Lattice Boltzmann simulations of liquid crystal hydrodynamics

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We describe a lattice Boltzmann algorithm to simulate liquid crystal hydrodynamics. The equations of motion are written in terms of a tensor order parameter. This allows both the isotropic and the nematic phases to be considered. Backflow effects and the hydrodynamics of topological defects are naturally included in the simulations, as are non-Newtonian flow properties such as shear thinning and shear banding.

I. INTRODUCTION

Liquid crystalline materials are often made up of long, thin, rodlike molecules [1]. The molecular geometry and interactions can lead to a wide range of equilibrium phases. Here we shall be concerned with two of the simplest phases: the isotropic phase, where the orientation of the molecules is random, and the nematic phase, where the molecules tend to align along a preferred direction.

The aim of this paper is to describe a numerical scheme that can explore the hydrodynamics of liquid crystals within both the isotropic and the nematic phases. There are two major differences between the hydrodynamics of simple liquids and that of liquid crystals. First, the geometry of the molecules means that they are rotated by gradients in the velocity field. Second, the equilibrium free energy is more complex than for a simple fluid and this in turn increases the complexity of the stress tensor in the Navier-Stokes equation for the evolution of the fluid momentum. This coupling between the elastic energy and the flow leads to rich hydrodynamic behavior. A simple example is the existence of a tumbling phase where the molecules rotate in an applied shear [2]. Other examples include shear banding, a nonequilibrium phase separation into coexisting states with different strain rates [3] and the possibility of Williams domains, convection cells induced by an applied electric field [1].

The equations of motion describing liquid crystal hydrodynamics are complex. There are several derivations broadly in agreement but differing in the detailed form of some terms. Here we follow the approach of Beris and Edwards [4] who wrote the equations of motion in terms of a tensor order parameter **Q** that can be related to the second moment of the orientational distribution function of the molecules. This has the advantage that the hydrodynamics of both the isotropic and the nematic phases, and of topological defects in the nematic phase can be included within the same formalism. Most other theories of liquid crystal hydrodynamics appear as limiting cases. In particular, the Ericksen-Leslie formulation of nematodynamics [5,6], widely used in the experimental liquid crystal literature, follows when uniaxiality is imposed and the magnitude of the order parameter is held constant.

Considerable analytic progress in understanding liquid crystal flow in simple geometries has been made but this is inevitably limited by the complexity of the equations of motion. Therefore it is useful to formulate a method of obtaining numerical solutions of the hydrodynamic equations to further explore their rich phenomenology. Moreover, we should like to be able to predict flow patterns for given viscous and elastic coefficients for comparison with experiments and to explore the effects of hydrodynamics when liquid crystals are used in display devices or during industrial processing.

Rey and Tsuji [2] have obtained interesting results on flow-induced ordering of the director field and on defect dynamics by solving the Beris-Edwards equation for the order parameter. However, the velocity field was imposed externally and no back-flows (effect of the director configuration on the velocity field) were included. Fukuda [7] used a Euler scheme to solve a model somewhat simpler than the full Beris-Edwards model but still including backflow, and studied the effect of hydrodynamics on phase ordering in liquid crystals. Otherwise most previous work on liquid crystal hydrodynamics has been limited to a constant order parameter (the Ericksen-Leslie-Parodi equations) and often restricted to one dimension.

Lattice Boltzmann schemes have recently proved very successful in simulations of complex fluids and it is this approach that we shall take here [8]. Such algorithms can be usefully and variously considered as a slightly unusual finite-difference discretization of the equations of motion or as a lattice version of a simplified Boltzmann equation. It is not understood why the approach is particularly useful for complex fluids but it may be related to the very natural way in which a free energy describing the equilibrium properties of the fluid can be incorporated in the simulations, drawing on ideas from statistical mechanics [9]. Recent applications have included phase ordering and flow in binary fluids [10] and self-assembly and spontaneous emulsification in amphiphilic fluids [11,12].

However, in applications so far, with the exception of [13], the order parameter has been a scalar and has coupled to the flow via a simple advective term. The liquid crystal equations of motion are written in terms of a tensor order parameter. This is responsible for the main new features of the lattice Boltzmann approach described in this paper. It also leads to the possibility of exploring non-Newtonian fluid behavior such as shear thinning and shear banding without the need to impose a constitutive equation for the stress [14].

In Sec. II we summarize the hydrodynamic equations of motion for liquid crystals. The lattice Boltzmann scheme is defined in Sec. III. A modified version of the collision operator is used to eliminate lattice viscosity effects. Section IV describes a Chapman-Enskog expansion that relates the numerical scheme to the hydrodynamic equations of motion. Numerical results for simple shear flows are presented in Sec. V and other possible applications of the approach are outlined in Sec. VI.

II. THE HYDRODYNAMIC EQUATIONS OF MOTION

We shall follow the formulation of liquid crystal hydrodynamics described by Beris and Edwards [4]. The continuum equations of motion are written in terms of a tensor order parameter $\mathbf{Q}$ that is related to the direction of individual molecules $\hat{\vec{n}}$ by $Q_{\alpha\beta} = \langle \hat{n}_\alpha \hat{n}_\beta - \frac{1}{3}\delta_{\alpha\beta}\rangle$ where the angular brackets denote a coarse-grained average. (Greek indices will be used to represent cartesian components of vectors and tensors and the usual summation over repeated indices will be assumed.) $\mathbf{Q}$ is a traceless symmetric tensor that is zero in the isotropic phase. We first write down a Landau free energy that describes the equilibrium properties of the liquid crystal and the isotropic-nematic transition. This appears in the equation of motion of the order parameter, which includes a Cahn-Hilliard-like term through which the system evolves towards thermodynamic equilibrium. It also includes a term coupling the order parameter to the flow. The order parameter is both advected by the flow and, because liquid crystal molecules are rodlike, rotated by velocity gradients.

We then write down the continuity and Navier-Stokes equations for the evolution of the flow field. In particular, the form of the stress appropriate to a tensor order parameter is discussed. A brief comparison is given to a similar formalism introduced by Doi [15] and extended by Olmsted and co-workers [16,17]. For a uniaxial nematic in the absence of any defects, the Beris-Edwards equations reduce to the Ericksen-Leslie-Parodi formulation of nematodynamics [1]. The hydrodynamic behavior of nematic liquid crystals is often characterized in terms of the Leslie coefficients and it is therefore useful to list them below. More details of the mapping between the Beris-Edwards and the Ericksen-Leslie-Parodi equations are given in Appendix A.

