Generalized drift velocity of a cholesteric texture in a temperature gradient

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We propose a general method to calculate the drift velocity of cholesteric textures subjected to a temperature gradient when the backflow effects are negligible. The textures may be Translationally Invariant Configurations (TICs) or localized structures such as cholesteric droplets or cholesteric fingers. For the TICs and for the droplets, the drift is rotational while for the fingers, the drift is translational. We show that for the TICs, the drift is only due to the thermomechanical coupling terms of Leslie (classical term) and of Akopyan and Zel'dovich (which are additional texture-dependent terms). For the localized structures, we show that another mechanism involving the temperature variations of the elastic constants and the existence of a transverse temperature gradient can lead to a drift which adds to the one due the classical thermomechanical effects.

1 Introduction

Cholesteric liquid crystals (LC) are chiral nematics. Under the action of a temperature gradient, their texture can drift in a permanent way. This drift can be rotational or translational. The most simple example of a rotational drift is the rotation of the planar texture obtained by orienting the cholesteric helix parallel to the temperature gradient and perpendicular to the glass plates treated for sliding planar anchoring.[1,2] In this geometry (usually called Leslie's geometry), the helix rotates at constant velocity under the action of the thermomechanical Leslie torque. This effect was observed both in compensated and diluted cholesteric mixtures. Another famous example is the rotation of cholesteric droplets when they coexist with their isotropic liquid at the melting temperature of the LC. This effect was discovered by Lehmann in 1900[3] and reproduced only recently.[4–7] This effect was first interpreted as due to the Leslie thermomechanical torque[8] but we recently showed that this interpretation is incomplete.[9,10] Cholesteric fingers (CF) are elongated, isolated structures that form in confined cholesteric samples treated for homeotropic (i.e. perpendicular) anchoring of the molecules at the surfaces. These textures can drift continuously when the sample is placed in a temperature gradient perpendicular to the plates. This phenomenon was first observed in a compensated mixture and was attributed to the

Leslie torque.[11] It was also observed in a diluted mixture close to the transition to the smectic phase, which is more surprising as we shall discuss later.[12]

The goal of the paper is to propose a general formalism to calculate the drift velocity of these textures. This method will enable us to show that other phenomena than the Leslie torque can lead to a drift. In particular, the role of the temperature variations of the elastic constants and of the "nematic like" thermomechanical coefficients[13,14] will be analyzed.

The plan of the article is the following. In Section 2, we establish the general formula for the drift velocity. This formula will then be applied to particular cases: – the rotation of the TICs (Translationally Invariant Configurations), the texture of which is uniform in the plane of the sample plates with planar sliding, homeotropic, or mixed boundary conditions (Section 3); – the drift of the cholesteric fingers (Section 4); and the rotation of the cholesteric droplets (Lehmann effect, Section 5). Conclusions will be drawn in Section 6.

2 Generalized drift velocity of a cholesteric texture in an external field

In this section, we focus on the special configurations where the total free energy $\mathcal{E}$ – including the bulk elastic energy $\mathcal{F}$ and the surface anchoring energy $\mathcal{W}$ on the boundaries – is invariant under a continuous transformation $\mathcal{T}_s$ parametrized by a parameter s, such that $\mathcal{T}_0$ is the identity. $\mathcal{E}$ is a functional of the director field $\left(\vec{n}, \vec{\nabla}\vec{n}\right)$, but may also explicitly depend on other fields such as the temperature field T. In practice, the elastic constants and the anchoring energy depend on the temperature

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so that $\mathcal{E}$ does explicitly depend on the temperature. A consequence of this invariance is that the configurations $\{\vec{n}, T\}$ and $\{\mathcal{T}_s\vec{n}, \mathcal{T}_s T\}$ can be deduced from each other by a global translation and (or) a solid rotation of the whole system.

By definition, $\mathcal{E}[\mathcal{T}_s\vec{n}, \mathcal{T}_s T]$ is independent of s. As a consequence,

$$\left.\frac{\partial \mathcal{E}[\mathcal{T}_s\vec{n}, \mathcal{T}_s T]}{\partial s}\right|_{s=0} = \int_V \left[-\vec{h}\cdot\frac{D\vec{n}}{Ds} + \frac{\delta\mathcal{F}}{\delta T}\frac{DT}{Ds}\right]dV$$

$$+ \int_S \left[\left(\underline{C}\cdot\vec{\nu} - \vec{h}_S\right)\cdot\frac{D\vec{n}}{Ds} + \frac{\delta\mathcal{W}}{\delta T}\frac{DT}{Ds}\right]dS = 0. \tag{1}$$

In these equations, $\vec{h} = -\dfrac{\delta\mathcal{F}}{\delta\vec{n}}$ is the molecular field of components $\dfrac{d}{dx_j}\dfrac{\partial f}{\partial n_{i,j}} - \dfrac{\partial f}{\partial n_i}$ by denoting by $f(n_i, n_{i,j}, T)$ the elastic free energy per unit volume (including the electric and magnetic free energy if an external field is applied), $\underline{C}$ is the elastic surface torque tensor of component $C_{ij} = \dfrac{\partial f}{\partial n_{i,j}}$, $\vec{h}_S = -\dfrac{\delta\mathcal{W}}{\delta\vec{n}}$ is the surface molecular field of components $-\dfrac{\partial w}{\partial n_i}$ by denoting by $w(n_i, T)$ the anchoring energy per unit surface. $\vec{\nu}$ is the unit vector perpendicular to the boundary of the LC and

$$\frac{D\vec{n}}{Ds} = \lim_{s\to 0}\frac{\mathcal{T}_s\vec{n} - \vec{n}}{s}, \quad \frac{DT}{Ds} = \lim_{s\to 0}\frac{\mathcal{T}_s T - T}{s}. \tag{2}$$

We now assume that the system is subjected to a temperature gradient, denoted by $\vec{G}$. By assuming that there is no flow of matter in the sample,† the torque equations for the director read[15,16]

$$\gamma_1\frac{\partial\vec{n}}{\partial t} = (\mathbb{I} - \vec{n}\otimes\vec{n})\cdot\left(\vec{h} + \vec{f}_{TM}\right) \tag{3}$$

in the bulk of the LC, and

$$\gamma_S\frac{\partial\vec{n}}{\partial t} = (\mathbb{I} - \vec{n}\otimes\vec{n})\cdot\left(\vec{h}_S - \underline{C}\cdot\vec{\nu}\right) \tag{4}$$

on the surface of the LC. Here, $\mathbb{I}$ is the identity matrix, $\otimes$ denotes the dyadic product of two vectors (with $\left(\vec{a}\otimes\vec{b}\right)_{ij} = a_i b_j$), γ_1 is the rotational viscosity, γ_S is a surface viscosity and $\vec{f}_{TM}$ is the thermomechanical force on the director. We propose the following form for $\vec{f}_{TM}$, in which the contribution of splay, twist and bend deformations is clear:

$$\vec{f}_{TM} = \bar{\xi}_1\left(\vec{\nabla}\cdot\vec{n}\right)\vec{G} + \left(\bar{\xi}_2\vec{n}\cdot\left[\vec{\nabla}\times\vec{n}\right] + \nu\right)\left(\vec{n}\times\vec{G}\right)$$

$$+ \bar{\xi}_3\left(\vec{n}\cdot\vec{G}\right)\left(\left[\vec{\nabla}\times\vec{n}\right]\times\vec{n}\right) \tag{5}$$

$$- \bar{\xi}_4\vec{\nabla}\cdot\left(\vec{G}\otimes\vec{n} - \left[\vec{G}\cdot\vec{n}\right]\mathbb{I}\right)$$

