Advances in Applied Mathematics and Mechanics
Adv. Appl. Math. Mech., Vol. **6**, No. 1, pp. 75-86

DOI: 10.4208/aamm.12-m12109
February 2014

Steady States of Sheared Active Nematics

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Received 23 August 2012; Accepted (in revised version) 23 May 2013

Available online 13 December 2013

Abstract. A continuum hydrodynamic model has been used to characterize flowing active nematics. The behavior of such a system subjected to a weak steady shear is analyzed. We explore the director structures and flow behaviors of the system in flow-aligning and flow tumbling regimes. Combining asymptotic analysis and numerical simulations, we extend previous studies to give a complete characterization of the steady states for both contractile and extensile particles in flow-aligning and flow-tumbling regimes. Another key prediction of this work is the role of the system size on the steady states of an active nematic system: if the system size is small, the velocity and the director angle files for both flow-tumbling contractile and extensile systems are similar to those of passive nematics; if the system is big, the velocity and the director angle files for flow-aligning contractile systems and tumbling extensile systems are akin to sheared passive cholesterics while they are oscillatory for flow-aligning extensile and tumbling contractile systems.

AMS subject classifications: 76A15, 76M45

Key words: Asymptotic expansion, active liquid crystals, hydrodynamics.

1 Introduction

Active liquid crystals are examples of active complex fluids receiving increasing theoretical and experimental attention. Such materials are called active because they continuously burn energy, for example, in the form of adenosine triphosphate (ATP), and this drives them out of thermodynamic equilibrium even when there is no external force. This is in sharp contrast to the physics of passive soft-matter systems where non-equilibrium

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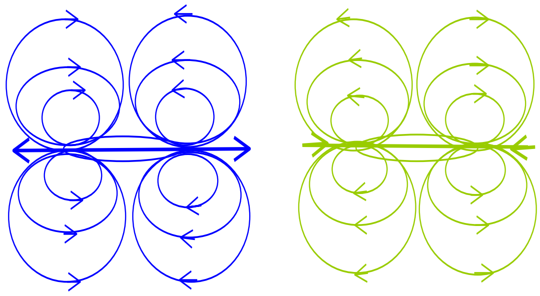

Figure 1: The dipolar flow fields surrounding a extensile (left) $(\delta<0)$ and a contractile (right) $(\delta>0)$ particle. The vertical arrows represent the director field, which is along the rod axis for rodlike swimmers.

behavior typically occurs only in the presence of an external driving force (such as shear). These systems are common in nature such as acto-myosin filaments, cytoskeletal gels interacting with motors, bacterial colonies, and swarming fishes [12, 13], but also occur in technological applications, as engineers have tried to design artificial swimmers to perform various functions [7, 11]. They are also interesting from a more fundamental perspective as their dynamic phenomenon such as bioconvection [6] and the spontaneous flow [8,17] are both physically fascinating and potentially of great biological significance.

Conventional liquid crystals exhibit a rich dynamic behavior when subject to external forcing, such as shear or applied magnetic and electric fields. This includes phase transitions, shear banding [16], and even the turbulent and chaotic behavior in the presence of shear [2]. Activity imparts non-trivial physical properties to an active system and leads to its peculiar phenomena such as bacterial swarming [10], bioconvection phenomenon or the so-called weak turbulence [6] and the spontaneous flow in the absence of externally applied forces, both stationary and oscillatory [8,9,14,17], in sharp contrast to their passive counterparts.

Active particles exert forces on the surrounding fluid, resulting in local extensile or contractile stresses proportional to the amount of orientational tensor: $\tau^a=\delta\mathbf{nn}$, where $\mathbf{n}$ is the orientation director in the nematic phase which is generally described by a unit vector, and δ is the amplitude of the dipolar forces exerted by the particle to swim. The sign of δ determines whether the dipolar flow field generated by the swimming suspension is extensile $(\delta<0)$ or contractile $(\delta>0)$, as illustrated in Fig. 1. In the swimmer literature, the former situation describes "pushers", i.e., most bacteria including E. Coli and Bacillus Subtilis, while the latter corresponds to "pullers" including Chlamydomonas. We note that this distinction is by no means exclusive, as certain highly symmetric organisms such as spherical multicellular algae (e.g., Volvox) may fall between the extensile-contractile or pusher-puller distinction.