Free energy: The equilibrium properties of a liquid crystal in solution can be described by a free energy [17]

$$\mathcal{F} = \int d^3r \left\{ \frac{a}{2}Q_{\alpha\beta}^2 - \frac{b}{3}Q_{\alpha\beta}Q_{\beta\gamma}Q_{\gamma\alpha} + \frac{c}{4}(Q_{\alpha\beta}^2)^2 + \frac{\kappa}{2}(\partial_\alpha Q_{\beta\lambda})^2 \right\}. \tag{2.1}$$

We shall work within the one elastic constant approximation. Although it is not hard to include more general elastic terms this simplification will not affect the qualitative behavior. The free energy (2.1) describes a first-order transition from the isotropic to the nematic phase.

Equation of motion of the nematic order parameter: The equation of motion for the nematic order parameter is [4]

$$(\partial_t + \vec{u}\cdot\vec{\nabla})\mathbf{Q} - \mathbf{S}(\mathbf{W},\mathbf{Q}) = \Gamma\mathbf{H}, \tag{2.2}$$

where Γ is a collective rotational diffusion constant. The first term on the left-hand side of Eq. (2.2) is the material derivative describing the usual time dependence of a quantity advected by a fluid with velocity $\vec{u}$. This is generalized by a second term

$$\mathbf{S}(\mathbf{W},\mathbf{Q}) = (\xi\mathbf{D}+\mathbf{\Omega})(\mathbf{Q}+\mathbf{I}/3) + (\mathbf{Q}+\mathbf{I}/3)(\xi\mathbf{D}-\mathbf{\Omega})$$
$$- 2\xi(\mathbf{Q}+\mathbf{I}/3)\mathrm{Tr}(\mathbf{QW}), \tag{2.3}$$

where $\mathbf{D} = (\mathbf{W}+\mathbf{W}^T)/2$ and $\mathbf{\Omega} = (\mathbf{W}-\mathbf{W}^T)/2$ are the symmetric part and the antisymmetric part, respectively, of the velocity gradient tensor $W_{\alpha\beta} = \partial_\beta u_\alpha$. $\mathbf{S}(\mathbf{W},\mathbf{Q})$ appears in the equation of motion because the order-parameter distribution can be both rotated and stretched by flow gradients. ξ is a constant that will depend on the molecular details of a given liquid crystal.

The term on the right-hand side of Eq. (2.2) describes the relaxation of the order parameter towards the minimum of the free energy. The molecular field $\mathbf{H}$ that provides the driving motion is related to the derivative of the free energy by

$$\mathbf{H} = -\frac{\delta\mathcal{F}}{\delta Q} + (\mathbf{I}/3)\mathrm{Tr}\frac{\delta\mathcal{F}}{\delta Q}$$
$$= -a\mathbf{Q} + b[\mathbf{Q}^2 - (\mathbf{I}/3)\mathrm{Tr}\,\mathbf{Q}^2] - c\mathbf{Q}\,\mathrm{Tr}\,\mathbf{Q}^2 + \kappa\nabla^2\mathbf{Q}. \tag{2.4}$$

Continuity and Navier-Stokes equations: The fluid momentum obeys the continuity

$$\partial_t\rho + \partial_\alpha\rho u_\alpha = 0, \tag{2.5}$$

where ρ is the fluid density and the Navier-Stokes equation

$$\rho\partial_t u_\alpha + \rho u_\beta\partial_\beta u_\alpha = \partial_\beta\tau_{\alpha\beta} + \partial_\beta\sigma_{\alpha\beta}$$
$$+ \frac{\rho\tau_f}{3}[\partial_\beta\{(\delta_{\alpha\beta}-3\partial_\rho P_0\delta_{\alpha\beta})\partial_\gamma u_\gamma$$
$$+ \partial_\alpha u_\beta + \partial_\beta u_\alpha\}]. \tag{2.6}$$

The form of the equation is not dissimilar to that for a simple fluid. However, the details of the stress tensor reflect the additional complications of liquid crystal hydrodynamics. There is a symmetric contribution

$$\sigma_{\alpha\beta} = -P_0\delta_{\alpha\beta} - \xi H_{\alpha\gamma}\left(Q_{\gamma\beta}+\frac{1}{3}\delta_{\gamma\beta}\right)$$
$$- \xi\left(Q_{\alpha\gamma}+\frac{1}{3}\delta_{\alpha\gamma}\right)H_{\gamma\beta} + 2\xi\left(Q_{\alpha\beta}+\frac{1}{3}\delta_{\alpha\beta}\right)Q_{\gamma\epsilon}H_{\gamma\epsilon}$$
$$- \partial_\beta Q_{\gamma\nu}\frac{\delta\mathcal{F}}{\delta\partial_\alpha Q_{\gamma\nu}} \tag{2.7}$$

and an antisymmetric contribution

$$\tau_{\alpha\beta} = Q_{\alpha\gamma}H_{\gamma\beta} - H_{\alpha\gamma}Q_{\gamma\beta}. \tag{2.8}$$

The pressure P_0 is taken to be

$$P_0 = \rho T - \frac{\kappa}{2}(\vec{\nabla}\mathbf{Q})^2. \qquad (2.9)$$

An earlier development of liquid crystal hydrodynamics in terms of a tensor order parameter was proposed by Doi [15]. The Doi theory is based upon a Smoluchowski evolution equation (similar to the Boltzmann equation for translational motion) for the orientational distribution function. The main advantage of the approach is the possibility of relating the phenomenological coefficients in the equations of motion to microscopic parameters. One omission is the lack of gradient terms in the free energy (but see [17]). Moreover, it is necessary to use closure approximations to obtain a tractable set of hydrodynamic equations. The Doi and Beris-Edwards equations are very similar: the main difference is in the symmetric contribution to the stress tensor. The Doi theory gives a simpler form that is incomplete in that it does not obey Onsager reciprocity. (Full molecular theories do not suffer from this inconsistency [18].)