Note that $\vec{f}_{TM}$ includes the classical Leslie term (proportional to the Leslie coefficient ν),[16,17] as well as "texture dependent" terms first

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† This means in particular that we neglect any flow induced by the rotation of the director, the so-called backflow effects.

introduced by Akopyan and Zel'dovich[13] and recalculated more rigorously by Pleiner and Brand.[14] This expression includes terms coming from the macroscopic deformation of the director field (terms proportional to $\bar{\bar{\xi}}_i$ and $\vec{\nabla}\vec{n}$) and a term coming from the phase chirality, here due to the microscopic chirality of the molecules (Leslie's term proportional to ν). Macro- and microscopic chirality may both play a key role depending on the LC properties and on the sample geometry[2,18–20] The correspondence with the formulation of Akopyan and Zel'dovich and that of Pleiner and Brand, is given in the appendix.

By replacing $\vec{h}$ and $\vec{h}_S + \underline{C}\cdot\vec{\nu}$ in eqn (1) by their expressions given by eqn (3) and (4), we obtain

$$\int_V \gamma_1\frac{\partial\vec{n}}{\partial t}\cdot\frac{D\vec{n}}{Ds}dV + \int_S \gamma_S\frac{\partial\vec{n}}{\partial t}\cdot\frac{D\vec{n}}{Ds}dS$$

$$= \int_V \vec{f}_{TM}\cdot\frac{D\vec{n}}{Ds}dV + \int_V \frac{\delta\mathcal{F}}{\delta T}\frac{DT}{Ds}dV + \int_S \frac{\delta\mathcal{W}}{\delta T}\frac{DT}{Ds}dS \tag{6}$$

Without the external field $\vec{G}$, the director field evolves to an equilibrium configuration $\vec{n}_0$ which minimizes the free energy $\mathcal{E}$. This solution is not unique because $\mathcal{T}_s\vec{n}_0$ is also a solution. This comes from the Curie symmetry principle according to which the set of solutions of the equations has the same symmetry as the equations. In the presence of $\vec{G}$, the system can evolve to a stationary state with a constant "drift" of the parameter s, such that

$$\vec{n}(t) = \mathcal{T}_{s(t)}\vec{n}(0) \tag{7}$$

with $s(t) = v_s t$ drifting at constant velocity v_s. In this stationary state,

$$\frac{\partial\vec{n}}{\partial t} = \frac{D\vec{n}}{Ds}v_s. \tag{8}$$

By replacing $\dfrac{\partial\vec{n}}{\partial t}$ by its expression in eqn (6), we calculate two contributions to v_s:

$$v_s = v_s^{TM} + v_s^E, \tag{9}$$

where v_s^{TM} is the drift velocity due to the thermomechanical cross coupling and v_s^E the drift velocity due to the variation of the free energy with the temperature:

$$v_s^{TM} = \frac{1}{I_\gamma}\int_V \vec{f}_{TM}\cdot\frac{D\vec{n}}{Ds}dV, \tag{10}$$

$$v_s^E = \frac{1}{I_\gamma}\left[\int_V \frac{\delta\mathcal{F}}{\delta T}\frac{DT}{Ds}dV + \int_S \frac{\delta\mathcal{W}}{\delta T}\frac{DT}{Ds}dS\right], \tag{11}$$

with

$$I_\gamma = \int_V \gamma_1\left(\frac{D\vec{n}}{Ds}\right)^2 dV + \int_S \gamma_S\left(\frac{D\vec{n}}{Ds}\right)^2 dS. \tag{12}$$

Formula (11) shows that, in addition to the thermomechanical terms, the variation in temperature of both the elastic constants and the anchoring energy can lead to a drift. At this level, it must be emphasized that f is defined within an additive constant $f_0(T)$ only function of temperature. This function does not contribute to the velocity because $\int_V \dfrac{df_0}{dT}\dfrac{DT}{Ds}dV = \int_V \dfrac{Df_0}{Ds}dV = \dfrac{\partial}{\partial s}\int_V f_0 dV = 0$ due to the s invariance. This can be

checked directly from the examples given below in Sections (3–5). The same holds for w that is defined within an additive constant $w_0(T)$ only function of temperature. It may also be noted that the $\bar{\bar{\xi}}_4$ term in v_s^{TM} can be put in the form $\frac{D}{Ds}\left[\left(\vec{G}\cdot\vec{n}\right)\left(\vec{\nabla}\cdot\vec{n}\right)\right] - \vec{\nabla}\cdot\left[\left(\vec{G}\cdot\vec{n}\right)\frac{D\vec{n}}{Ds}\right]$ if $\vec{G}$ is assumed uniform and the derivatives $\frac{D}{Ds}$ and $\vec{\nabla}$ commute, which is the case for the rotational and translational drift phenomena addressed in the next three sections. In this case, the integral of the $\bar{\bar{\xi}}_4$ term also reduces to surface contributions which vanish for strong zenithal anchoring and in the absence of singularities like disclinations.

In practice, the LC sample of thickness d is prepared between two parallel glass plates of total thickness $h \gg d$ and the temperature gradient $\vec{G}$ is obtained by imposing a temperature difference ΔT between the two external faces of the sample. In the limit $\Delta T \to 0$, the local gradient $\vec{G}$ in the LC is proportional to the imposed temperature gradient $\hat{G} = \Delta T/h$. The same holds for $\vec{f}_{TM}$ and $\frac{DT}{Ds}$. This defines the linear regime in which

$$v_s \propto \hat{G} = \frac{\Delta T}{h} \tag{13}$$

This proportionality is generally observed in experiments, so our calculations can be restricted to first order in $\hat{G}$. In this case, all integrals in eqn (10)–(12) can be evaluated in the equilibrium configuration $\vec{n}_0$ and with equilibrium values of the material constants.