A striking property of active liquid crystal films is the onset of spontaneous flow above a critical film thickness first identified by Voituriez et al. [17]. Marenduzzo et al. [14,15] have numerically studied the active nematic hydrodynamics in both 1D and 2D geometry based on the conformation tensor theory of Beris and Edwards [1]. Edwards et al. [8] used Leslie-Ericken continuum theory to extend this study in quasi-1D active nematics by numerically exploring the range of possible steady states. They distinguished six spontaneous flow states. However, there are few works in characterization of such a system under an imposed shear.

Our aim in this paper is therefore to study steady structures and flow states of active nematics subjected to a small shear rate. We focus on an a apolar system composed of symmetric rods and neglect any variations in the number density. Besides, we evaluate the role of the gap width on the steady states. The rest of this paper is structured as follows. The model is presented in Section 2. Section 3 investigates the sheared steady states and conducts their stability analysis. We focus on rod-like active particle systems. Section 4 contains conclusions and perspectives for future study.

2 Model formulation

We adopt the Erickson-Leslie-Parodi model [3,8], in which the nematic order parameter is a fixed-magnitude unit vector field $\overrightarrow{\mathbf{n}}$ which evolves according to

$$\frac{\partial \overrightarrow{\mathbf{n}}}{\partial t}+\overrightarrow{\mathbf{v}}\cdot\nabla\overrightarrow{\mathbf{n}}=\lambda\mathbf{D}\cdot\overrightarrow{\mathbf{n}}-\boldsymbol{\Omega}\cdot\overrightarrow{\mathbf{n}}+\Gamma\overrightarrow{\mathbf{h}}, \tag{2.1}$$

where $\overrightarrow{\mathbf{v}}$ is the velocity field of the solvent; λ is the flow alignment parameter, Γ is a rotational viscosity; $\overrightarrow{\mathbf{h}}=K\Delta\overrightarrow{\mathbf{n}}$ is the molecular field and K is the Frank elasticity constant (single constant approximation), $\Omega=(\nabla\mathbf{v}-\nabla\mathbf{v}^T)/2$ and $\mathbf{D}=(\nabla\mathbf{v}+\nabla\mathbf{v}^{\mathbf{T}})/\mathbf{2}$ are the rate-of vorticity and the rate-of-strain tensors, respectively.

The first two terms on the right-hand side of Eq. (2.1) describe alignment (or tumbling) of the director field by local shear flow. The third term accounts for the tendency of the ordered nematic to resist distortions, and arises ultimately from excluded volume interactions between individual particles. The flow field $\overrightarrow{\mathbf{v}}$ obeys the Navier-Stokes equation

$$\rho\Big(\frac{\partial\overrightarrow{\mathbf{v}}}{\partial t}+\overrightarrow{\mathbf{v}}\cdot\nabla\overrightarrow{\mathbf{v}}\Big)=\frac{\partial p}{\partial x}\mathbf{I}+\nabla\cdot(\tau+2\eta\mathbf{D}) \tag{2.2}$$

with the continuity equation $\nabla\cdot\overrightarrow{\mathbf{v}}=0$ to guarantee incompressibility, the stress tensor given by the passive and active contributions, $\tau=\tau^p+\tau^a$,

$$\tau^p=-\frac{\lambda}{2}[\overrightarrow{\mathbf{n}}\,\overrightarrow{\mathbf{h}}+(\overrightarrow{\mathbf{n}}\,\overrightarrow{\mathbf{h}})^T]+\frac{1}{2}[\overrightarrow{\mathbf{n}}\,\overrightarrow{\mathbf{h}}-(\overrightarrow{\mathbf{n}}\,\overrightarrow{\mathbf{h}})^T], \tag{2.3}$$

where ρ is the fluid density and η is the viscosity and λ is the flow-alignment parameter. The magnitude of λ controls how the director field responds to a shear flow. $|\lambda|>1$ corresponds to flow aligning regime in which the director tends to align to the flow direction at the Leslie alignment angle $\theta_L=\cos^{-1}\lambda^{-1}/2$ while $|\lambda|<1$ corresponds to flow tumbling regime in which the director continuously rotates under shear. The value of λ is mainly determined by the shape of the active particles. $\lambda>0$ corresponds to a rod-shaped particle, $\lambda<0$ for a disc-shaped particle and $\lambda=0$ for a spherical particle.

