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Research Article

Monotonicity of a Key Function Arised in Studies of Nematic Liquid Crystal Polymers

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We revisit a key function arised in studies of nematic liquid crystal polymers. Previously, it was conjectured that the function is strictly decreasing and the conjecture was numerically confirmed. Here we prove the conjecture analytically. More specifically, we write the derivative of the function into two parts and prove that each part is strictly negative.

1. Introduction

In our previous study of steady states and dynamics of two-dimensional nematic liquid crystal polymers under an imposed weak shear [1], we carried out multiscale asymptotic expansions [2, 3] to reveal the slow time evolution of the polymer orientation distribution. In the two-dimensional case, the orientation of a polymer rod is represented by angle θ [4–6]. Let $\rho(\theta,t)$ denote the probability density of the orientation of the polymer rod ensemble. Our multiscale asymptotic analysis on the Smoluchowski equation which governs the evolution of the probability density [1] demonstrates that, to the leading term, the probability density $\rho(\theta,t)$ behaves like a travelling wave with nonuniform velocity

$$\rho(\theta,t)=\rho^{(0)}(\theta-\alpha(t))+\cdots. \tag{1.1}$$

Here $\rho^{(0)}(\theta)$ is a given function and the phase angle $\alpha(t)$ evolves according to

$$\frac{d\alpha(t)}{dt}=\epsilon\, c_1\left(\sin^2(\alpha(t))-c_2\right), \tag{1.2}$$

where ϵ is the Peclet number. For a weak shear, the Peclet number is small. c_1 is a positive constant independent of ϵ and α. The expression of c_2 is given by

$$c_2 = \frac{h(r)}{2g(r)}. \tag{1.3}$$

From the evolution equation (1.2), we see that the sign of c_2 determines the behavior of polymer orientation distribution: for $0 < c_2 < 1$, the polymer orientation distribution will converge to a steady state while for $c_2 < 0$, the polymer orientation distribution will keep rotating (tumbling). Function $g(r)$ is defined as

$$g(r) \equiv \left(\frac{1}{2\pi}\int_0^{2\pi} \exp(r\cos 2\theta)d\theta\right)^2. \tag{1.4}$$

Function $h(r)$ is defined as

$$h(r) \equiv \frac{1}{\langle \cos 2\theta\rangle}\left(1 - g(r)\left(1 - \langle \cos 2\theta\rangle\right)\right). \tag{1.5}$$

Here $\langle \cos 2\theta\rangle$ denotes the average of random variable $\cos 2\theta$ defined as

$$\langle \cos 2\theta\rangle \equiv \int_0^{2\pi} \cos 2\theta \rho(\theta, r)d\theta, \tag{1.6}$$

where the probability density used in the average is given by

$$\rho(\theta, r) \equiv \frac{\exp(r\cos 2\theta)d\theta}{\int_0^{2\pi}\exp(r\cos 2\theta)d\theta}. \tag{1.7}$$

It is clear that $\langle \cos 2\theta\rangle$ is a function of r. But for conciseness, we will simply write $\langle \cos 2\theta\rangle$ instead of writing $\langle \cos 2\theta\rangle(r)$. In the discussion here, r is treated as an independent variable for mathematical convenience. From physical considerations, a more meaningful quantity is, U, the normalized polymer concentration. In [1], we showed that r is a strictly increasing function of U, so there is a one-to-one correspondence between U and r.

Since function $g(r)$ is always positive, the sign of c_2 is completely determined by function $h(r)$. In [1], by doing expansions at $r = 0$ and at $r = \infty$, we showed

$$\begin{aligned} h(0) &= 1, \\ h'(0) &= -1, \\ h(r) &= \frac{-1}{4\pi r^2}\exp(2r) + \cdots \quad \text{as } r \longrightarrow +\infty. \end{aligned} \tag{1.8}$$

In [1], we made a conjecture that $h(r)$ is a strictly decreasing function of r for $r > 0$. Based on the conjecture, we concluded that there is a threshold r_0 such that $h(r) > 0$ for $r < r_0$ and $h(r) < 0$ for $r > r_0$. Because of the one-to-one correspondence between U and r, the conclusion in r leads to the conclusion that there is a threshold U_0 for the normalized polymer concentration: for $U < U_0$, the polymer orientation distribution will converge to a steady state while for $U > U_0$, the polymer orientation distribution will keep rotating (tumbling).