3 Application to translationaly invariant configurations

3.1 General configuration

If the texture is invariant by translation in the plane (x, y) with the z-axis perpendicular to the plates located at $z = 0$ and $z = d$, there are no distortions in the (x, y) plane. The equations of the system are thus invariant by a rotation of the director around $\vec{e}_z$ by the same angle Φ everywhere. Furthermore, $\vec{G}$ is parallel to $\vec{e}_z$ and the temperature field is independent of Φ. Taking $s = \Phi$, we find $\frac{D\vec{n}}{D\Phi} = \vec{e}_z \times \vec{n}$ and $\frac{DT}{D\Phi} = 0$. Hence, in these geometries, only the thermomechanical couplings contribute to the angular drift and

$$\omega = \frac{d\Phi}{dt} = v_\Phi = v_\Phi^{TM}. \tag{14}$$

The director components are

$$\vec{n} = \begin{pmatrix} \sin\alpha\cos\phi \\ \sin\alpha\sin\phi \\ \cos\alpha \end{pmatrix}, \tag{15}$$

where the angles α and ϕ are assumed to only depend on z. The angular drift velocity can be decomposed into three terms:

$$\omega = \frac{1}{I_\gamma}(I_\nu + I_2 + I_3) \tag{16}$$

with

$$I_\nu = -\int_0^d G\nu\sin^2\alpha\,dz, \tag{17}$$

$$I_2 = \int_0^d G\bar{\bar{\xi}}_2\phi_{,z}\sin^4\alpha\,dz, \tag{18}$$

$$I_3 = \int_0^d G\bar{\bar{\xi}}_3\phi_{,z}\cos^2\alpha\sin^2\alpha\,dz, \tag{19}$$

and

$$I_\gamma = \int_0^d \gamma_1\sin^2\alpha\,dz + \gamma_S(0)\sin^2\alpha(0) + \gamma_S(d)\sin^2\alpha(d) \tag{20}$$

The temperature gradient G may depend on z in general because of the anisotropy of the heat conductivity. The heat flux J, on the other hand, is independent of z in the stationary regime. Strictly speaking, there is a linear cross coupling between J and ω ($J \approx \kappa G + \nu\omega$ where κ is the heat conductivity of the LC and $\omega \approx \nu G/\gamma_1$). However, this coupling is completely negligible because it gives a relative correction to the heat flux of order $\nu^2/\kappa\gamma_1 \sim 3 \times 10^{-12}$ by taking $\kappa \approx 0.15$ W m^{-1} K^{-1},[16] $\gamma_1 \approx 0.02$ Pa s[16] and $\nu \approx 10^{-7}$ kg K^{-1} s^{-2}.[2] So we can write $J = (\kappa_\perp\sin^2\alpha + \kappa_\parallel\cos^2\alpha)G \approx \kappa_g\hat{G}$ (since $h \gg d$) by denoting by $\kappa_\perp$ ($\kappa_\parallel$) the heat conductivity perpendicular (parallel) to the director and by κ_g the heat conductivity of the glass plates limiting the sample. This gives

$$G = \frac{\kappa_g}{\kappa_\perp\sin^2\alpha + \kappa_\parallel\cos^2\alpha}\hat{G}. \tag{21}$$

In the following, we apply eqn (16) to particular configurations, starting with the simplest one first described by Leslie.[21]

3.2 Rotation of the planar texture under sliding anchoring conditions

It is known[2,22] that the director rotates continuously in planar cholesteric samples when the surfaces are treated for sliding anchoring and a temperature gradient is applied perpendicularly to the plates (Leslie's configuration[21]). The director remains planar with $\alpha = \pi/2$. By using eqn (16), we obtain:

$$\omega = \hat{G}\frac{\kappa_g}{\kappa_\perp}\frac{\int_0^d\left(\bar{\bar{\xi}}_2\phi_{,z} - \nu\right)dz}{\int_0^d\gamma_1\,dz + \gamma_S(0) + \gamma_S(d)}. \tag{22}$$

In the linear regime, $\phi_{,z}$ can be replaced by its equilibrium value q_0 and the material constants γ_1, ν and $\bar{\bar{\xi}}_2$ can be taken

independent of z, yielding to the simplified equation

$$\omega = \hat{G}\frac{\kappa_\mathrm{g}}{\kappa_\perp}\frac{\bar{\xi}_2 q_0 - \nu}{\gamma_1 + \frac{1}{d}[\gamma_\mathrm{S}(0) + \gamma_\mathrm{S}(d)]}. \quad (23)$$

This equation shows that the thermomechanical coefficient measured experimentally in this geometry is not ν but $\bar{\nu} = \nu - \bar{\xi}_2 q_0.$‡ It is important to note that in this geometry the director remains planar. As a consequence there are only twist deformations and the backflow disappears.[15,16] This means that the no-flow approximation is exact in this particular case and that formula (3) is exact in the Leslie's configuration.

3.3 Rotation of the TIC under homeotropic anchoring conditions

We now consider a cholesteric LC of negative dielectric anisotropy sandwiched between two parallel electrodes treated for strong homeotropic anchoring. Let $C = d/p$ denote the confinement ratio (d is the sample thickness and $p = 2\pi/q_0$ the equilibrium cholesteric pitch). It can be shown that if $C < C^\star = K_{32}/2$ where $K_{32} = K_3/K_2$ is the ratio of the bend and twist constants, the cholesteric phase unwinds and forms a homeotropic nematic phase. Conversely, it is possible to wind again the cholesteric phase by applying a destabilizing AC electric field $E = V/d$. If the sample is thin enough, the configuration which develops above the critical voltage

$$V_\mathrm{c}^2 = \frac{4\pi^2 K_3}{-\varepsilon_\mathrm{a}}\left(\frac{1}{4} - \frac{C^2}{K_{32}^2}\right) \quad (24)$$

is translationaly invariant in the plane of the sample (TIC) with its helical axis perpendicular to the electrodes. This configuration, shown in Fig. 1, develops when $C < C_\mathrm{tr} < C^\star$ where C_tr defines the position of a triple point in the parameter plane (E, C).[16,23] In this regime, the Nematic-to-TIC transition is second order. As the consequence, the tilt angle α of the director with respect to the z axis is small just above the onset of instability and $\vec{n}$ has for components $(\alpha \cos\phi, \alpha \sin\phi, 1 - \alpha^2)$ at second order in α.

We now assume that a temperature gradient is applied perpendicularly to the electrodes. By using eqn (16), we get at lowest order in α:

$$\omega = \hat{G}\frac{\kappa_\mathrm{g}}{\kappa_\|}\frac{\int_0^d (\bar{\xi}_3 \phi_{,z} - \nu)\alpha^2 \mathrm{d}z}{\int_0^d \gamma_1 \alpha^2 \mathrm{d}z}. \quad (25)$$

It can be shown that $\phi_{,z} = q_0/K_{32}$ at equilibrium.[16,23] In the linear regime, the thermomechanical and elastic coefficients

‡ It must be emphasized that in our previous papers, we "regularized" the expression of $\vec{f}_\mathrm{TM}$ in the cholesteric phase by replacing the term $\xi_2 (\vec{n} \cdot \vec{\nabla} \times \vec{n})(\vec{n} \times \vec{G})$ of the Akopyan and Zel'dovich equation by $\xi_2 (\vec{n} \cdot \vec{\nabla} \times \vec{n} + q_0)(\vec{n} \times \vec{G})$ in order that $\vec{f}_\mathrm{TM}$ vanishes in the cholesteric phase when the helix is not distorted. With this choice, the measured quantity is ν in the linear regime[10,11]. *A posteriori*, we think that this choice is not justified because the system is out of equilibrium as long as the cholesteric phase is subjected to a temperature gradient, even when the helix is not distorted. This is the reason why we do not regularize $\vec{f}_\mathrm{TM}$ in this paper.
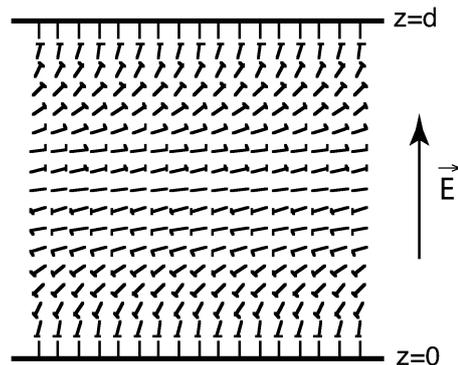