The active contribution can be expressed as [3,8,9],

$$\tau^a=\delta\overrightarrow{\mathbf{n}}\,\overrightarrow{\mathbf{n}}. \tag{2.4}$$

The sign of δ determines whether the particles are extensile $(\delta<0)$ or contractile $(\delta>0)$.

In order to study the role of the gap width of the experimental geometry, we keep the governing system (2.1) and (2.2) in dimensional form.

3 Weak shear flows

We consider shear flow between two parallel plates located at $y=\pm H$ and moving with corresponding velocity

$$\mathbf{v}=(\pm v_0,0,0). \tag{3.1}$$

We assume strong particle anchoring at the plates given by

$$\mathbf{n_0}=(\cos\varphi_0,\sin\varphi_0,0), \tag{3.2}$$

where $\mathbf{n_0}$ is the initial director across the plates in absence of shear flow. Fig. 2 depicts the cross section of the shear flow on the (x,y) plane. Variations in the direction of flow (x) and primary vorticity direction (z), and transport in the vertical (y) direction are suppressed.

We now look for the steady states of an active nematic in a confined geometry. We consider the in-plane orientation of an active nematic confined to the shearing plane (x,y)

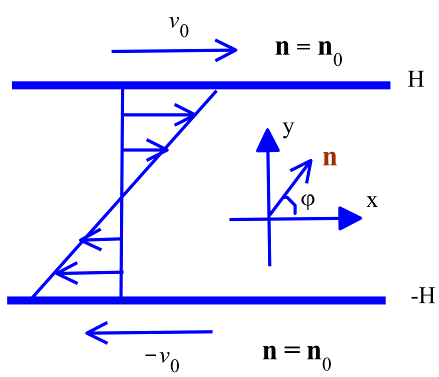

Figure 2: Plane shear flow geometry. The boundary anchoring for the director is assumed to equal to its quiescent nematic equilibrium value and the velocity boundary condition is no-slip $v(\pm H)=0$. The director field n is measured by the orientation angle φ such that $\varphi=0$ is parallel to the walls, and $\varphi=\pi/2$ is perpendicular.

and strong anchoring boundary conditions. The director $\mathbf{n}$ confined to the shearing plane (x,y) and parameterized by the director angle φ,

$$\mathbf{n}=(\cos\varphi,\sin\varphi,0).$$

We only consider here a rodlike particle system and the tangential anchoring boundary condition where the director at the confining surfaces is parallel to the flow direction, i.e., $\varphi=0$. Other cases will be the subject of future work.

We seek asymptotic solutions of the governing system of equations with the boundary conditions given by (3.1) and (3.2). We consider the in-plane orientation of active suspensions confined to the shearing plane (x,y).

The director $\mathbf{n}$ confined to the shearing plane (x,y) and parameterized by the director angle φ,

$$\mathbf{n}=(\cos\varphi,\sin\varphi,0). \tag{3.3}$$

We propose the solution ansatz

$$v_x=\sum_{k=1}^{\infty}v_x^{(k)}v_0^k,\varphi=\varphi_0+\sum_{k=1}^{\infty}\varphi^{(k)}v_0^k. \tag{3.4}$$