Hydrodynamic equations for the nematic phase were formulated by Ericksen and Leslie [5,6,1]. These are widely used as the Leslie coefficients provide a useful measure of the viscous properties of the liquid crystal fluid. The Beris-Edwards equations reduce to those of Ericksen and Leslie in the uniaxial nematic phase when the magnitude of the order parameter remains constant. Hence a limitation of the Ericksen-Leslie theory is that it cannot include the hydrodynamics of topological defects. For convenience we list below the relationship between the Leslie coefficients and the parameters appearing in the equations of motion (2.2) and (2.6). An outline of their derivation from the Beris-Edwards approach is given in Appendix A.

$$\alpha_1 = -\frac{2}{3}q^2(3+4q-4q^2)\xi^2/\Gamma, \qquad (2.10)$$

$$\alpha_2 = \left\{ -\frac{1}{3}q(2+q)\xi - q^2 \right\} \Big/ \Gamma, \qquad (2.11)$$

$$\alpha_3 = \left\{ -\frac{1}{3}q(2+q)\xi + q^2 \right\} \Big/ \Gamma, \qquad (2.12)$$

$$\alpha_4 = \frac{4}{9}(1-q)^2\xi^2/\Gamma + \eta, \qquad (2.13)$$

$$\alpha_5 = \left\{ \frac{1}{3}q(4-q)\xi^2 + \frac{1}{3}q(2+q)\xi \right\} \Big/ \Gamma, \qquad (2.14)$$

$$\alpha_6 = \left\{ \frac{1}{3}q(4-q)\xi^2 - \frac{1}{3}q(2+q)\xi \right\} \Big/ \Gamma, \qquad (2.15)$$

where q is the magnitude of the nematic order parameter and $\eta = \rho\tau_f/3$.

A detailed comparison of the theories of liquid crystal hydrodynamics can be found in Beris and Edwards [4].

III. A LATTICE BOLTZMANN ALGORITHM FOR LIQUID CRYSTAL HYDRODYNAMICS

We now define a lattice Boltzmann algorithm that solves the hydrodynamic equations of motion of a liquid crystal, Eqs. (2.2), (2.5), and (2.6). Lattice Boltzmann algorithms are defined in terms of a set of continuous variables, usefully termed partial distribution functions, which move on a lattice in discrete space and time. They were first developed as mean-field versions of cellular automata simulations but can also usefully be viewed as a particular finite-difference implementation of the continuum equations of motion [8].

Lattice Boltzmann approaches have been particularly successful in modeling fluids that evolve to minimize a free energy [9]. It has not been proved why this is the case, but one can surmise that the existence of an H theorem, which governs the approach to equilibrium, helps to enhance the stability of the scheme [19,20].

The simplest lattice Boltzmann algorithm, which describes the Navier-Stokes equations of a simple fluid, is defined in terms of a single set of partial distribution functions that sum on each site to give the density. For liquid crystal hydrodynamics, this must be supplemented by a second set, which are tensor variables, and which are related to the tensor order parameter $\mathbf{Q}$. A description of the algorithm is given in Sec. III A and the continuum limit is taken in Sec. III B. A Chapman-Enskog expansion [21] showing how the algorithm reproduces the liquid crystal equations of motion follows in Sec. III C.

A. The lattice Boltzmann algorithm

We define two distribution functions, the scalars $f_i(\vec{x})$ and the symmetric traceless tensors $\mathbf{G}_i(\vec{x})$ on each lattice site $\vec{x}$. Each f_i, $\mathbf{G}_i$ is associated with a lattice vector $\vec{e}_i$. We choose a nine-velocity model on a square lattice with velocity vectors $\vec{e}_i = (\pm 1,0),(0,\pm 1),(\pm 1,\pm 1),(0,0)$. Physical variables are defined as moments of the distribution function

$$\rho = \sum_i f_i, \quad \rho u_\alpha = \sum_i f_i e_{i\alpha}, \quad \mathbf{Q} = \sum_i \mathbf{G}_i. \qquad (3.1)$$

The distribution functions evolve in a time step Δt according to

$$f_i(\vec{x}+\vec{e}_i\Delta t, t+\Delta t) - f_i(\vec{x},t)$$
$$= \frac{\Delta t}{2}[\mathcal{C}_{fi}(\vec{x},t,\{f_i\}) + \mathcal{C}_{fi}(\vec{x}+\vec{e}_i\Delta t, t+\Delta t,\{f_i^*\})], \qquad (3.2)$$

$$\mathbf{G}_i(\vec{x}+\vec{e}_i\Delta t, t+\Delta t) - \mathbf{G}_i(\vec{x},t)$$
$$= \frac{\Delta t}{2}[\mathcal{C}_{\mathbf{G}i}(\vec{x},t,\{\mathbf{G}_i\}) + \mathcal{C}_{\mathbf{G}i}(\vec{x}+\vec{e}_i\Delta t, t+\Delta t,\{\mathbf{G}_i^*\})]. \qquad (3.3)$$

This represents free streaming with velocity $\vec{e}_i$ and a collision step that allows the distribution to relax towards equilibrium. f_i^* and $\mathbf{G}_i^*$ are first-order approximations to $f_i(\vec{x}+\vec{e}_i\Delta t,t+\Delta t)$ and $\mathbf{G}_i(\vec{x}+\vec{e}_i\Delta t,t+\Delta t)$, respectively. They are obtained from Eqs. (3.2) and (3.3) but with f_i^* and $\mathbf{G}_i^*$ set to f_i and $\mathbf{G}_i$. Discretizing in this way, which is similar to a predictor-corrector scheme, has the advantages that lattice viscosity terms are eliminated to second order and that the stability of the scheme is improved.

