$ with $\gamma = 40$. For very small detachment length $\delta L \to 0$ the straight filament becomes absolutely stable and $\alpha_c \to \infty$.

C. Wall Effect on the Sliding Speed and Buckling Dynamics of a Single Straight Filament

In the motility assay the filament distance $h$ to the bottom wall is no larger than $1/10$ of the filament contour length, a limit set by the maximum length of the motor proteins that are actuated on the assays. As a result equation 12 is no longer valid when the filament-wall interaction is taken into account, and the filament speed $U$ depends on filament slenderness $\beta$ and the distance $h$. Such dependencies are illustrated in figures 6 (a) and (b) from simulation for a single filament of length $L = 1$ in a constant polar forcing landscape with $\alpha = 10$.

Figure 6(a) shows that, at a fixed distance $h = 0.01$, the filament speed $U$ is inversely proportional to $\beta$ ($U = 20$ for $\beta = 0$ as predicted by equation 12.) At a fixed distance, the interaction between the
filament and the wall increases in magnitude with $\beta$, and consequently the filament speed $U$ decreases due to the increasing drag force from the bottom wall. For a typical value of filament slenderness $\beta = 0.08$ (typical for the actin filaments), the filament speed increases with the distance to bottom wall $h$ as shown in the inset of figure 6(b). The ratio $\alpha/U$ is plotted as a function of distance to the wall. The dashed line in figure 6(b) is the drag coefficient along the long axis of the filament in the absence of the wall.

Results in figures 6 suggest that the interaction with the wall reduces the gliding velocity, and hence the straight polar filament becomes more stable. For example, in the sinusoidal forcing landscape (equation 18) the critical forcing amplitude $\alpha_c \sim 105$ for $W/L = \pi/2$ in the absence of the bottom wall. In the presence of the bottom wall and with a filament slenderness $\beta = 0.08$ (which corresponds to an aspect ratio of $\epsilon \sim 1/1000$), $\alpha_c \sim 133$ at $h = 0.1$ and $\alpha_c \sim 265$ at $h = 0.01$ from the numerical simulation of the straight filament motion. Thus we conclude that interaction with the wall has stabilizing effects on the buckling of the filament: The closer the filament is to the wall, the higher the critical forcing amplitude $\alpha_c$ for buckling instability.

IV. BUCKLING OF A POLAR FILAMENT

The dimensionless slender-body equations, equations 1-7, are re-cast in terms of a curvature in the natural coordinate system along the centerline via the Hasimoto transformation [30–32]. The resultant fourth-order nonlinear integro-differential equation for the complex curvature and the second-order equation for the line tension are discretized using a second-order semi-implicit time-stepping scheme, and second-order divided differences to discretize the spatial derivatives. The self-interaction integral $K$ (equation 3) is regularized using the scheme [27] that is consistent with the spatial discretization.
FIG. 7: Snapshots of a filament undergoing buckling instability with $L = 1$, $W/L = \pi/2$ and $\alpha = 3000$. Time goes from top to bottom then left to right, and the filament deformation travels from head to tail. The direction of filament translation is altered due to the buckling instability.

scheme. The filament centerline position is reconstructed from the complex curvature and the three unit vectors in the natural coordinate system with the updated filament end points from the markers. More details of the numerical implementation can be found in [33]. In the following we present results from the numerical simulations of a polar filament that undergoes buckling instability in different forcing landscapes: In § IV A we show buckling dynamics in a forcing landscape that varies periodically. In § IV B we show how a partially detached filament buckles in a constant forcing landscape.

A. A polar filament in a sinusoidal forcing landscape

In this subsection we show the detailed buckling dynamics of a polar filament in the sinusoidal forcing landscape $\alpha (1 + \delta \cos(kx))$. As discussed in § III A, the straight polar filament is susceptible to buckling instability at locations where the line tension is sufficiently negative. At these locations the critical forcing amplitude is computed and the dependencies of $\alpha_c$ on $\delta$, filament angle $\theta$, and $W/L$ (or $k$) are quantified in § III A.