The solution is sensitive to the choice of boundary conditions, we restrict to tangential $(\varphi_0=0)$ and homeotropic $(\varphi_0=\pi/2)$ anchoring conditions. At the first order of the asymptotic scheme, the flow and orientational director dynamics dominate. We present the results at tangential anchoring and comment on those at homeotropic anchoring. We drop the subscript on φ for brevity and use v_x to express $v_x^{(1)}$. At the first order $\mathcal{O}(v_0)$, the system reduces to

$$\frac{\partial\varphi}{\partial t}=A\frac{\partial^2\varphi}{\partial y^2}+B\frac{\partial v_x}{\partial y},\quad \rho\frac{\partial v_x}{\partial t}=\frac{\partial\tau_{xy}}{\partial y},\quad \tau_{xy}=C\frac{\partial^2\varphi}{\partial y^2}+D\frac{\partial v_x}{\partial y}+\delta\varphi, \tag{3.5}$$

where

$$A=\Gamma K,\quad B=\frac{\lambda-1}{2},\quad C=-KB,\quad D=\eta. \tag{3.6}$$

The majority of the symbolic and numerical calculations presented in this paper were performed using the software MAPLE 12 by Waterloo Maple. The values of main parameters used in this paper are taken from [8]: Γ=0.2,K=0.04 and η=1.27. For a flow-aligning system, $\lambda=1.5$ and for a tumbling system $\lambda=0.7$.

3.1 Steady states, their continuity with respect to the activity and their stability

The steady state of the system (3.5) is given

$$v_x=\frac{\sinh ry}{\sinh rH},\quad \varphi=-\frac{B\coth rH}{Ar}\Big(\frac{\cosh ry}{\cosh rH}-1\Big), \tag{3.7}$$

where $r=\sqrt{(\lambda-1)\delta/2(AD-BC)}$. It is real (imaginary) if $(\lambda-1)\delta>0$ (<0). This implies a remarkable duality for the steady state structures: *A contractile (extensile) system with* $\lambda>1$ *is the same as a extensile (contractile) system with* $\lambda<1$.

Note that, in the activity limit $\delta=0$, the system (3.5) is reduced to the governing system for passive nematics and the steady solutions are

$$v_{xp}=\frac{y}{H},\quad \varphi_p=\frac{BH}{A}\Big(1-\frac{y^2}{H^2}\Big). \tag{3.8}$$

Proposition 3.1. The steady state (3.7) is continuous at $\delta=0$. Thus (3.7) is a continuous function of δ on $(-\infty,\infty)$.

Proof. By simple calculation, we have

$$\lim_{\delta\to 0}v_x=\frac{y}{H},\quad \lim_{\delta\to 0}\varphi=\frac{BH}{A}\Big(1-\frac{y^2}{H^2}\Big).$$

Hence, (3.7) is continuous at $\delta=0$. The proof is completed. □

It is important to consider the stability of the steady state (3.7) because it may result orientational or phase transitions in the system and thus affects the rheology of the system. To study this, we consider the transient solution for v_x and φ (the difference between the time-dependent solution and the steady state) obeys the following linear partial differential equations with a zero boundary condition

$$\frac{\partial\varphi}{\partial t}=A\frac{\partial^2\varphi}{\partial y^2}+B\frac{\partial v_x}{\partial y},\quad \rho\frac{\partial v_x}{\partial t}=\frac{\partial \tau_{xy}}{\partial y}. \tag{3.9}$$

Its behavior dictates the stability of the steady state (3.7) within the asymptotic balance model: the steady state is asymptotically stable if the transient solution vanishes as $t\to\infty$. The author [3] proved the following theorem.

Theorem 3.1. *The steady state is stable for a tangential anchoring if* $(\lambda-1)\delta>0$. *If* $(\lambda-1)\delta<0$, *then the steady state is stable for* $|\delta|\ll 1$, *i.e., in a low activity regime.*

For readers' convenience, we provide the main idea of the proof as follows:

We note that

$$A=\Gamma K>0,\quad BC=-K\Big(\frac{\lambda-1}{2}\Big)^2<0\quad \text{and}\quad D=\eta>0.$$

We use φ_y, φ_{yy}, $v_{x,y}$ and $v_{x,yy}$ to express $d\varphi/dy$, $d^2\varphi/dy^2$, dv_x/dy and d^2v_x/dy^2, respectively.

Extending the first equation of (3.5) to the boundary and accounting for the boundary condition $\varphi(-H,t)=\varphi(H,t)=0$, we have

$$(A\varphi_{yy}y+Bv_{x,y})|_{y=\pm 1}=0. \tag{3.10}$$

We introduce a Liapunov function

$$I(t)=\int_{-H}^{H}[\gamma_1\varphi_y^2+\gamma_2 v_x^2+\gamma_3\varphi^2]dy \tag{3.11}$$

with $\gamma_1>0$, $\gamma_2>0$ and $\gamma_3>0$.