Fig. 1 Director field in the TIC induced by a vertical electric field. Tilted molecules are represented by nails, proportional in length to the director projection in the plane of the drawing. The head of the nails is below the plane of the drawing and their points are directed towards the observer.

can again be taken as constant, and the integrals of α^2 simplify. Finally, it remains:

$$\omega = \hat{G}\frac{\kappa_\mathrm{g}}{\kappa_\|}\frac{\bar{\xi}_3 \frac{q_0}{K_{32}} - \nu}{\gamma_1}. \quad (26)$$

3.4 Application to the rotation of the TIC under mixed anchoring conditions

In practice, it is possible to combine the two previous geometries by treating one plate (for instance the top one at $z = d$) for strong sliding planar anchoring and the other at $z = 0$ for strong homeotropic anchoring. With these boundary conditions, a TIC forms if the sample is thin enough, typically when $C = d/p < 1/2$. For larger thickness, stripes develop and the texture is no longer invariant by translation.[24] Using eqn (16) in the linear regime, where the material constants can be taken constant over the sample thickness, yields

$$\omega = \hat{G}\frac{\kappa_\mathrm{g}}{\kappa_\|}\frac{\bar{\xi}_2 q_0 \bar{I}_2 + \bar{\xi}_3 q_0 \bar{I}_3 - \nu \bar{I}_\nu}{\gamma_1 \bar{I}_\gamma + \frac{1}{d}\gamma_\mathrm{S}(d)} \quad (27)$$

with the dimensionless integrals

$$\bar{I}_\nu = \frac{1}{d}\int_0^d \frac{\sin^2 \alpha}{1 - \varepsilon \sin^2 \alpha}\mathrm{d}z, \quad (28)$$

$$\bar{I}_2 = \frac{1}{q_0 d}\int_0^d \frac{\phi_{,z} \sin^4 \alpha}{1 - \varepsilon \sin^2 \alpha}\mathrm{d}z, \quad (29)$$

$$\bar{I}_3 = \frac{1}{q_0 d}\int_0^d \frac{\phi_{,z} \cos^2 \alpha \sin^2 \alpha}{1 - \varepsilon \sin^2 \alpha}\mathrm{d}z, \quad (30)$$

$$\bar{I}_\gamma = \frac{1}{d}\int_0^d \sin^2 \alpha \, \mathrm{d}z. \quad (31)$$

Here, $\varepsilon = 1 - \kappa_\perp/\kappa_\|$ is the relative anisotropy of thermal conductivity. The integrals can be computed numerically with Mathematica once the two differential equations that describe the static torque balance: $\frac{\delta \mathcal{F}}{\delta \alpha} = 0$ and $\frac{\delta \mathcal{F}}{\delta \phi} = 0$ are solved.
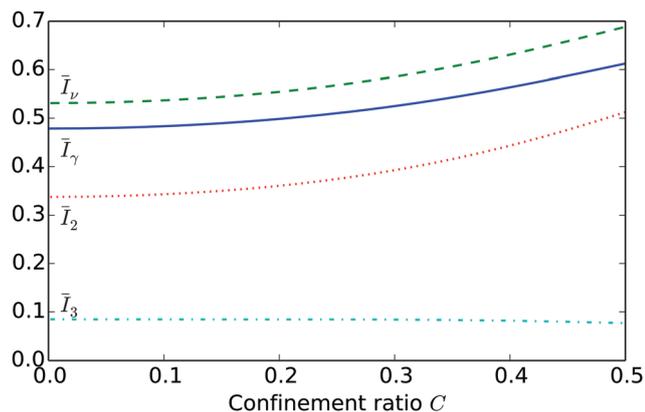
Fig. 2 Integrals $\bar{I}_\gamma$, $\bar{I}_\nu$, $\bar{I}_2$ and $\bar{I}_3$ as a function of the confinement ratio $C = d/p$. Values calculated for MBBA at the transition to the isotropic liquid.

We performed the calculation for different values of C by choosing K_1 = 1.87 pN, K_2 = 1.15 pN, K_3 = 2.64 pN and ε = 0.13. These values correspond to MBBA at the nematic to isotropic phase transition.[25,26] This choice was dictated by the fact that MBBA is a very classical LC with a negative dielectric anisotropy. The results are shown in Fig. 2.

These calculations show that measuring ω in the three geometries described above should allow, in principle, to determine ν, $\bar{\bar{\xi}}_2$ and $\bar{\bar{\xi}}_3$.

4 Application to the drift of cholesteric fingers

In homeotropic samples, cholesteric fingers of the first type (CF1) form when the confinement ratio $C = p/d$ is close to 1.[27] The CF1s are elongated, isolated textures that minimize the frustration created by the boundary conditions. Their structure is invariant by translation along their long axis and is shown in Fig. 3. Previous experiments have shown that the CF1s can drift perpendicularly to their axis and form spirals when they are subjected to a temperature gradient. This effect was first observed in compensated mixtures where isolated CF1s form when the temperature is close to the compensation
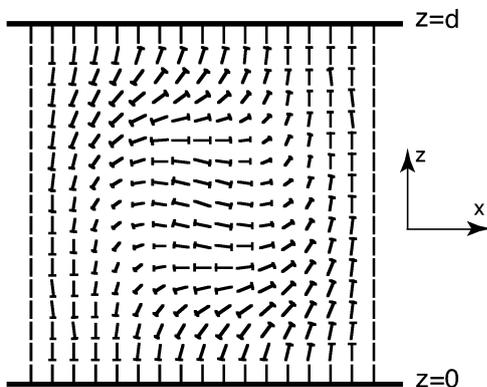

Fig. 3 Director field inside a cholesteric finger of the first type (CF1).

temperature.[11] In this case, the drift is mainly due to the Leslie torque acting on the director. In the next paragraph, we show how to recover this result from our general formulation of the problem.