The collision operators are taken to have the form of a single relaxation time Boltzmann equation [8] together with a forcing term

$$\mathcal{C}_{fi}(\vec{x},t,\{f_i\})=-\frac{1}{\tau_f}[f_i(\vec{x},t)-f_i^{eq}(\vec{x},t,\{f_i\})]+p_i(\vec{x},t,\{f_i\}),$$
$$(3.4)$$

$$\mathcal{C}_{\mathbf{G}i}(\vec{x},t,\{\mathbf{G}_i\})=-\frac{1}{\tau_g}\{\mathbf{G}_i(\vec{x},t)-\mathbf{G}_i^{eq}(\vec{x},t,\{\mathbf{G}_i\})\}$$
$$+\mathbf{M}_i(\vec{x},t,\{\mathbf{G}_i\}). \qquad (3.5)$$

The form of the equations of motion and thermodynamic equilibrium follow from the choice of the moments of the equilibrium distributions f_i^{eq} and $\mathbf{G}_i^{eq}$ and the driving terms p_i and $\mathbf{M}_i$. f_i^{eq} is constrained by

$$\sum_i f_i^{eq}=\rho,\quad \sum_i f_i^{eq}e_{i\alpha}=\rho u_\alpha,$$

$$\sum_i f_i^{eq}e_{i\alpha}e_{i\beta}=-\sigma_{\alpha\beta}+\rho u_\alpha u_\beta, \qquad (3.6)$$

where the zeroth and first moments are chosen to impose conservation of mass and momentum. The second moment of f^{eq} controls the symmetric part of the stress tensor whereas the moments of p_i

$$\sum_i p_i=0,\quad \sum_i p_ie_{i\alpha}=\partial_\beta\tau_{\alpha\beta},\quad \sum_i p_ie_{i\alpha}e_{i\beta}=0 \quad (3.7)$$

impose the antisymmetric part of the stress tensor. For the equilibrium of the order-parameter distribution, we choose

$$\sum_i \mathbf{G}_i^{eq}=\mathbf{Q},\quad \sum_i \mathbf{G}_i^{eq}e_{i\alpha}=\mathbf{Q}u_\alpha,\quad \sum_i \mathbf{G}_i^{eq}e_{i\alpha}e_{i\beta}=\mathbf{Q}u_\alpha u_\beta.$$
$$(3.8)$$

This ensures that the order parameter is convected with the flow. Finally, the evolution of the order parameter is most conveniently modeled by choosing

$$\sum_i \mathbf{M}_i=\Gamma\mathbf{H}(\mathbf{Q})+\mathbf{S}(\mathbf{W},\mathbf{Q})\equiv\hat{\mathbf{H}},\quad \sum_i \mathbf{M}_ie_{i\alpha}=\left(\sum_i \mathbf{M}_i\right)u_\alpha,$$
$$(3.9)$$

which ensures that the fluid minimizes its free energy at equilibrium.

Conditions (3.6)–(3.9) can be satisfied as is usual in lattice Boltzmann schemes by writing the equilibrium distribution functions and forcing terms as polynomial expansions in the velocity [8]

$$f_i^{eq}=A_s+B_su_\alpha e_{i\alpha}+C_su^2+D_su_\alpha u_\beta e_{i\alpha}e_{i\beta}+E_{s\alpha\beta}e_{i\alpha}e_{i\beta},$$

$$\mathbf{G}_i^{eq}=\mathbf{J}_s+\mathbf{K}_su_\alpha e_{i\alpha}+\mathbf{L}_su^2+\mathbf{N}_su_\alpha u_\beta e_{i\alpha}e_{i\beta},$$

$$p_i=T_s\partial_\beta\tau_{\alpha\beta}e_{i\alpha},$$

$$\mathbf{M}_i=\mathbf{R}_s+\mathbf{S}_su_\alpha e_{i\alpha}, \qquad (3.10)$$

where $s=\vec{e}_i^{\,2}\in\{0,1,2\}$ identifies separate coefficients for different absolute values of the velocities. A suitable choice is

$$A_2=(\sigma_{xx}+\sigma_{yy})/16,\quad A_1=2A_2,\quad A_0=\rho-12A_2,$$

$$B_2=\rho/12,\quad B_1=4B_2,$$

$$C_2=-\rho/16,\quad C_1=-\rho/8,\quad C_0=-3\rho/4,$$

$$D_2=\rho/8,\quad D_1=\rho/2,$$

$$E_{2xx}=(\sigma_{xx}-\sigma_{yy})/16,\quad E_{2yy}=-E_{2xx},\quad E_{2xy}=E_{2yx}=\sigma_{xy}/8,$$

$$E_{1xx}=4E_{2xx},\quad E_{1yy}=4E_{2yy},$$

$$\mathbf{J}_0=\mathbf{Q},$$

$$\mathbf{K}_2=\mathbf{Q}/12,\quad \mathbf{K}_1=4\mathbf{K}_2,$$

$$\mathbf{L}_2=-\mathbf{Q}/16,\quad \mathbf{L}_1=-\mathbf{Q}/8,\quad \mathbf{L}_0=-3\mathbf{Q}/4,$$

$$\mathbf{N}_2=\mathbf{Q}/8,\quad \mathbf{N}_1=\mathbf{Q}/2,$$

$$T_2=1/12,\quad T_1=4T_2,$$

$$\mathbf{R}_2=\hat{\mathbf{H}}/9,\quad \mathbf{R}_1=\mathbf{R}_0=\mathbf{R}_2,$$

$$\mathbf{S}_2=\hat{\mathbf{H}}/12,\quad \mathbf{S}_1=4\mathbf{S}_2, \qquad (3.11)$$

where any coefficients not listed are zero.

B. Continuum limit

We write down the continuum limit of the lattice Boltzmann evolution equations (3.2) and (3.3) showing, in particular, that the predictor-corrector form of the collision integral eliminates lattice viscosity effects to second order.

Consider Eq. (3.2). Taylor expanding $f_i(\vec{x}+\vec{e}_i\Delta t,t+\Delta t)$ gives

$$f_i(\vec{x}+\vec{e}_i\Delta t,t+\Delta t)=f_i(\vec{x},t)+\Delta tDf_i(\vec{x},t)+\frac{\Delta t^2}{2}D^2f_i(\vec{x},t)$$
$$+O(\Delta t^3), \qquad (3.12)$$

where $D\equiv\partial_t+e_{i\alpha}\partial_\alpha$. Similarly, expanding the collision term equation (3.4),

$$\mathcal{C}_{fi}(\vec{x}+\vec{e}_i\Delta t,t+\Delta t,[f_i+\Delta t\mathcal{C}_{fi}(\vec{x},t,\{f_i\})])$$
$$=\mathcal{C}_{fi}(\vec{x},t,\{f_i\})+\Delta tD\mathcal{C}_{fi}(\vec{x},t,\{f_i\})+O(\Delta t^2)$$

$$(3.13)$$

and substituting into Eq. (3.2) gives

$$Df_i(\vec{x},t)=\mathcal{C}_{fi}(\vec{x},t,\{f_i\})-\frac{\Delta t}{2}[D^2f_i(\vec{x},t)-D\mathcal{C}_{fi}(\vec{x},t,\{f_i\})]$$

$$+O(\Delta t^2). \qquad (3.14)$$

We see immediately that

$$Df_i(\vec{x},t)=\mathcal{C}_{fi}(\vec{x},t,\{f_i\})+O(\Delta t). \qquad (3.15)$$