If $(\lambda-1)\delta>0$, then B and δ have same signs. We choose $\gamma_1=|C|$, $\gamma_2=|B|\rho$ and $\gamma_3=|B|\delta/B$ and integrating by parts, the time derivative of the nonnegative functional $I(t)$ can be estimated:

$$\begin{aligned}\frac{dI(t)}{dt}=&-2\int_{-H}^{H}\left[\gamma_1 A\varphi_{yy}^2+(\gamma_1 B+\gamma_2 C)\varphi_{yy}v_{x,y}+\gamma_2 D v_{x,y}^2+\gamma_3 A\varphi_y^2+(\gamma_3 B-\gamma_2\delta)\varphi_y v_x\right]dy\\ =&-2\int_{-H}^{H}\Big[|C|A\varphi_{yy}^2+|B|Dv_{x,y}^2+A|B|\frac{\delta}{B}\varphi_y^2\Big]dy<0. \end{aligned} \tag{3.12}$$

Thus the steady solution of the system is stable.

If $(\lambda-1)\delta<0$, then B and δ have opposite signs. We choose $\gamma_1=|C|$, $\gamma_2=|B|\rho$ and $\gamma_3=0$, then

$$\frac{dI(t)}{dt}=-2\int_{-H}^{H}\left[|C|A\varphi_{yy}^2+|B|Dv_{x,y}^2\right]dy+2\delta|B|\int_{-H}^{H}\varphi_y v_x dy. \tag{3.13}$$

If $|\delta|\ll 1$, i.e., in a low activity regime, then the first integral of the right-hand side of (3.13) is dominant, and since it is negative, $dI(t)/dt<0$. Hence the steady solution of the system is stable.

3.2 Numerical experiments

Now we turn to numerical studies of the steady state (3.7). We will consider flow-aligning and flow tumbling regimes. We will also study the effects of the gap width on the steady solutions.

3.2.1 Flow-aligning regime

For $\lambda=1.5$, the system is flow aligning. Fig. 3 depict the typical velocity and director profiles for flow-aligning active rodlike swimmers. Figs. 3(a) and (b) depict the typical velocity and director profiles for flow-aligning rodlike contractile swimmers. When $\delta=0.001$, the velocity and the director structure is similar to sheared passive nematics. When $\delta=0.01$, the velocity is zero and the director is a constant near the center of the plates. When $\delta=0.1$, the flow velocity is zero and the director angle is a constant except near the plates, which is akin to permeation in passive cholesteric liquid crystals [5]. Figs. 3 (c) and (d) depict the typical velocity and director profiles for flow-aligning rodlike extensile swimmers. When $\delta=-0.001$, the velocity and the director structure is similar to sheared passive nematics. When $\delta=0.01$, the velocity and the director become oscillatory. When $\delta=0.1$, the flow velocity and the director angle are highly oscillatory. We summarize our findings as follows:

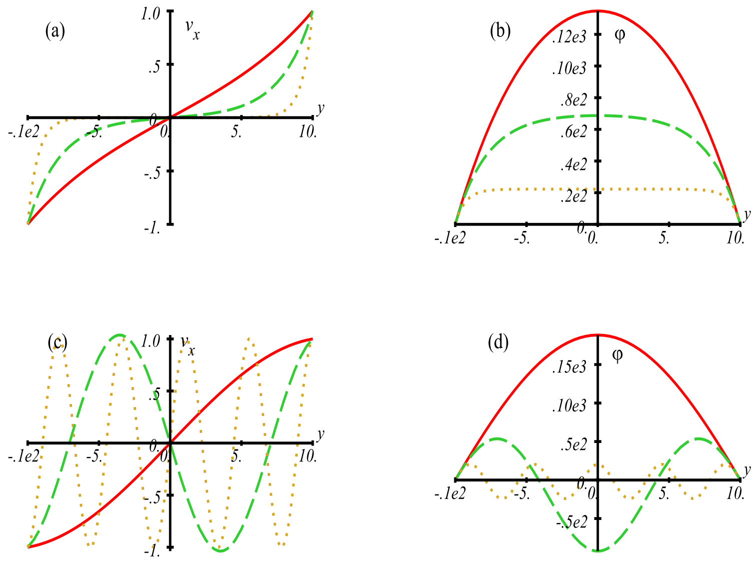

Figure 3: The steady states for a tangential anchoring at different values of the activity. (a) and (b) depict the velocity and the director profiles for the flow-aligning rodlike contractile swimmers: solid, dashed and dotted lines correspond to $\delta=0.001,0.01,0.1$. (c) and (d) depict the velocity and the director profiles for the flow-aligning rodlike extensile swimmers: solid, dashed and dotted lines correspond to $\delta=-0.001,-0.01,-0.1$.

- At low activity regime, the velocity and the director angle files for both flow-aligning contractile and extensile systems are similar to those of passive systems.
- At high activity regime, the velocity and the director angle files are similar to passive cholesterics for flow-aligning contractile systems while they are oscillatory for flow-aligning contractile systems.

3.2.2 Flow-tumbling regime

For $\lambda=0.7$, the system is flow tumbling. Fig. 4 depicts the typical velocity and director profiles for flow-tumbling rodlike swimmers. Figs. 4(a) and (b) depict the typical velocity and director profiles for flow-tumbling rodlike contractile swimmers. When $\delta=0.001$, the velocity and the director structure are similar to sheared passive nematics. When $\delta=0.01$, the flow velocity and the director angle are moderately oscillatory. When $\delta=0.1$, the flow velocity and the director angle are highly oscillatory. Figs. 4(c) and (d) depict the typical velocity and director profiles for flow-aligning rodlike extensile swimmers. When $\delta=-0.001$, the velocity and the director structure is similar to sheared passive nematics. When $\delta=-0.01$, the velocity is zero and the director is a constant near the center of the plates. When $\delta=-0.1$, the flow velocity is zero and the director angle is a constant except near the plates, which is similar to sheared passive cholesteric liquid crystals [5]. We summarize our results as follows:

- At low activity regime, the velocity and the director angle files for both flow-tumbling contractile and extensile systems are similar to those of passive systems.

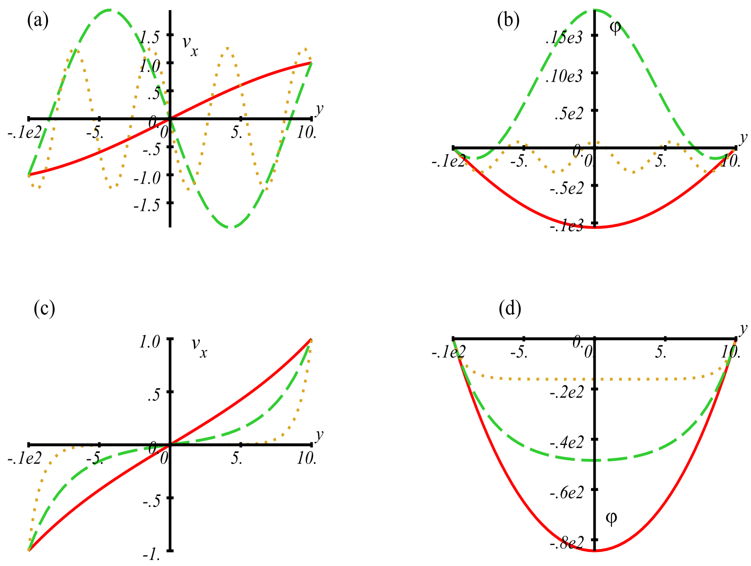

Figure 4: The steady states for a tangential anchoring at different values of the activity. (a) and (b) depict the velocity and the director profiles for the flow-tumbling rodlike contractile swimmers: solid, dashed and dotted lines correspond to $\delta=0.001,0.01,0.1$. (c) and (d) depict the velocity and the director profiles for the flow-tumbling rodlike extensile swimmers: solid, dashed and dotted lines correspond to $\delta=-0.001,-0.01,-0.1$.