4.1 Finger drift in compensated mixtures: model based on the existence of the thermomechanical terms of Leslie, Akopyan and Zel'dovich

In this paragraph, we focus on the thermomechanical contribution ν^{TM} to the drift velocity. For simplicity, we assume that the homeotropic anchoring is very strong. As a result, $\vec{n}$ does not change on the plates and the surface dissipation becomes negligible. We now consider a straight isolated CF1 with the axis parallel to the $\vec{e}_y$ axis (Fig. 3). The plates are perpendicular to the $\vec{e}_z$ axis. We denote by $\vec{n}_0$ the equilibrium solution obtained when $\vec{G} = 0$ and by $\vec{n}$ the general solution when $\vec{G} \neq 0$. The system equations are invariant by any translation X along $\vec{e}_x$. By using $s = X$, it comes $\frac{D\vec{n}}{DX} = \lim_{X \to 0} \frac{\vec{n}(x - X) - \vec{n}(x)}{X} = -\frac{\partial \vec{n}}{\partial x}$. By definition, the generalized velocity $\nu^{TM} = dX/dt$ given by the general eqn (10) is the drift velocity ν of the finger. It reads by taking into account the assumptions made at the beginning of the paragraph:

$$\nu^{TM} = -\frac{\int_V \vec{f}_{TM} \cdot \frac{\partial \vec{n}}{\partial x} dV}{\int_V \gamma_1 \left(\frac{\partial \vec{n}}{\partial x}\right)^2 dV} \tag{32}$$

The formula further simplifies neglecting the anisotropy of thermal conductivity, *i.e.* by assuming that the temperature gradient is little different from the average gradient $\hat{G}\frac{\kappa_g}{\kappa_\parallel}\vec{e}_z$. In the linear regime, $\vec{n}$ can also be replaced by the equilibrium solution $\vec{n}_0$ and the material constants γ_1, ν and $\bar{\bar{\xi}}_i$ (i = 1–4) are independent of the temperature. Under these assumptions, we obtain by using the expression of $\vec{f}_{TM}$ given in eqn (5):

$$\nu^{TM} = -d\hat{G}\frac{\kappa_g}{\kappa_\parallel} \frac{\nu J_\nu + \bar{\bar{\xi}}_1 q_0 J_1 + \bar{\bar{\xi}}_2 q_0 J_2 + \bar{\bar{\xi}}_3 q_0 J_3}{\gamma_1 J_\gamma} \tag{33}$$

where the dimensionless integrals J_i are defined by

$$J_\nu = \frac{1}{d}\int (\vec{n}_0 \times \vec{e}_z) \cdot \frac{\partial \vec{n}_0}{\partial x} dxdz, \tag{34}$$

$$J_1 = \frac{1}{q_0 d}\int \left(\vec{\nabla} \cdot \vec{n}_0\right)\vec{e}_z \cdot \frac{\partial \vec{n}_0}{\partial x} dxdz, \tag{35}$$

$$J_2 = \frac{1}{q_0 d}\int \left(\vec{n}_0 \cdot \left[\vec{\nabla} \times \vec{n}_0\right]\right)(\vec{n}_0 \times \vec{e}_z) \cdot \frac{\partial \vec{n}_0}{\partial x} dxdz, \tag{36}$$

$$J_3 = \frac{1}{q_0 d}\int (\vec{n}_0 \cdot \vec{e}_z)\left(\left[\vec{\nabla} \times \vec{n}_0\right] \times \vec{n}_0\right) \cdot \frac{\partial \vec{n}_0}{\partial x} dxdz, \tag{37}$$

$$J_\gamma = \int \left(\frac{\partial \vec{n}_0}{\partial x}\right)^2 dxdz. \tag{38}$$

This formula generalizes a formula already given in ref. 11 and 28 where the thermomechanical coefficients $\bar{\bar{\xi}}_i$ were neglected.§

It must be noted that the fingers exist when $C \approx 1$. As a consequence, all these dimensionless integrals are only functions of the ratios of the elastic constants. This shows that the drift velocity is proportional to d. Another important point to emphasize is that, for symmetry reasons, these integrals do not change sign when q_0 changes sign.¶

This calculation shows that the thermomechanical terms $\bar{\bar{\xi}}_i$ may lead to a drift of the CF1s. In the compensated mixtures, the dominating term is the Leslie term since the others in $\bar{\bar{\xi}}_i q_0$ are expected to be small close to the compensation temperature where $q_0 = 0$. This explanation of the drift of the CF1s was proposed in ref. 11 and was confirmed by the fact that the drift velocity is almost the same on both sides of the compensation temperature. In addition, the value of ν interpolated from these measurements of the drift velocity is compatible with the value of ν measured directly in the Leslie's geometry at the compensation temperature.

4.2 Finger drift in diluted cholesteric mixtures: model based on the temperature variation of the elastic constants

In the diluted mixtures, the CF1s usually do not drift in a measurable way. This is expected from the previous model because the coefficient $\bar{\nu}$ (which we suppose to be of the same order of magnitude as ν and $\bar{\bar{\xi}} q_0$) is too small, typically 10 to 100 times smaller than the coefficient ν measured in the compensated mixtures. This is due to the fact that in the diluted mixtures the concentration of chiral molecules is also 10 to 100 times smaller than in the compensated mixtures (usually obtained by mixing a LC with a large concentration of cholesteryl chloride, up to 60% by mass).

There is nonetheless an exception that was observed in an eutectic mixture of 8CB and 8OCB doped with a small amount of R811. This mixture has a smectic A phase at low temperature. In this mixture, it was observed that the CF1s start to drift in a measurable way when the temperature approaches the transition temperature to the smectic phase. This is very surprising because the viscosity γ_1 diverges in this limit,[29] which could lead to a fast decrease of the drift velocity. The only possibility to explain this observation within the previous model of Section 4.1 would be that the thermomechanical coefficients diverge faster than γ_1. In order to test this hypothesis, we measured the Leslie coefficient in the diluted mixture 8CB + 1 wt% R811 and found that ν does not diverge at the transition.‖ This result shows that the previous model cannot explain the drift of the fingers close to the smectic phase. Another explanation must be found.

It turns out that the general eqn (11) contains another explanation. Indeed, this expression shows that two other

terms, that we neglect so far, can lead to a drift. The first one is a volume term proportional to $\dfrac{\delta\mathcal{F}}{\delta T}$ and the second one a surface term proportional to $\dfrac{\delta\mathcal{W}}{\delta T}$. Both are proportional to the horizontal temperature gradient since $\dfrac{DT}{DX} = \lim_{X \to 0} \dfrac{T(x-X) - T(x)}{X} = -\dfrac{\partial T}{\partial x}$. These two terms can dominate the thermomechanical terms if $\mathcal{F}$ and (or) $\mathcal{W}$ strongly depend on temperature. This is expected close to the transition to the smectic phase as explained below. In this situation, the drift velocity reads:

$$v^E = -\frac{\int \dfrac{\delta\mathcal{F}}{\delta T}\dfrac{\partial T}{\partial x}\mathrm{d}x\mathrm{d}z + \int \dfrac{\delta\mathcal{W}}{\delta T}(0,d)\dfrac{\partial T}{\partial x}\mathrm{d}x}{\int \gamma_1 \left(\dfrac{\partial \vec{n}}{\partial x}\right)^2 \mathrm{d}x\mathrm{d}z + \int \gamma_S(0,d)\left(\dfrac{\partial \vec{n}}{\partial x}\right)^2 \mathrm{d}x}. \tag{39}$$

This formula simplifies if the anchoring energy is very large and if the thermal conductivity of the plates is much larger than that of the LC. In this case, the two surface integrals in γ_S and can be neglected because $\dfrac{\partial \vec{n}}{\partial x} \approx 0$ and $\dfrac{\partial T}{\partial x} \approx 0$ on the plates. This gives:

$$v^E = -\frac{\int \dfrac{\delta\mathcal{F}}{\delta T}\dfrac{\partial T}{\partial x}\mathrm{d}x\mathrm{d}z}{\int \gamma_1 \left(\dfrac{\partial \vec{n}}{\partial x}\right)^2 \mathrm{d}x\mathrm{d}z} \tag{40}$$

This new model shows that the temperature variations of the elastic constants can lead to a drift. In general, the elastic constants change little with temperature and this effect is negligible. The situation is different close to the transition to the smectic phase where the bend and the twist constants K_3 and K_2 diverge because of the presence of smectic cybotactic groups.[29] This divergence could explain the drift observed experimentally.