Using Eq. (3.15) in the expansion (3.14), it follows that there are no terms of order Δt in Eq. (3.14) and

$$Df_i(\vec{x},t)=\mathcal{C}_{fi}(\vec{x},t,\{f_i\})+O(\Delta t^2). \qquad (3.16)$$

A similar expansion of Eq. (3.3) leads to

$$D\mathbf{G}_i(\vec{x},t)=\mathcal{C}_{\mathbf{G}i}(\vec{x},t,\{\mathbf{G}_i\})+O(\Delta t^2). \qquad (3.17)$$

In the standard lattice, Boltzmann-discretization terms of order Δt appear in Eqs. (3.16) and (3.17). These are of similar forms to those that arise from the Chapman-Enskog expansion and have been subsumed into the viscosity. However, this is not generally possible and it is convenient to use the predictor-corrector form for the collision term assumed in Eqs. (3.4) and (3.5) to eliminate them at this stage.

C. Chapman-Enskog expansion

We can now proceed with a Chapman-Enskog expansion, an expansion of the distribution functions about equilibrium, which assumes that successive derivatives are of increasingly high order [21]. The aim is to show that Eq. (3.17) reproduces the evolution equation of the liquid crystal order parameter (2.2), Eq. (3.16), and the continuity and Navier-Stokes Eqs. (2.5) and (2.6) to second order in derivatives. Writing

$$\mathbf{G}_i=\mathbf{G}_i^{(0)}+\mathbf{G}_i^{(1)}+\mathbf{G}_i^{(2)}+\cdots \qquad (3.18)$$

and substituting into Eq. (3.17) using the form for the collision term (3.5) gives, to zeroth order

$$\mathbf{G}_i^{(0)}=\mathbf{G}_i^{eq}+\tau_g\mathbf{M}_i. \qquad (3.19)$$

Summing over i and using, from Eqs. (3.1) and (3.8),

$$\sum_i\mathbf{G}_i\equiv\mathbf{Q}=\sum_i\mathbf{G}_i^{eq} \qquad (3.20)$$

shows that the zeroth moment of $\mathbf{M}_i$ appears at first order in the Chapman-Enskog expansion. This is as expected because from Eq. (3.9), $\Sigma_i\mathbf{M}_i$ is related to free energy derivatives that will be zero in equilibrium. The first moment will also be first order in derivatives.

It then follows, from substituting Eq. (3.18) into Eq. (3.17), that the first and second-order deviations of the distribution function from equilibrium are

$$\mathbf{G}_i^{(1)}=-\tau_gD\mathbf{G}_i^{eq}+\tau_g\mathbf{M}_i, \qquad (3.21)$$

$$\mathbf{G}_i^{(2)}=\tau_g^2D^2\mathbf{G}_i^{eq}-\tau_g^2D\mathbf{M}_i. \qquad (3.22)$$

Using Eq. (3.21) in Eq. (3.18), summing over i, and using Eqs. (3.20), (3.8), and (3.9) give, to first order,

$$\partial_t\mathbf{Q}+\partial_\alpha(\mathbf{Q}u_\alpha)=\hat{\mathbf{H}}+O(\partial^2). \qquad (3.23)$$

The second-order term (3.22) gives after a lengthy calculation, described in Appendix B, a correction

$$-\tau_g\left\{\partial_\alpha\left(\frac{\mathbf{Q}}{\rho}\partial_\eta P_0\right)\right\}. \qquad (3.24)$$

This additional term is a feature common to most lattice Boltzmann models of complex fluids. It is not known whether it has a physical origin, but it is very small in all the cases tested so far and has no effect upon the behavior of the fluid.

A similar expansion for the partial density distribution functions f_i gives the continuity and Navier-Stokes equations. Writing

$$f_i=f_i^{(0)}+f_i^{(1)}+f_i^{(2)}+\cdots, \qquad (3.25)$$

substituting into Eq. (3.16) and using the collision operator (3.4) give

$$f_i^{(0)}=f_i^{eq}+\tau_fp_i, \qquad (3.26)$$

$$f_i^{(1)}=-\tau_fDf_i^{eq}-\tau_f^2Dp_i, \qquad (3.27)$$

$$f_i^{(2)}=\tau_f^2D^2f_i^{eq}+\tau_f^3D^2p_i. \qquad (3.28)$$

Summing f_i over i and using the constraints on the moments of f_i, f_i^{eq}, and p_i from Eqs. (3.1), (3.6), and (3.7), respectively,

$$\left(\partial_t\rho+\partial_\alpha\rho u_\alpha+\tau_f\partial_\alpha\sum_i p_ie_{i\alpha}\right)$$

$$=\tau_f\partial_t\left[\partial_t\rho+\partial_\alpha\rho u_\alpha+\tau_f\partial_\alpha\sum_i p_ie_{i\alpha}\right]$$

$$+\tau_f\partial_\alpha\left[\partial_t\rho u_\alpha+\partial_\beta\sum_i f_i^{eq}e_{i\alpha}e_{i\beta}+\tau_f\partial_t\sum_i p_ie_{i\alpha}\right].$$

$$(3.29)$$

The first term in square brackets is second order in derivatives. Therefore

$$\left(\partial_t\rho+\partial_\alpha\rho u_\alpha+\tau_f\partial_\alpha\sum_i p_i e_{i\alpha}\right)$$

$$=\tau_f\partial_\alpha\left[\partial_t\rho u_\alpha+\partial_\beta\sum_i f_i^{eq}e_{i\alpha}e_{i\beta}+\tau_f\partial_t\sum_i p_i e_{i\alpha}\right]$$

$$+O(\partial^3). \tag{3.30}$$

We now multiply Eq. (3.25) by $e_{i\alpha}$ and sum over i. Using the constraints (3.6), (3.7), and the definitions (3.1),

$$\left(\partial_t\rho u_\alpha+\partial_\beta\sum_i f_i^{eq}e_{i\alpha}e_{i\beta}+\tau_f\partial_t\sum_i p_i e_{i\alpha}\right)$$

$$=\sum_i p_i e_{i\alpha}+\tau_f\partial_t\left[\partial_t\rho u_\alpha+\partial_\beta\sum_i f_i^{eq}e_{i\alpha}e_{i\beta}\right.$$

$$+\tau_f\partial_t\sum_i p_i e_{i\alpha}\right]+\tau_f\partial_\beta\left[\partial_t\sum_i f_i^{eq}e_{i\alpha}e_{i\beta}\right.$$

$$+\partial_\gamma\sum_i f_i^{eq}e_{i\alpha}e_{i\beta}e_{i\gamma}+\tau_f\partial_\gamma\sum_i p_i e_{i\alpha}e_{i\beta}e_{i\gamma}\right]. \tag{3.31}$$