- At high activity regime, the velocity and the director angle files are similar to passive cholesterics for tumbling extensile systems while they are oscillatory for tumbling contractile systems.

3.2.3 Effects of the gap width

We now study the role of the gap width on the steady states. Fig. 5 depicts the velocity and director profiles for flow-aligning rodlike contractile and extensile swimmers. When $H=1$, for both flow-aligning rodlike contractile and extensile swimmers, the flow velocities are nearly linear and the director angle profiles are parabolic. These are like sheared passive nematics. When $H=10$, for the flow-aligning rodlike contractile system, the flow velocity is zero and the director angle is a constant near the center of the gap; for the flow-aligning rodlike extensile system, both the flow velocity and the director angle are moderately oscillatory. When $H=100$, for the flow-aligning rodlike contractile system, the flow velocity is zero and the director angle is a constant through the gap except near the plates; for the flow-aligning rodlike extensile system, both the flow velocity and the director angle are highly oscillatory.

Fig. 6 depicts the velocity and director profiles for flow-tumbling rodlike contractile and extensile swimmers. When $H=1$, for both tumbling rodlike contractile and extensile swimmers, the flow velocities is linear and the director profiles are parabola. These are similar to sheared passive nematics. When $H=10$, for the tumbling rodlike contractile systems, both the flow velocity and the director angle are oscillatory, for the tumbling

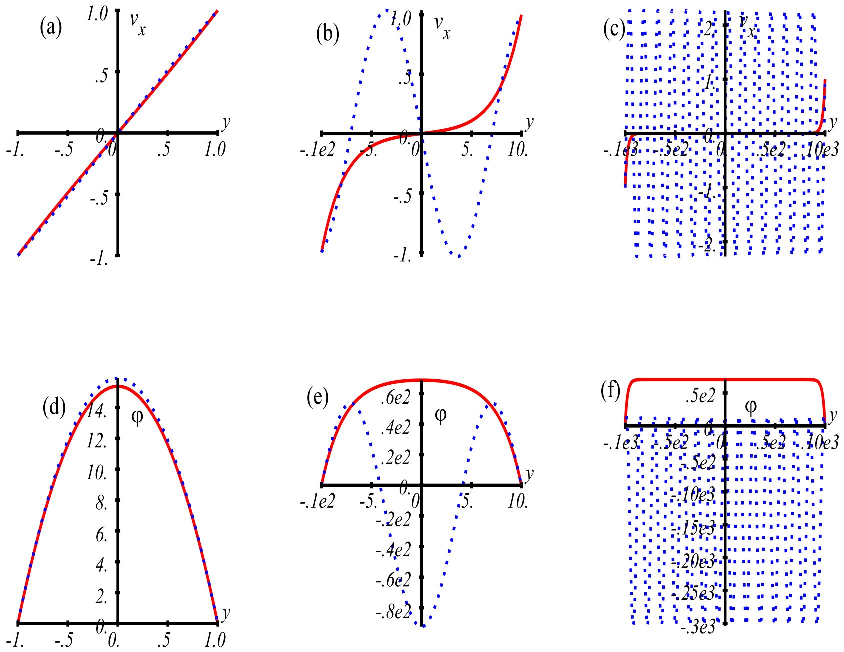

Figure 5: The steady velocity and director angle profiles for flow-aligning rodlike swimmers at different gap width H. (a) and (d) depict the velocity and director profiles for flow-aligning rodlike contractile (solid line) and extensile (dotted line) swimmers for $H=1$. (b) and (e) depict the velocity and director profiles for flow-aligning rodlike contractile (solid line) and extensile (dotted line) swimmers for $H=10$. (c) and (f) depict the velocity and director profiles for flow-aligning rodlike contractile (solid line) and extensile (dotted line) swimmers for $H=100$. For a contractile system, the values of parameters are $\lambda=1.5$ and $\delta=0.01$. For a extensile system, the values of parameters are $\lambda=1.5$ and $\delta=-0.01$.

rodlike extensile systems, the flow velocity is zero and the director angle is a constant near the center of the gap. When $H=100$, for the tumbling rodlike contractile systems, both the flow velocity and the director angle are highly oscillatory; for the tumbling rodlike extensile system, the flow velocity is zero and the director angle is a constant away the plates. Here is the summary of our results:

- At a low gap width, the velocity and the director angle files for both flow-tumbling contractile and extensile systems are similar to those of passive systems.
- At high gap width, the velocity and the director angle files for flow-aligning contractile systems and tumbling extensile systems are akin to sheared passive cholesterics while they are oscillatory for flow-aligning extensile and tumbling contractile systems.