Another important point of the model is that it is not the vertical temperature gradient, but the horizontal one $\dfrac{\partial T}{\partial x}$, that is directly responsible for the drift. This gradient appears as long as the finger is subjected to an average temperature gradient along $\vec{e}_z$. The reason is that the thermal field lines are distorted inside the finger because of the anisotropy of the thermal conductivity. In addition, a finger has no mirror symmetry because the cholesteric phase is chiral. As a consequence, the temperature field also has no mirror symmetry so that one side (in the x-direction) of the finger must be colder than the other.

The drift can be qualitatively explained as follows: because the elastic constants of the cholesteric LC depend on temperature, the free energy of the finger is sensible to the temperature field. For this reason, the finger prefers to shift to the side where it has the lower energy. In return, the temperature field follows the finger as a propagating wave. This pushes the finger forward like a surfer on a wave. This effect must be especially strong close to the smectic transition where the twist and bend elastic constants diverge.

To conclude this paragraph, let us estimate the drift velocity. The first question is to calculate the horizontal gradient.

---

§ We mention that there is an error of sign in eqn (3) of ref. 11. On the other hand, all the rest is correct in the paper, in particular the numerical value of the constant A calculated from this equation.

¶ When q_0 changes sign, the equilibrium configuration is changed to its mirror image in a (y, z) plane.

‖ P. Oswald, unpublished results.

At small $\hat{G}$ (linear regime) it is obtained by solving the heat equation. At first order in $\hat{G}$, this equation reads

$$\vec{\nabla} \cdot \left(\kappa_\perp \vec{\nabla} T + \kappa_a \left(\vec{n}_0 \cdot \vec{\nabla} T \right) \vec{n}_0 \right) = 0 \qquad (41)$$

where $\kappa_a = \kappa_\parallel - \kappa_\perp$ is the anisotropy of conductivity. Note that in this equation, the heat production due to the rotation of the director has been neglected as well as the non stationary term $\frac{\partial T}{\partial t}$ as the calculation is done in the equilibrium configuration $\vec{n}_0$. We can always decompose the temperature field as $T(x,z) = T_0 + \hat{G}\frac{\kappa_g}{\kappa_\parallel}(z + gd)$ by introducing the relative perturbation of temperature $g(x, z)$ due to the finger and by denoting by T_0 the temperature of the bottom plate. With this notation, it comes $\frac{\partial T}{\partial x} = \hat{G}\frac{\kappa_g}{\kappa_\parallel}d\frac{\partial g}{\partial x}$. By assuming that the conductivities are constant, the equation for g reads

$$\vec{\nabla} \cdot \left(\vec{\nabla} g + \frac{\kappa_a}{\kappa_\perp}\left[\vec{n}_0 \cdot \vec{\nabla} g + \frac{\vec{n}_0 \cdot \vec{e}_z}{d} \right] \vec{n}_0 \right) = 0, \qquad (42)$$

with the boundary condition $g = 0$ on both plates. This equation, which can be solved numerically, shows that $g \neq 0$ as long as $\kappa_a \neq 0$. Knowing that $\frac{\partial T}{\partial x} = \hat{G}\frac{\kappa_g}{\kappa_\parallel}d\frac{\partial g}{\partial x}$, eqn (40) becomes:

$$v^E = -\hat{G}\frac{\kappa_g}{\kappa_\parallel}d\frac{\int \frac{\delta\mathcal{F}}{\delta T}\frac{\partial g}{\partial x}dxdz}{\int \gamma_1 \left(\frac{\partial \vec{n}_0}{\partial x}\right)^2 dxdz}, \qquad (43)$$

where $\vec{n}$ has been replaced by $\vec{n}_0$ (linear regime).

This equation shows that the temperature gradient along x generates a constant drift velocity proportional to the applied temperature gradient, in the same way as the thermomechanical coupling. In other words, this new mechanism acts as an effective Leslie coupling characterized by an effective coefficient ν_{eff}. We can estimate the order of magnitude of ν_{eff} for a CF1 by writing that

$$\nu_{eff}\left(\frac{\partial \vec{n}}{\partial x} \times \vec{n}\right) \cdot \vec{e}_z \sim d\frac{\delta\mathcal{F}}{\delta T}\frac{\partial g}{\partial x}. \qquad (44)$$

This gives

$$\nu_{eff} \sim \frac{\delta\mathcal{F}}{\delta T}dg. \qquad (45)$$

By taking $\nabla \vec{n} \sim q_0 \sim \frac{1}{d}$, $\frac{\delta\mathcal{F}}{\delta T} \sim \frac{\partial K}{\partial T}(\nabla \vec{n})^2$ (with K a typical elastic constant) and $\frac{g}{d} \sim \frac{\kappa_a}{\kappa_\perp}\nabla \vec{n}$ according to eqn (42), we finally obtain

$$\nu_{eff} \sim \frac{\partial K}{\partial T}\frac{\kappa_a}{\kappa_\perp}q_0. \qquad (46)$$

This formula again shows that the drift disappears if $\kappa_a = 0$ because the horizontal gradient disappears in this case. More important, the eqn (46) states clearly that the sign of ν_{eff} depends on the sign of q_0. Indeed, under the transformation $x \rightarrow -x$, $n_x \rightarrow -n_x$

corresponding to a mirror symmetry with respect to the plane (y, z), $\vec{e}_z \cdot \left(\frac{\partial \vec{n}}{\partial x} \times \vec{n}\right)$ is invariant whereas $\frac{\partial g}{\partial x}$ changes sign. As a result, ν_{eff} changes sign when q_0 changes sign, contrary to the Leslie coefficient ν, the sign of which is independent of the sign of q_0. In addition, ν_{eff} is inversely proportional to d because q_0d of the order of 2π in a finger (this is the condition of existence of a finger).

Finally, the drift velocity is obtained from eqn (33) and (46) and reads to within a numerical factor:

$$v^E \sim -\hat{G}\frac{\kappa_g}{\kappa_\parallel}\frac{\partial K}{\partial T}\frac{\kappa_a}{\kappa_\perp}\frac{q_0d}{\gamma_1} \qquad (47)$$

This model could explain the drift of the CF1s close to a smectic phase transition. The role of the anchoring is more difficult to grasp because there is no study in the literature of the anchoring energy close to a smectic phase. On the other hand, it has been shown that the smectic phase wets the plates over a thickness of the order of the smectic correlation length.[30] This could lead to additional drift due to a strong variation of W as a function of the temperature.