The buckling instability of a polar filament in the sinusoidal forcing landscape is depicted in figures 7
FIG. 8: Trajectories of a polar filament undergoing buckling instability with $L = 1$ and $W/L = \pi/2$ and three different values of $\alpha$. Without buckling the polar filament moves from left to right, in a direction parallel to the $x$-axis. The direction of filament translation is altered due to the buckling instability.

from a simulation with the filament length $L = 1$, the length ratio $W/L = \pi/2$, a forcing amplitude $\alpha = 3000$, and the wall drag is neglected. The filament deformation initiates from the head and travels from head to tail as it grows in amplitude (see figures 7(a)-(e)). This growing traveling disturbance leads to a change in the direction of motion (see figures 7(f)-(j)). This finding is consistent with experimental observations in in vitro motility assays: Actin filaments change their directions of motion when they deform around defects in the motility assay.

Figure 8 shows the trajectory of the filament center-of-mass for three values of $\alpha$ from the simulations, where the initial filament is oriented along the $x$-axis, moving from left to right. As the polar filament undergoes the buckling instability it changes its direction of motion, and over long time the filament trajectory deviates significantly from the straight trajectory. For larger value of $\alpha$ significant filament deformation is found at locations where the line tension is most negative, and consequently more significant deflection from the straight trajectory.

Figure 9 elucidates how buckling dynamics leads to a change in the direction of filament motion. During the buckling process the deformation of the polar filament amplifies, giving rise to a non-trivial normal force density

$$\hat{n} \cdot [-x_{ssss} + (Tx_s)_s + f_x_s] = -\kappa_{ss} + \kappa^3 + T\kappa, \quad x_{ss} = \kappa\hat{n},$$

as shown in the top left panel of figure 9(a). The peaks in the normal force density correspond to the maximum filament curvature (and hence the filament deformation). The normal force changes the filament angle, which, for a polar filament, is equivalent to the change in its direction of motion. The filament angle (averaged over the center line) $\langle \theta \rangle$ is shown in the left bottom panel of figure 9(a). As the polar filament goes through the buckling dynamics, the filament speed deviates from that of the straight filament as shown in the right panels of figure 9: At the supercritical forcing amplitude ($\alpha = 3000$ for panel (c)) the filament buckles when the line tension is strongly negative. When the
FIG. 9: Buckling of a filament with $L = 1$, $W/L = \pi/2$ and $\alpha = 6000$. (a): Average normal force versus time. (c): Average filament angle $\theta$ (with respect to the $x$-axis) versus time. (b) and (d): Speed of filament center (solid lines) for two values of $\alpha$: $\alpha = 3000$ (top) and $\alpha = 1000$ (bottom). Dashed lines are the speed for the straight filament.

filament buckles the filament speed (dashed line) deviates most from that of the straight filament (solid line). At the sub-critical forcing amplitude $\alpha = 1000$ (panel (d)) the filament does not buckle, and therefore the filament speed is the same as the analytic filament speed in equation 19.

B. Buckling of a partially detached polar filament

The non-homogeneous binding between the polar filament and the motor proteins gives rise to a compressive tension as shown in III B. Depending on the degree of detachment, the polar filament becomes susceptible to buckling instability at different critical forcing amplitude. When the forcing amplitude is above the critical value the line tension becomes significantly negative and the filament buckles. From III B, the critical forcing amplitude decreases with increasing $\delta L$, the length of detached segment (see figures 5(a) and (b)).

Figures 10 are snapshots of a buckling filament from a simulation with $\delta L = 0.8$ and $\alpha = 3000 > \alpha_c$ ($\sim 1600$ for $\delta L = 0.8$). In a uniform forcing landscape with a sub-critical forcing amplitude ($\alpha < \alpha_c$), the partially detached filament moves in a straight line from tail to head. At a supercritical forcing amplitude (such as $\alpha = 3000$ in figures 10) the partial detachment gives rise to a sufficiently large gradient in polar forcing that leads to growing filament undulation traveling from head to tail, and thus the oscillation amplitude is larger at the tail than at the head, as shown in figure 11 that plots the traces of filament head (top panel) and tail (bottom panel) over time.