So to first order in derivatives

$$\left(\partial_t\rho u_\alpha+\partial_\beta\sum_i f_i^{eq}e_{i\alpha}e_{i\beta}+\tau_f\partial_t\sum_i p_i e_{i\alpha}\right)$$

$$=\sum_i p_i e_{i\alpha}+O(\partial^2). \tag{3.32}$$

Placing Eq. (3.32) into the square brackets in Eq. (3.30), we obtain the continuity equation (2.5) to second order in derivatives

$$(\partial_t\rho+\partial_\alpha\rho u_\alpha)=0+O(\partial^3). \tag{3.33}$$

Substituting Eq. (3.32) into the first square brackets in Eq. (3.31) and imposing the constraints on the first moment of p_i and the second moment of f_i^{eq}, Eqs. (3.7) and (3.6), gives

$$\partial_t(\rho u_\alpha)+\partial_\beta(\rho u_\alpha u_\beta)$$

$$=\partial_\beta\sigma_{\alpha\beta}+\partial_\beta\tau_{\alpha\beta}+\tau_f\partial_\beta\left[-\partial_t\sigma_{\alpha\beta}+\partial_t(\rho u_\alpha u_\beta)\right.$$

$$+\partial_\gamma\sum_i f_i^{eq}e_{i\alpha}e_{i\beta}e_{i\gamma}+\tau_f\partial_\gamma\sum_i p_i e_{i\alpha}e_{i\beta}e_{i\gamma}\right] \tag{3.34}$$

showing immediately that the equation of motion (2.6) is reproduced to Euler level (first order in derivatives).

From the definitions (3.11),

$$\sum_i f_i^{eq}e_{i\alpha}e_{i\beta}e_{i\gamma}=\frac{\rho}{3}(u_\alpha\delta_{\beta\gamma}+u_\beta\delta_{\alpha\gamma}+u_\gamma\delta_{\alpha\beta}), \tag{3.35}$$

$$\sum_i p_i e_{i\alpha}e_{i\beta}e_{i\gamma}=\frac{1}{3}(\partial_\delta\tau_{\delta\alpha}\delta_{\beta\gamma}+\partial_\delta\tau_{\delta\beta}\delta_{\alpha\gamma}+\partial_\delta\tau_{\delta\gamma}\delta_{\alpha\beta}). \tag{3.36}$$

Using Eqs. (3.35) and (3.36), the viscous terms in the square brackets in Eq. (3.34) can be simplified. We assume that the fluid is incompressible, ignore terms of third order in the velocities, and furthermore, assume that within these second-order terms, the stress tensor can be approximated by minussing the equilibrium pressure P_0. We consider each term in the square brackets in turn.

(1) The first term can be rewritten as

$$\partial_t\sigma_{\alpha\beta}=-(\partial_\rho P_0)(\partial_t\rho)\delta_{\alpha\beta}=\rho(\partial_\rho P_0)\partial_\gamma u_\gamma\delta_{\alpha\beta}, \tag{3.37}$$

where the last step follows using the continuity equation (2.5).

(2) Rewriting

$$\partial_t(\rho u_\alpha u_\beta)=\partial_t(\rho u_\alpha)u_\beta+u_\alpha\partial_t(\rho u_\beta) \tag{3.38}$$

and replacing the time derivatives with space derivatives using the Euler terms in Eq. (3.34), one sees that this term is zero given the assumptions listed above.

(3) Using Eq. (3.35),

$$\partial_\gamma\sum_i f_i^{eq}e_{i\alpha}e_{i\beta}e_{i\gamma}=\frac{\rho}{3}(\partial_\beta u_\alpha+\partial_\alpha u_\beta+\partial_\gamma u_\gamma\delta_{\alpha\beta}). \tag{3.39}$$

(4) From Eq. (3.36) the fourth term is of third order in derivatives and can be neglected.

Replacing the square brackets in Eq. (3.34) with contributions from (1) and (3), we obtain the incompressible Navier-Stokes equation (2.6).

IV. NUMERICAL RESULTS

The primary aim of this paper is to describe the details of a numerical algorithm for simulating liquid crystal hydrodynamics. Therefore we restrict ourselves here to presenting a few brief test cases aimed at checking the approach. Further numerical applications are listed in the summary of the paper and will be presented in detail elsewhere.

In equilibrium with no flow, the free energy (2.1) is minimized. For a generic lyotropic liquid crystal, we take $a=(1-\gamma/3)$ and $b=c=\gamma$, where $\gamma=\phi L\nu_2/\alpha$ is Doi's excluded volume parameter [15,4]. [L is the molecular aspect ratio, ϕ the concentration, and ν_2 and α are $O(1)$ geometrical prefactors.] At $a=b^2/(27c)$ or $\gamma=2.7$ for the generic lyotropic, there is a first-order transition to the nematic phases and as γ is increased further, the nematic order parameter q increases. The variation of q with γ can be calculated analytically. The agreement with simulation results is excellent as shown in Fig. 1.

Imposing a shear on the system in the nematic phase will act to align the director field along the flow gradient. Assuming a steady state, homogeneous flow, and a uniaxial nematic
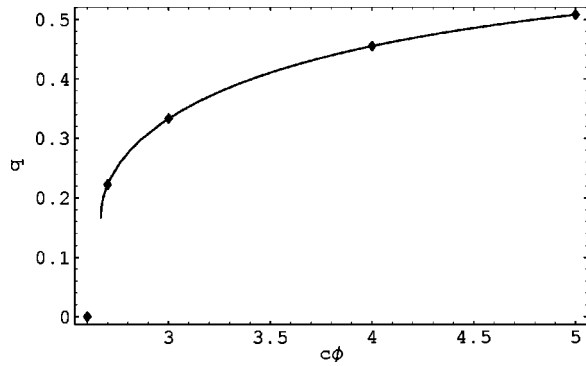
FIG. 1. Equilibrium order parameter q versus $c\phi$. The points are from a simulation and the line is the analytic result.

state, it follows from Eq. (2.2) that the angle between the direction of flow and the director θ is given by [4]

$$\xi \cos 2\theta = \frac{3q}{2+q}. \tag{4.1}$$

The simulations reproduce this relation well as shown in Fig. 2 for different values of q and ξ.