5 Application to the rotation of cholesteric droplets (Lehmann effect)

To end this paper we could question whether this new mechanism introduced to explain the drift of the fingers close to a smectic transition could not also explain the rotation of cholesteric droplets in the isotropic liquid, the famous Lehmann effect. Indeed, the general eqn (6) also holds in this system when the invariance under a "solid rotation" of the texture without flow of matter, is used. Note that the absence of flow of matter is sustained by recent experiments of fluorescence recovery after photobleaching (FRAP) in the vicinity of the droplets.[31] In this case, $s = \Theta$ – the angle of solid rotation around the axis parallel to $\vec{e}_z$ and passing through the center of the droplet, $\frac{DT}{D\Theta} = -\frac{\partial T}{\partial \vartheta}$ and $\frac{D\vec{n}}{D\Theta} = \vec{e}_z \times \vec{n} - \frac{\partial \vec{n}}{\partial \vartheta}$ by denoting by ϑ the polar angle in cylindrical coordinates.

So far we only considered the role of the Leslie coupling. In this case, our general formula gives in the linear regime and by assuming that $\vec{G} = G\vec{e}_z$ is constant inside the droplet and by neglecting the surface dissipation, which we expect to be very small at the cholesteric–isotropic interface:

$$\omega = \frac{d\Theta}{dt} = G\frac{\nu L_\nu + \bar{\xi}_1 q_0 L_1 + \bar{\xi}_2 q_0 L_2 + \bar{\xi}_3 q_0 L_3}{\gamma_1 L_\gamma} \qquad (48)$$

with the dimensionless integrals

$$L_\gamma = \frac{1}{V}\int_V \left(\frac{D\vec{n}_0}{D\Theta}\right)^2 dV, \qquad (49)$$

$$L_\nu = \frac{1}{V}\int_V (\vec{n}_0 \times \vec{e}_z) \cdot \frac{D\vec{n}_0}{D\Theta}dV, \qquad (50)$$

$$L_1 = \frac{1}{q_0 V}\int_V \left(\vec{\nabla} \cdot \vec{n}_0\right)\vec{e}_z \cdot \frac{D\vec{n}_0}{D\Theta}dV, \qquad (51)$$

$$L_2 = \frac{1}{q_0 V}\int_V \left(\vec{n}_0 \cdot \left[\vec{\nabla} \times \vec{n}_0\right]\right)(\vec{n}_0 \times \vec{e}_z)\cdot\frac{D\vec{n}_0}{D\Theta}\mathrm{d}V, \quad (52)$$

$$L_3 = \frac{1}{q_0 V}\int_V (\vec{n}_0 \cdot \vec{e}_z)\left(\left[\vec{\nabla} \times \vec{n}_0\right] \times \vec{n}_0\right)\cdot\frac{D\vec{n}_0}{D\Theta}\mathrm{d}V. \quad (53)$$

In banded droplets for instance ("banded" because of their striped contrast under the microscope), in which the helical axis is perpendicular to the temperature gradient, the cholesteric layers are little deformed[5,6] which means that the local twist is close to q_0. In this case, there are no splay nor bend deformations, so that $L_1 = L_3 = 0$ and $L_2 = -L_\nu$ since $\vec{n}_0 \cdot \left[\vec{\nabla} \times \vec{n}_0\right] = -q_0$. Then eqn (48) simplifies to

$$\omega = \frac{\bar{\nu} G L_\nu}{\gamma_1 L_\gamma}, \quad (54)$$

where $\bar{\nu} = \nu - \bar{\bar{\xi}}_2 q_0$ is the thermomechanical coefficient measured in the planar TIC (Leslie geometry). This is the formula given in ref. 4.** From this formula and the measurements of the rotation velocity of the droplets, a value of $\bar{\nu}$ was obtained. The problem is that this value is always much larger (by a factor of 10 in the compensated mixture to 1000 in the diluted mixtures) than the value measured in the Leslie's configuration. This observation and the fact that the sign of the rotation velocity is not always given by the sign of $\bar{\nu}$[22] led us to the conclusion that the Leslie coupling is not directly responsible for the Lehmann rotation. On the other hand, in all cases, the sign of ω is given by the sign of q_0.[10,32] One possibility to explain this observation would be that the helix is slightly deformed inside the droplets and that thermomechanical coefficients $\bar{\bar{\xi}}_i$ are responsible for the rotation, even if the $\bar{\nu}$ terms plays a negligible role. This explanation is sustained by recent observations of the rotation of twisted bipolar droplets observed in a chromonic nematic LC.[20] In this case, $\nu = 0$ (we are dealing with a nematic phase), but the director field inside the droplets is twisted because of the elastic anisotropy of the phase ($K_2 \ll K_1$ and K_3). In these conditions, only the terms in $\bar{\bar{\xi}}_i$ can lead to a rotation.

Another possibility would be that the terms proportional to $\frac{\delta\mathcal{F}}{\delta T}$ and $\frac{\delta\mathcal{W}}{\delta T}$ are responsible for the rotation. In this case, the general formula gives:

$$\omega^E = -\frac{\int_V \frac{\delta\mathcal{F}}{\delta T}\frac{\partial T}{\partial\vartheta}\mathrm{d}V + \int_S \frac{\delta\mathcal{W}}{\delta T}\frac{\partial T}{\partial\vartheta}\mathrm{d}S}{\gamma_1 L_\gamma} \quad (55)$$

As in the case of the finger drift, it appears that it is the horizontal temperature gradient (more precisely its orthoradial component), and not directly the vertical gradient, that is responsible for the rotation. This component exists because of the anisotropy of the thermal conductivities and must be proportional to $\hat{G}$. Another important point is that $\frac{\partial T}{\partial\vartheta}$ changes sign when q_0 is changed to $-q_0$. This model thus predicts that the sense of rotation is given by the sign of q_0, as observed

experimentally. For the moment, it is difficult to give the order of magnitude of ω because we do not know how $\mathcal{F}$ and $\mathcal{W}$ vary with temperature in the coexistence zone. A specific study is required to answer this question. On the other hand, the previous equation shows that it should be possible to explain the Lehmann rotation – both in cholesteric and nematic phases – without introducing the thermomechanical terms.

6 Conclusion

To summarize, we have established a very general formula that allows to calculate the drift velocity of a cholesteric texture subjected to a temperature gradient. This formula applies if the backflow effects are negligible. This is the case for the TIC textures described in Section 3. In these three examples, the thermomechanical terms are directly responsible for the rotation of the director. The theory predicts that these textures do not rotate at the same velocity if the nematic-like coefficients $\bar{\bar{\xi}}_i$ are taken into account.

We then applied our general formula to the case of the cholesteric fingers of the first type. These fingers are observed in homeotropic samples and drift under the action of a temperature gradient. We confirm that the drift observed in the compensated mixtures close to the compensation temperature is mainly due to the Leslie thermomechanical term. By contrast, the thermomechanical terms cannot explain the drift observed in diluted mixtures in the vicinity of a smectic A phase. For this reason, we propose a new model based on the divergence of the bend and twist elastic constants and on the existence of a horizontal temperature gradient inside the fingers.