Figure 12(a) shows the filament center speed normalized by the speed of the straight filament $U$ in equation 31. Buckling of filament leads to a larger filament speed, and the larger the forcing amplitude $\alpha$ the more the enhancement in filament speed. In addition the filament undulation depends on $\alpha$: A sub-harmonic is found to emerge for large $\alpha$. At $\alpha = 5000$ the sub-harmonic is found, and it persists for large $\alpha$ as shown in figure 12(b).
FIG. 10: Motion of a partially detached filament with $\alpha = 3000$ and $\delta L = 0.8$ in a uniform forcing landscape. The polar filament is moving from left to right. Undulation of a partially detached filament is clearly demonstrated over time.

V. EFFECT OF BUCKLING INSTABILITY ON TRANSPORT OF FILAMENTS IN POLAR FORCING

Our stability analysis for a straight polar filament predicts that, provided that the spatial fluctuation is sufficiently large, the polar filament may buckle and the ensuing deformation from the instability leads to change in the direction of motion. For stiff filaments and low motor protein concentration ($\alpha < \alpha_c$), no buckling instability is expected and the polar filament remains straight and moves across space in a straight line. For floppy filaments and high motor concentrations ($\alpha \geq \alpha_c$), negative line tension arises due to polar forcing gradient, and the polar filament may undergo the buckling instability. The ensuing large filament deformation results in a change in the direction of motion. As the deformed filament relaxes, it soon resumes a straight trajectory until the next buckling occurs. The resultant filament transport consists of straight line segments of different orientations.

Figures 13 show the trajectory of a polar filament in a two-dimensional forcing landscape

$$F = 1 + \delta \cos(k_x x) \cos(k_y y),$$

(33)

where $2\pi/k_x$ and $2\pi/k_y$ are the characteristic forcing length scales in $x$- and $y$-directions, respectively. Along the trajectory, the average forcing $\langle F \rangle$, the average filament curvature $\langle \kappa \rangle$, and the average filament line tension $\langle \sigma \rangle$ are shown in panels (a), (b) and (c), respectively. First we note that the filament trajectory consists of straight segments with $\langle \kappa \rangle \sim 0$. These straight segments have different orientations (angles) and are joined by small intervals where $\langle \kappa \rangle$ and $\langle \sigma \rangle$ are high. The association
FIG. 11: Traces of filament head and tail with $\alpha = 3000$ and $\delta L = 0.8$. Filament head (top panel) oscillates with a smaller amplitude than filament tail (bottom panel).

FIG. 12: (a) Filament speed (normalized by $U$) for $\alpha = 3000$ and $\alpha = 64000$. (b) Bifurcation diagram in terms of $\alpha$.

between change in interval orientation and high curvature (or line tension) is expected from results in § IV. Thus the filament trajectory appears to be similar to the trajectory of a random walker over certain characteristic length scale. Does this imply that the long-time transport of polar filament may be described by a diffusive transport?

Random walks of a semi-flexible filament due to its deformation have been observed when the filament is immersed in a periodic cellular flow that contains many stagnation points, where the flow exerts strong compression that gives rise to filament buckling. Such a buckling instability of the semi-flexible filament around a stagnation point in the extensional flow is termed the “stretch-coil” transition in relevance to the “coil-stretch” transition of a flexible filament. The repetition of “stretch-coil” transitions in the periodic cellular flow gives rise to the diffusive filament transport in the absence of Brownian noises and hydro-dynamic interaction [20]. The effective filament diffusivity may be
FIG. 13: (a) Forcing profile $F$ along the filament trajectory. (b) Averaged filament curvature $\langle \kappa \rangle$ along the filament trajectory. (c) Averaged filament tension $\langle \sigma \rangle$ along the filament trajectory.

computed based on the characteristic length and associated residence time within a vorticity cell.