When there is no solution to Eq. (4.1), the director tumbles in the flow or may move out of the plane to form a log-rolling state [1,2]. Figure 3 gives an example of this type of behavior showing the director angle as a function of time.

Olmsted and Goldbart [16] have argued that shear stress acts to favor the nematic over the isotropic phase. Hence application of shear moves the phase boundary, which extends from the first-order equilibrium transition at zero shear along a line of first-order transitions that end at a nonequilibrium critical point. Numerical results for this boundary are shown in Fig. 4. The results are qualitatively similar to those of [16,17] who obtained the phase boundary for a slightly different model using an interface stability argument.

On the coexistence line the liquid crystal prefers to phase separate into shear bands [16,17,3], coexisting regions of different strain rate running parallel to the shear direction. Such shear banding occurs spontaneously in the simulations reported here. An example is shown in Fig. 5.
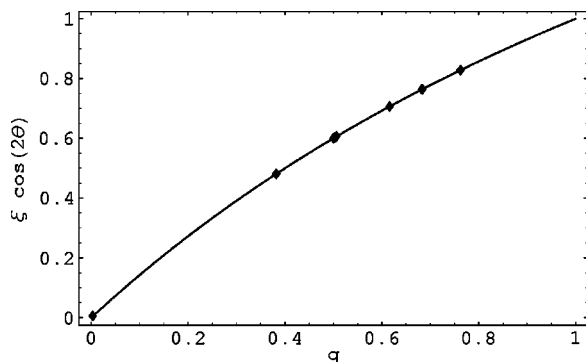

FIG. 2. ξ times the cosine of twice the angle between the director and the flow $\xi \cos 2\theta$ versus the magnitude of the order parameter q. The points are from simulations and the line is the expected value $3q/(2+q)$ from Eq. (4.1).
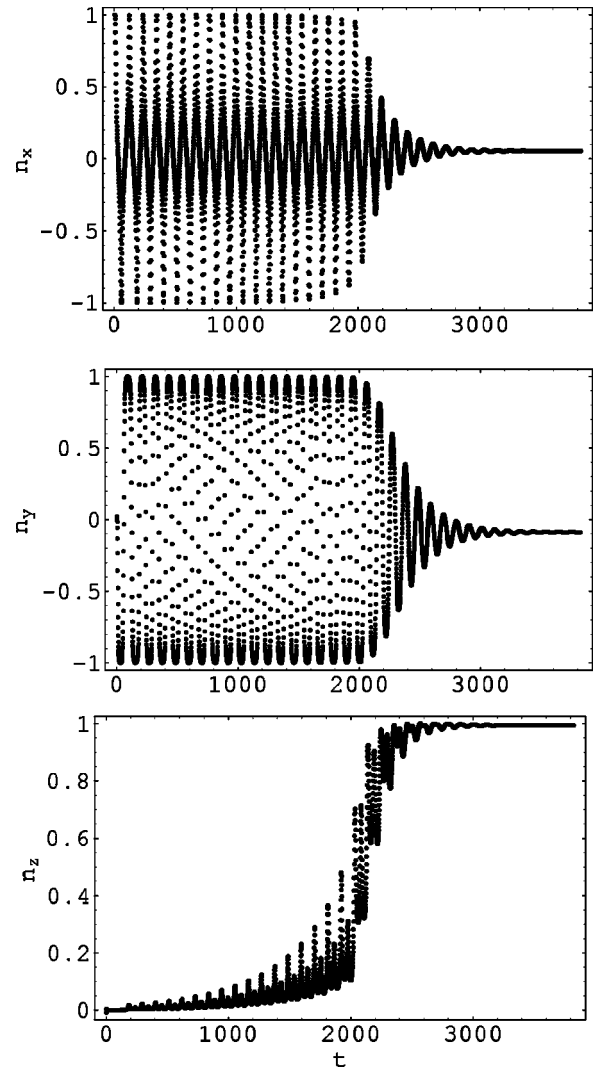

FIG. 3. The components of the director as a function of time for a system changing from a metastable tumbling state to a stable log-rolling state.

V. SUMMARY AND DISCUSSION

In this paper we described in detail a lattice Boltzmann algorithm to simulate liquid crystal hydrodynamics. In the continuum limit we recover the Beris-Edwards formulation within which the liquid crystal equations of motion are written in terms of a tensor order parameter. The equations are applicable to the isotropic, uniaxial nematic, and biaxial nematic phases. Working within the framework of a variable tensor order parameter, it is possible to simulate the dynamics of topological defects and nonequilibrium phase transitions between different flow regimes.

Lattice Boltzmann simulations have worked well for complex fluids where a free energy can be used to define thermodynamic equilibrium. However, previous work has concentrated on self-assembly with much less attention being paid to more complex flow properties. The algorithm described here includes coupling between the order parameter and the flow. This allows the investigation of non-Newtonian effects such as shear thinning and shear banding. Examples are given in Sec. IV.
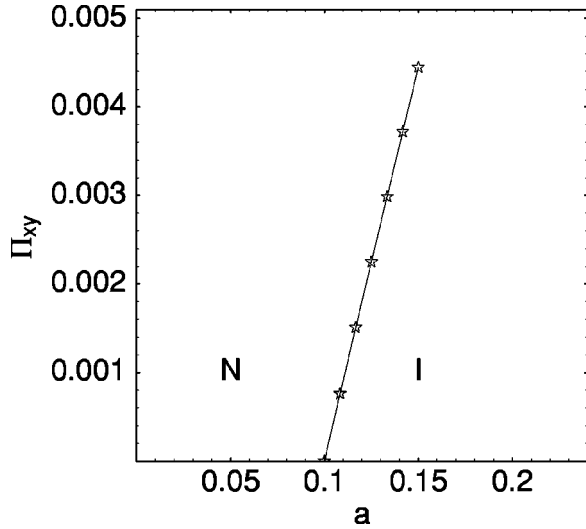
FIG. 4. Phase diagram in the shear stress Π_{xy}, effective temperature a plane. [a is the coefficient of the quadratic term in the free energy (2.1).]