Finally, we applied our general formula to the Lehmann droplets. We confirm that the Leslie thermomechanical coupling cannot explain alone their rotation. On the other hand, two alternatives could be envisaged if the director field inside the droplets is distorted by the surface effects. The first one involves the "texture-dependent" Akopyan and Zel'dovich thermomechanical terms, while the second considers the temperature variations of the elastic and (or) anchoring energy and the existence of an orthoradial temperature gradient inside the droplets.

For the time being, these new models which we propose for the fingers and the Lehmann droplets are qualitative. To test them and explicitly calculate the corresponding velocities, numerical simulations of the director and temperature fields are required. Systematic measurements of the thermomechanical coefficients $\bar{\bar{\xi}}_i$ would also be desirable, for instance by using the results on the TICs, to determine whether their order of magnitude is compatible with the observed velocities of the Lehmann droplets. Such simulations and experiments are planned in the future.

Appendix: equivalent expressions for the thermomechanical force

The general expression of the thermomechanical force was first given by Akopyan and Zel'dovich[13] and was then derived more

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** With $\bar{\nu}$ replacing ν since, in our previous publications, we neglected the $\bar{\bar{\xi}}_2 q_0$ contribution.

rigorously by Pleiner and Brand.[14,33] In this paper, we give a different, but more physical form of $\vec{f}_{TM}$. This form was derived from an analogy with the terms in $\vec{h}$ (denoted by $\vec{h}_{\nabla K}$) that come from the spatial variations of the elastic constants. These thermomechanical terms are responsible for a static distortion of the texture, but do not contribute to the drift velocity of the texture. A straightforward calculation gives:

$$
\begin{aligned}
\vec{h}_{\nabla K} &= \left(\vec{\nabla}\cdot\vec{n}\right)\vec{\nabla}K_1 + \left(\vec{n}\cdot\vec{\nabla}\times\vec{n}\right)\left(\vec{n}\times\vec{\nabla}K_2\right)\\
&+ \vec{n}\times\vec{\nabla}(K_2 q_0) + \left(\vec{n}\cdot\vec{\nabla}K_3\right)\left(\left[\vec{\nabla}\times\vec{n}\right]\times\vec{n}\right)\\
&- \vec{\nabla}\cdot\left(\vec{\nabla}K_4\otimes\vec{n} - \left[\vec{\nabla}K_4\cdot\vec{n}\right]\mathbb{1}\right)
\end{aligned}
\tag{56}
$$

by taking the elastic energy under the form

$$
\begin{aligned}
f &= \frac{1}{2}K_1\left(\vec{\nabla}\cdot\vec{n}\right)^2 + \frac{1}{2}K_2\left(\vec{n}\cdot\vec{\nabla}\times\vec{n}\right)^2 + \frac{1}{2}K_3\left(\vec{n}\times\left[\vec{\nabla}\times\vec{n}\right]\right)^2\\
&- \frac{1}{2}K_4\vec{\nabla}\cdot\left(\left[\vec{\nabla}\cdot\vec{n}\right]\vec{n} + \vec{n}\times\left[\vec{\nabla}\times\vec{n}\right]\right).
\end{aligned}
\tag{57}
$$

In this expression, the K_i's are the splay ($i = 1$), twist ($i = 2$), bend ($i = 3$) and saddle-splay ($i = 4$) Frank elastic constants.

The eqn (56) is equivalent to eqn (5) given in the body of the paper on condition to replace the $\xi_i\vec{G}$ by $\vec{\nabla}K_i$ for $i = 1\dots3$ and $\nu\vec{G}$ by $\vec{\nabla}(K_2 q_0)$.

In their paper, Akopyan and Zel'dovich give the following expression for the thermomechanical force:††[13]

$$
\begin{aligned}
\vec{f}_{TM} &= \left(-\xi_1 + \frac{1}{2}\xi_3\right)\left(\vec{\nabla}\cdot\vec{n}\right)\vec{G}\\
&+ \xi_2\left(\vec{n}\cdot\vec{\nabla}\times\vec{n}\right)\vec{n}\times\vec{G}\\
&+ (\xi_3 - \xi_4)\left(\vec{n}\cdot\vec{G}\right)\underline{\underline{m}}\cdot\vec{n}\\
&- \xi_3\underline{\underline{m}}\cdot\vec{G} + \nu\vec{n}\times\vec{G},
\end{aligned}
\tag{58}
$$

with $\underline{\underline{m}}_{ij} = \frac{1}{2}(n_{i,j} + n_{j,i})$. This expression is equivalent to our eqn (5) with

$$
\begin{array}{c|c}
\bar{\xi}_1 = -\xi_1 - \frac{1}{2}\xi_3 & \xi_1 = \frac{1}{2}\bar{\xi}_4 - \bar{\xi}_1\\[4pt]
\bar{\xi}_2 = \xi_2 - \frac{1}{2}\xi_3 & \xi_2 = \bar{\xi}_2 - \frac{1}{2}\bar{\xi}_4\\[4pt]
\bar{\xi}_3 = -\frac{1}{2}\xi_4 & \xi_3 = -\bar{\xi}_4\\[4pt]
\bar{\xi}_4 = -\xi_3 & \xi_4 = -2\bar{\xi}_3
\end{array}
\tag{59}
$$

Brand and Pleiner pointed out a flaw in Akopyan and Zel'dovich reasoning[33] and gave the following expression for the thermomechanical force:[14]

$$
\begin{aligned}
\vec{f}_{TM} &= -\gamma_1\Big(\pi_1\left[\vec{\nabla}\cdot\vec{n}\right]\vec{G} + \pi_2\vec{\nabla}\vec{n}\cdot\vec{G} + \pi_3\left[\vec{G}\cdot\vec{\nabla}\right]\vec{n}\\
&+ [\pi_4 - \pi_3]\left[\vec{n}\cdot\vec{G}\right]\left[\vec{n}\cdot\vec{\nabla}\right]\vec{n}\Big)
\end{aligned}
\tag{60}
$$

This expression is also equivalent to that of Akopyan and Zel'dovich. The correspondence with our eqn (5) is obtained with

$$
\begin{array}{c|c}
\bar{\xi}_1 = -\gamma_1(\pi_1 + \pi_2 + \pi_3) & \pi_1 = \frac{1}{\gamma_1}(\bar{\xi}_4 - \bar{\xi}_1)\\[6pt]
\bar{\xi}_2 = -\gamma_1\pi_3 & \pi_2 = \frac{1}{\gamma_1}(\bar{\xi}_2 - \bar{\xi}_4)\\[6pt]
\bar{\xi}_3 = -\gamma_1\pi_4 & \pi_3 = -\frac{1}{\gamma_1}\bar{\xi}_2\\[6pt]
\bar{\xi}_4 = -\gamma_1(\pi_2 + \pi_3) & \pi_4 = -\frac{1}{\gamma_1}\bar{\xi}_3
\end{array}
\tag{61}
$$

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†† Note that this expression is the same as that of Akopyan and Zel'dovich with a minus sign in front of the texture dependent terms in order to conform with our definition of the thermomechanical force.

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