2. Proof of the conjecture

In [1], the conjecture that $h(r)$ is a strictly decreasing function of r for $r > 0$ is only numerically confirmed. In this study, we prove this conjecture analytically. We start by writing function $h(r)$ in a slightly different form:

$$h(r) = \frac{-(g(r)-1)}{\langle \cos 2\theta \rangle} + g(r). \tag{2.1}$$

We calculate the derivative of $\rho(\theta, r)$:

$$\begin{aligned} \frac{d}{dr}\rho(\theta,r) &= \frac{\cos 2\theta \exp(r\cos 2\theta)}{\int_0^{2\pi} \exp(r\cos 2\theta)d\theta} \\ &\quad - \frac{\exp(r\cos 2\theta)\int_0^{2\pi}\cos 2\theta \exp(r\cos 2\theta)d\theta}{\left(\int_0^{2\pi}\exp(r\cos 2\theta)d\theta\right)^2} \\ &= \left(\cos 2\theta - \langle \cos 2\theta \rangle\right)\rho(\theta,r). \end{aligned} \tag{2.2}$$

Using this result, we compute the derivative of $\langle \cos 2\theta \rangle$:

$$\begin{aligned} \frac{d}{dr}\langle \cos 2\theta \rangle &= \langle \cos 2\theta(\cos 2\theta - \langle \cos 2\theta \rangle)\rangle \\ &= \langle \cos^2 2\theta \rangle - \langle \cos 2\theta \rangle^2 \\ &= \operatorname{var}(\cos 2\theta) > 0, \end{aligned} \tag{2.3}$$

where $\operatorname{var}(\cos 2\theta)$ denotes the variance of random variable $\cos 2\theta$ and is always positive for finite values of r. The derivative of function $g(r)$ is given by

$$\begin{aligned} \frac{d}{dr}g(r) &= \frac{2}{4\pi^2}\int_0^{2\pi}\exp(r\cos 2\theta)d\theta \int_0^{2\pi}\cos 2\theta \exp(r\cos 2\theta)d\theta \\ &= 2\left(\frac{1}{2\pi}\int_0^{2\pi}\exp(r\cos 2\theta)d\theta\right)^2 \frac{\int_0^{2\pi}\cos 2\theta\exp(r\cos 2\theta)d\theta}{\int_0^{2\pi}\exp(r\cos 2\theta)d\theta} \\ &= 2g(r)\langle \cos 2\theta \rangle. \end{aligned} \tag{2.4}$$

Differentiating both sides of (2.1) with respect to r and using (2.3) and (2.4) yield

$$\begin{aligned} \frac{d}{dr}h(r) &= -(g(r)-1)\frac{d}{dr}\left(\frac{1}{\langle \cos 2\theta \rangle}\right) - \frac{dg(r)}{dr}\frac{1}{\langle \cos 2\theta \rangle} + \frac{dg(r)}{dr} \\ &= (g(r)-1)\frac{\operatorname{var}(\cos 2\theta)}{\langle \cos 2\theta \rangle^2} - 2g(r) + 2g(r)\langle \cos 2\theta \rangle \\ &= \left(g(r) - 1 - 2g(r)\langle \cos 2\theta \rangle^2\right)\frac{\operatorname{var}(\cos 2\theta)}{\langle \cos 2\theta \rangle^2} \\ &\quad + 2g(r)\left(\operatorname{var}(\cos 2\theta) - 1 + \langle \cos 2\theta \rangle\right) \\ &\equiv Q_1(r)\frac{\operatorname{var}(\cos 2\theta)}{\langle \cos 2\theta \rangle^2} + 2g(r)Q_2(r). \end{aligned} \tag{2.5}$$

In this study, our goal is to prove $dh(r)/dr < 0$ for $r > 0$. Since in (2.5), both $g(r)$ and $\text{var}(\cos 2\theta)/\langle \cos 2\theta\rangle^2$ are always positive, to achieve our goal, we only need to prove the two theorems below.

Theorem 2.1.

$$Q_1(r) \equiv g(r) - 1 - 2g(r)\langle \cos 2\theta\rangle^2 < 0 \quad \textit{for } r > 0. \tag{2.6}$$

Theorem 2.2.

$$Q_2(r) \equiv \text{var}(\cos 2\theta) - 1 + \langle \cos 2\theta\rangle < 0 \quad \textit{for } r > 0. \tag{2.7}$$

Remark 2.3. The conclusion that function $h(r)$ is strictly decreasing for $r > 0$ follows directly from these two theorems.

To facilitate the proofs of these two theorems, we introduce a functional. Specifically, the functional maps a function of θ to a function of r defined as [5]

$$F[q(\theta)](r) \equiv \int_0^{2\pi} q(\theta) \exp(r\cos 2\theta)d\theta. \tag{2.8}$$

The derivative of $F[q(\theta)](r)$ is given by

$$\begin{aligned}\frac{d}{dr}F[q(\theta)](r) &= \int_0^{2\pi} q(\theta)\cos 2\theta \exp(r\cos 2\theta)d\theta \\ &= F[q(\theta)\cos 2\theta](r).\end{aligned} \tag{2.9}$$