In the following it is illustrated that the ballistic transport of a polar filament may be replaced by a diffusive transport due to a sequence of filament buckling. We will demonstrate this effect of buckling instability in both a doubly-periodic forcing landscape and random forcing landscape.

A. Dispersion of Polar Filaments in Periodic and Random Forcing Landscapes

In a uniform forcing landscape polar filaments (without detachment from the motor proteins) remain straight and move in straight lines at a constant speed. The resultant filament transport is ballistic with a dispersion that scales quadratically with time. A spatial gradient in the polar forcing gives rise to a negative line tension and the possibility for the buckling instability provided that $\alpha > \alpha_c$.

When polar filaments buckle they change their direction of motion as shown in figure 13. To examine the transport of filaments that buckle under a compressive polar forcing gradient, 160 non-interacting filaments with different orientations are released around $(0, 0)$ and the filament dispersion is collected over a long duration of time. The filament dispersion is defined as

$$\overline{d^2} = \overline{x^2} - \overline{x}^2,$$

where the bar $\overline{\cdot}$ indicates average over all filaments. The long-time transport of floppy polar filaments in the doubly-periodic forcing landscape may differ significantly from ballistic transport. For diffusive transport, the dispersion scales linearly with time with a factor that is proportional to the effective diffusivity $D$: $\overline{d^2} \rightarrow 2nDt$ as $t \rightarrow \infty$, where $n$ is the spatial dimension of the forcing landscape. An example of such diffusive transport is the “stretch-coil” transition around stagnation points in the periodic cellular flow [20].

Figure 14(a) shows the trajectories of all 160 filaments in the two-dimensional periodic forcing landscape (equation 33). From the filament trajectories we find that a lot of filaments spend a significant amount of time moving diagonally. This is because the polar filament is least susceptible to buckling when its angle $\theta = \pm \pi/4$ in the two-dimensional periodic forcing landscape in equation 33. Therefore
FIG. 14: (a) Filament trajectories of 160 non-interacting filaments in a doubly-periodic forcing landscape with \( \alpha = 32000, \delta = 1 \) and \( W_x/L = W_y/L = \pi/2 \). (b) Filament dispersion (solid lines) averaged over filaments. The dashed line is a quadratic fit to early dispersion, and the dash-dotted line indicates the late-time dispersion with the diffusion coefficient \( D \) from the mean-free-path and the associated average duration between buckling events.

the filament can travel for longer durations in the diagonal directions without buckling and changing their direction of motion.

Figure 14(b) shows the corresponding filament dispersion. An initial ballistic transport is found (indicated by the dashed line). Over long time the dispersion deviates from the ballistic transport and approaches the diffusive transport (dash-dotted line). Results in figures 13 suggest that filament buckling leads to changes in its direction, and between buckling the filament is straight, moving along straight lines. The mean-free-path and the average duration between buckling events can be calculated by collecting the average distance traveled between two buckling events: From the simulations we find that the mean-free-path \( \Delta l \sim 290.63 \), and average duration is \( \Delta t \sim 0.0085 \), which gives a filament transport diffusivity (slope of the dash-dotted line) \( D \sim 10^{-2}D_0 \), where \( D_0 = U^2/l \) with \( U \) the speed of a straight filament and \( l \) is the characteristic forcing length scale. The filament dispersion from the simulation oscillates around the dash-dotted line, and the general trend indicates the diffusive nature of filament transport.

Figure 15(a) show the trajectories of all 160 filaments in the two-dimensional random forcing landscape with a characteristic length scale \( W/L \sim 0.5 \). The random forcing landscape is constructed by randomizing the phase \( \varphi_i \) of the Fourier modes of \( F \)

\[
F = a_0 + \sum_{i=1} a(k_i)e^{i(k_ix+\varphi_i)}, \tag{35}
\]

with \( |k_i| = 2i\pi \) and \( a(k_i) = a_0|k_i|^{-r} \), where \( a_0 \) and \( r \) are two positive constants that determine the forcing length scale \( W/L \). The forcing landscape in equation 35 is smooth and the numerical accuracy and convergence are retained by adjusting the time-step in the simulations. The filament
FIG. 15: (a) Filament trajectories of 160 non-interacting filaments in a random forcing landscape with $\langle \alpha F \rangle = 6000$ and a correlation length $W/L \sim 0.5$. (b) Filament dispersion (solid lines) averaged over filaments. The dashed line is a quadratic fit to early dispersion, and the dash-dotted line indicates the late-time dispersion with the diffusion coefficient $D$ from the mean-free-path and the associated average duration between buckling events.