4 Conclusions

We have derived the governing equations for flowing active nematics based on Leslie-Ericken-Parodi continuum model. We establish the asymptotic formulas of the steady

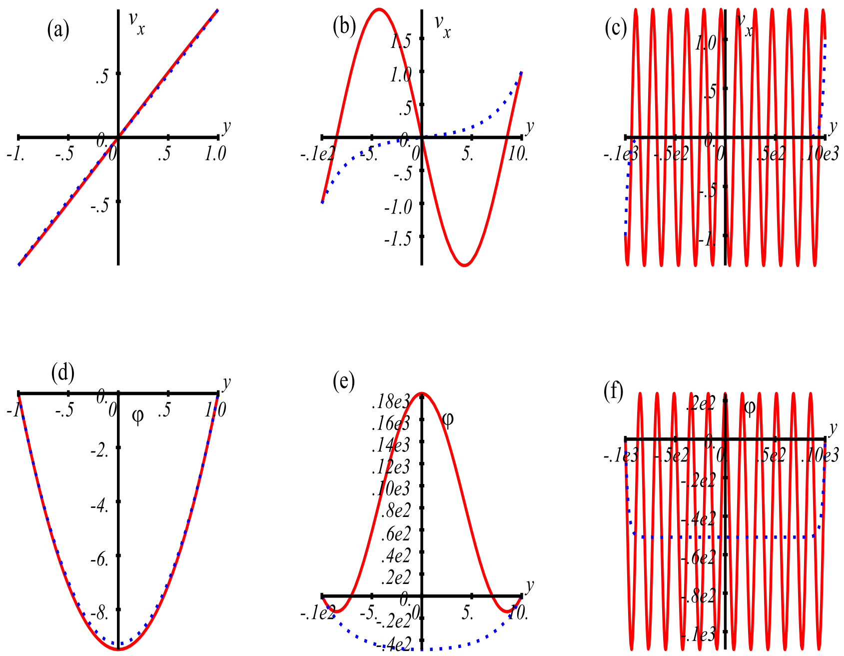

Figure 6: The steady velocity and director angle profiles for flow-tumbling rodlike swimmers at different gap width H. (a) and (d) depict the velocity and director profiles for flow-tumbling rodlike contractile (solid line) and extensile (dotted line) swimmers for $H=1$. (b) and (e) depict the velocity and director profiles for flow-aligning rodlike contractile (solid line) and extensile (dotted line) swimmers for $H=10$. (c) and (f) depict the velocity and director profiles for flow-tumbling rodlike contractile (solid line) and extensile (dotted line) swimmers for $H=100$. For a contractile system, the values of parameters are $\lambda=1.5$ and $\delta=0.01$, for a extensile system the values of parameters are $\lambda=0.7$ and $\delta=-0.01$.

boundary-value problem subject to a steady weak shear and give numerical analysis of the steady structures. We explore the steady states for contractile and extensile nematics. These results demonstrate a remarkable richness in the steady-state hydrodynamic behaviors of active nematics to an external forcing. They are consistent with the previous results on active rodlike particle system [4, 8]. Clearly, more dedicated controlled experiments with active suspensions of different shapes and further generalizations of the obtained results to more general flow geometries are needed and we expect more tests of these predictions in experiments on active liquid crystals.

Acknowledgments

Zhenlu Cui's work is supported in part by NSF through grant HBCU-UP-1036257 and Fayetteville State University. Xiaoming Zeng's work is supported in part by the National Science Foundation of China (Grant No. 61170324). Jianbing Su's work is supported in part by the National Science Foundation of China (Grant No. 11171285).

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