With the notation of functional, $\langle \cos 2\theta\rangle$ and $g(r)$ can be written as

$$\begin{aligned}\langle \cos 2\theta\rangle &= \frac{F[\cos 2\theta](r)}{F[1](r)}, \\ g(r) &= \frac{F[1]^2(r)}{4\pi^2}.\end{aligned} \tag{2.10}$$

Proof of Theorem 2.1.
Step 1. Using the notation of functional, we express function $Q_1(r)$ as

$$Q_1(r) = \frac{1}{4\pi^2}\left(F[1]^2(r) - 4\pi^2 - 2F[\cos 2\theta]^2(r)\right). \tag{2.11}$$

It is straightforward to verify that $Q_1(0) = 0$. Thus, to prove $Q_1(r) < 0$ for $r > 0$, we only need to prove $dQ_1(r)/dr < 0$ for $r > 0$. Taking the derivative of $Q_1(r)$ and with the help of (2.9), we get

$$\frac{d}{dr}Q_1(r) = \frac{2F[\cos 2\theta](r)}{4\pi^2}\left(F[1](r) - 2F[\cos^2 2\theta](r)\right). \tag{2.12}$$

Using the fact that the functional $F[\bullet]$ is linear and using the identity $\cos^2 2\theta = 1 - \sin^2 2\theta$, we obtain

$$\frac{d}{dr}Q_1(r) = \frac{2F[\cos 2\theta](r)}{4\pi^2}\left(2F[\sin^2 2\theta](r) - F[1](r)\right). \tag{2.13}$$

Since $F[\cos 2\theta](0) = 0$ and $dF[\cos 2\theta](r)/dr = F[\cos^2 2\theta](r) > 0$, we have $F[\cos 2\theta](r) > 0$ for $r > 0$. As a result, to prove $dQ_1(r)/dr < 0$ for $r > 0$, we only need to prove $2F[\sin^2 2\theta](r) - F[1](r) < 0$ for $r > 0$.

Step 2. We now prove $2F[\sin^2 2\theta](r) - F[1](r) < 0$ for $r > 0$.

Using the Taylor expansion

$$\exp(r\cos 2\theta) = \sum_{n=0}^{\infty} \frac{r^n \cos^n 2\theta}{n!}, \tag{2.14}$$

and using the fact that $\int_0^{2\pi} \cos^{2n+1} 2\theta d\theta = \int_0^{2\pi} \sin^2 2\theta \cos^{2n+1} 2\theta d\theta = 0$ to get rid of terms of odd powers in the sum, we write the expression $2F[\sin^2 2\theta](r) - F[1](r)$ as

$$\begin{aligned} &2F[\sin^2 2\theta](r) - F[1](r) \\ &\quad = \sum_{n=0}^{\infty} \frac{r^{2n}}{(2n)!} \int_0^{2\pi} (2\sin^2 2\theta \cos^{2n} 2\theta - \cos^{2n} 2\theta) d\theta. \end{aligned} \tag{2.15}$$

Applying integration by parts, we obtain

$$\begin{aligned} \int_0^{2\pi} 2\sin^2 2\theta \cos^{2n} 2\theta d\theta &= -\int_0^{2\pi} \sin 2\theta \frac{d(\cos^{2n+1} 2\theta)}{2n+1} \\ &= \frac{2}{2n+1} \int_0^{2\pi} \cos^{2n+2} 2\theta d\theta \\ &= \begin{cases} \displaystyle\int_0^{2\pi} \cos^{2n} 2\theta d\theta, & n = 0 \\ \displaystyle< \frac{2}{2n+1} \int_0^{2\pi} \cos^{2n} 2\theta d\theta, & n > 1. \end{cases} \end{aligned} \tag{2.16}$$

Substituting (2.16) into (2.15), we arrive at

$$\begin{aligned} &2F[\sin^2 2\theta](r) - F[1](r) \\ &\quad < -\sum_{n=1}^{\infty} \frac{r^{2n}}{(2n)!} \left(\frac{2n-1}{2n+1}\right) \int_0^{2\pi} \cos^{2n} 2\theta d\theta < 0. \end{aligned} \tag{2.17}$$

This completes the proof of Theorem 2.1. □

Proof of Theorem 2.2.