The trajectories show no preferred orientations due to the randomness in the forcing. The corresponding filament dispersion is shown in figure 15(b). In this simulation the filament length is larger than the characteristic forcing length scale, thus the randomness in forcing averages out over the entire filament. As a result the filaments undergo the buckling instability and change their directions of motion less often than those in the periodic forcing. This explains the longer duration for the initial ballistic transport in the filament dispersion in figure (15)(b). Similar to the periodic forcing case, an initial ballistic transport is indicated by the dashed line, while at late time the dispersion deviates away from the ballistic transport and approaches the diffusive transport (dash-dotted line). The filament diffusivity (slope of the dash-dotted line) $D \sim 7 \times 10^{-3} D_0$ based on the mean-free-path $\Delta l \sim 106.85$ and the average duration between buckling events in the random forcing landscape $\Delta t \sim 0.0137$. $D_0 \equiv (\alpha F)^2 / W/L$ is based on the characteristic velocity of a straight filament $\alpha F = 6000$ and a characteristic forcing length scale $W/L = 0.5$.

VI. CONCLUSION

In this work we formulate a continuum model for the dynamics of a semi-flexible polar filament driven by motor proteins in the motility assays using the slender-body framework, which allows us to obtain an explicit expression of the force-velocity relationship for a straight filament in any forcing landscape. The line tension for the straight filament can be computed from an integral of the polar force density along the filament. The linear analysis shows that the straight polar filament is subject to the buckling instability if its line tension is sufficiently negative due to the spatial gradient in the polar forcing. The
viscous drag from the bottom wall leads to a reduced filament speed, which results in a higher critical myosin concentration for buckling instability. Results from the linear stability analysis for a straight polar filament indicate that spatial gradient in the polar forcing landscape (either due to spatial variation or partial detachment) is essential to the buckling instability. At the supercritical forcing amplitude or above, the straight polar filament undergoes buckling instability, leading to filament deformation, undulation and deflection from the original direction of motion.

A direct consequence of the filament buckling instability is that the subsequent filament transport is no longer ballistic: Instead the filament transport becomes diffusive, much similar to the transport of elastic filaments undergoing “stretch-coil” transitions in the periodic cellular flows [20]. Results in [20] suggest that the filament diffusivity can be estimated from the characteristic length $l$ in the flow and the residence time of the filament in a flow cell of size $l$. In the present case of polar filament transport across a forcing landscape, the characteristic length $l$ is the mean-free-path of the polar filament and the characteristic time is the average duration between two buckling events. Such an estimate (dash-dotted lines in figures 14(b) and figures 15(b)) gives reasonable values for the filament diffusivity in both cases.

The mean-free-path for a polar filament undergoing buckling in a forcing landscape is similar to the trajectory persistence length of a polar filament in a channel. Both filament deflection from the channel sidewall and filament buckling in a forcing landscape are associated with filament deformation. By monitoring the filament elastic energy one can quantify the mean-free-path and the time duration between filament deformation and deflection. Thus it would be interesting to see if the trajectory persistence length for a filament interacting with the channel sidewalls can be computed in our continuum model when we take into account the filament interaction with the sidewalls and the thermal fluctuations. Preliminary studies have shown that the thermal forces are essential to filament deflection from the channel sidewalls, and further studies are now underway to quantify the trajectory persistence length in a narrow channel. These results will be useful to designing micro-fluidic tracks for directed transport of microtubules in integrated microdevices.

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