Step 1. Using the definition $\mathrm{var}(\cos 2\theta) = \langle \cos^2 2\theta \rangle - \langle \cos 2\theta \rangle^2$, the relation $\langle \cos^2 2\theta \rangle - 1 = -\langle \sin^2 2\theta \rangle$, and the notation of functional, we write function $Q_2(r)$ as

$$\begin{aligned} Q_2(r) &= -\langle \sin^2 2\theta \rangle - \langle \cos 2\theta \rangle^2 + \langle \cos 2\theta \rangle \\ &= -\frac{F[\sin^2 2\theta](r)}{F[1](r)} - \frac{F[\cos 2\theta]^2(r)}{F[1]^2(r)} + \frac{F[\cos 2\theta](r)}{F[1](r)}. \end{aligned} \tag{2.18}$$

Applying integration by parts to $F[\sin^2 2\theta](r)$, we have

$$\begin{aligned} F[\sin^2 2\theta](r) &= \int_0^{2\pi} \sin^2 2\theta \exp(r\cos 2\theta)d\theta \\ &= \frac{-1}{2r}\int_0^{2\pi} \sin 2\theta d(\exp(r\cos 2\theta)) \\ &= \frac{1}{r}\int_0^{2\pi} \cos 2\theta \exp(r\cos 2\theta)d\theta \\ &= \frac{1}{r}F[\cos 2\theta](r). \end{aligned} \tag{2.19}$$

Substituting (2.19) into (2.18), using the fact that the functional $F[\bullet]$ is linear and using the relation $\cos 2\theta = 1 - 2\sin^2\theta$, we obtain

$$\begin{aligned} Q_2(r) &= \frac{F[\cos 2\theta](r)}{F[1]^2(r)}\left(\left(1-\frac{1}{r}\right)F[1](r) - F[\cos 2\theta](r)\right) \\ &= \frac{1}{r}\cdot\frac{F[\cos 2\theta](r)}{F[1]^2(r)}\left(2F[r\sin^2\theta](r) - F[1](r)\right). \end{aligned} \tag{2.20}$$

In the proof of Theorem 2.1, we have shown that $F[\cos 2\theta](r) > 0$ for $r > 0$. It follows that to prove $Q_2(r) < 0$ for $r > 0$, we only need to show $2F[r\sin^2\theta](r) - F[1](r) < 0$ for $r > 0$.
Step 2. We now prove $2F[r\sin^2\theta](r) - F[1](r) < 0$ for $r > 0$.

Using $\cos 2\theta = 2\cos^2\theta - 1$, we rewrite and expand $\exp(r\cos 2\theta)$ as

$$\begin{aligned} \exp(r\cos 2\theta) &= \exp(-r)\exp(2r\cos^2\theta) \\ &= \exp(-r)\sum_{n=0}^{\infty}\frac{(2r)^n\cos^{2n}\theta}{n!}. \end{aligned} \tag{2.21}$$

Using this result, we write $2F[r\sin^2\theta](r) - F[1](r)$ as

$$\begin{aligned} &2F[r\sin^2\theta](r) - F[1](r) \\ &\quad= \exp(-r)\left[\sum_{n=0}^{\infty}\frac{(2r)^{n+1}}{n!}\int_0^{2\pi}\sin^2\theta\cos^{2n}\theta d\theta - \sum_{n=0}^{\infty}\frac{(2r)^n}{n!}\int_0^{2\pi}\cos^{2n}\theta d\theta\right] \\ &\quad= \exp(-r)\left[\sum_{n=0}^{\infty}\frac{(2r)^{n+1}}{n!}\int_0^{2\pi}\sin^2\theta\cos^{2n}\theta d\theta - 2\pi - \sum_{m=0}^{\infty}\frac{(2r)^{m+1}}{(m+1)!}\int_0^{2\pi}\cos^{2(m+1)}\theta d\theta\right] \\ &\quad= \exp(-r)\left[\sum_{n=0}^{\infty}\frac{(2r)^{n+1}}{n!}\int_0^{2\pi}\left(\sin^2\theta\cos^{2n}\theta - \frac{\cos^{2n+2}\theta}{n+1}\right)d\theta - 2\pi\right]. \end{aligned} \tag{2.22}$$

Integrating by parts, we obtain

$$\begin{aligned} \int_0^{2\pi}\sin^2\theta\cos^{2n}\theta d\theta &= -\int_0^{2\pi}\sin\theta\frac{d(\cos^{2n+1}\theta)}{2n+1} \\ &= \frac{1}{2n+1}\int_0^{2\pi}\cos^{2n+2}\theta d\theta. \end{aligned} \tag{2.23}$$

Substituting (2.23) into (2.22), we arrive at

$$\begin{aligned}&2F[r\sin^2\theta](r)-F[1](r)\\&\quad=\exp(-r)\left[-\sum_{n=1}^{\infty}\frac{(2r)^{n+1}}{n!}\frac{n}{(2n+1)(n+1)}\int_0^{2\pi}\cos^{2n+2}\theta d\theta-2\pi\right]<0\quad\text{for } r>0.\end{aligned}\tag{2.24}$$

This completes the proof of Theorem 2.2. □

3. Concluding remarks

We provide a rigorous proof on the monotonicity of a key function in the study of nematic liquid crystal polymers. This monotonicity has enabled us to establish analytically the tumbling region of shear-driven nematic liquid crystal polymers [1]. This paper serves as a theoretical advance in our studies of complex fluids.

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