There are many directions for further research opened up by the rich physics inherent in liquid crystal hydrodynamics and the generality of the Beris-Edwards equations. For example, results for liquid crystals under Poiseuille flow show that the director configuration can depend on the sample history as well as the viscous coefficients and thermodynamic parameters [22]. The effect of hydrodynamics on phase ordering is being investigated [23] and it would be interesting to study the pathways by which different dynamic states transform into each other. The addition of an electric field to the equations of motion will allow problems relevant to liquid crystal displays to be addressed. Numerical investigations are proving vital as the complexity of the equations makes analytic progress difficult.

APPENDIX A

We outline how the Beris-Edwards equations reduce to those of Ericksen, Leslie, and Parodi in the uniaxial nematic
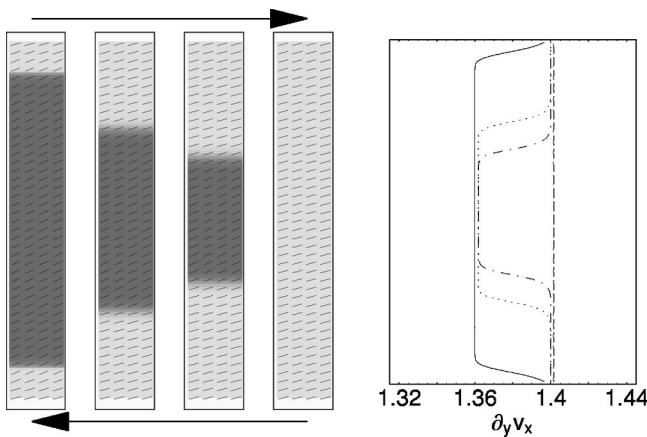

FIG. 5. Shear bands for a range of strain rates. The bands are formed by the coexistence of isotropic (darker) and nematic states. The variation of the strain rate across the system, scaled by 100Γ to make it dimensionless, is also shown.

phase when the magnitude of the order parameter remains constant. Hence we obtain expressions for the Leslie coefficients in terms of the parameters appearing in the equations of motion (2.2) and (2.6) [4].

Taking $\vec{n}$ to represent the order-parameter field, the Ericksen-Leslie stress tensor and the equation of motion for the order parameter are, respectively, [5,6,1]

$$\sigma_{\alpha\beta}^{EL}=\alpha_1 n_\alpha n_\beta n_\mu n_\rho D_{\mu\rho}+\alpha_4 D_{\alpha\beta}+\alpha_5 n_\beta n_\mu D_{\mu\alpha}$$
$$+\alpha_6 n_\alpha n_\mu D_{\mu\beta}+\alpha_2 n_\beta N_\alpha+\alpha_3 n_\alpha N_\beta, \tag{A1}$$

$$h_\mu^{EL}=\gamma_1 N_\mu+\gamma_2 n_\alpha D_{\alpha\mu} \tag{A2}$$

together with the relations

$$\gamma_1=\alpha_3-\alpha_2, \tag{A3}$$

$$\gamma_2=\alpha_6-\alpha_5=\alpha_2+\alpha_3. \tag{A4}$$

The second of these, known as Parodi's relation, is a result of Onsager reciprocity. [Note that, following the convention in Eq. (2.6), the stress tensor is written so that in the corresponding Navier-Stokes equation one contracts on the second index when taking the divergence.]

The N_α are corotational derivatives

$$N_\alpha=\partial_t n_\alpha+u_\beta\partial_\beta n_\alpha-\Omega_{\alpha\mu}n_\mu. \tag{A5}$$

The molecular field $\vec{h}$ is given by

$$h_\mu=-\frac{\delta\mathcal{F}}{\delta n_\mu}=\kappa^{EL}\nabla^2 n_\mu+\zeta(\mathbf{r})n_\mu, \tag{A6}$$

where the last line assumes the one-elastic constant approximation and ζ is a Lagrange multiplier to impose $\vec{n}^2=1$.

To obtain the Ericksen-Leslie-Parodi equations from the tensor formalism, uniaxial symmetry is imposed on the order parameter

$$Q_{\alpha\beta}=q(n_\alpha n_\beta-1/3\delta_{\alpha\beta}). \tag{A7}$$

We first obtain an expression for κ^{EL} in terms of κ and show that Eq. (2.4) reduces to the form (A6). Using the chain rule

$$h_\mu^{EL}=-\frac{\delta\mathcal{F}}{\delta n_\mu}=-\frac{\delta\mathcal{F}}{\delta Q_{\alpha\beta}}\frac{\partial Q_{\alpha\beta}}{\partial n_\mu}=q(H_{\mu\beta}n_\beta+n_\alpha H_{\alpha\mu}). \tag{A8}$$

Substituting **H** from Eq. (2.4) into Eq. (A8), writing **Q** in uniaxial form and simplifying gives after some algebra

$$h_\mu^{EL}=2q^2\kappa\nabla^2 n_\mu. \tag{A9}$$

The terms proportional to n_μ have been omitted as these will only change the magnitude of the order parameter, and the Lagrange multipier ζ will adjust to prevent this. Hence comparing Eqs. (A6) and (A9),

$$\kappa^{EL}=2q^2\kappa. \tag{A10}$$

Consider now the equation of motion for the order parameter (A2). Solving the **Q**-evolution equation (2.2) for **H** and writing **Q** in uniaxial form give

$$\Gamma H_{\alpha\beta} = q(n_\beta N_\alpha + n_\alpha N_\beta) - q\xi(D_{\alpha\gamma}n_\gamma n_\beta + n_\alpha n_\gamma D_{\gamma\beta})$$

$$+ \frac{2}{3}(q-1)\xi D_{\alpha\beta} + 2q^2\xi n_\alpha n_\beta D_{\gamma\nu}n_\nu n_\gamma$$

$$+ \frac{2}{3}q(1-q)\xi\delta_{\alpha\beta}D_{\gamma\nu}n_\nu n_\gamma. \tag{A11}$$

Substituting this into Eq. (A8) yields, after some algebra,

$$h_\mu = 2q^2 N_\mu - \frac{2}{3}q(q+2)\xi n_\alpha D_{\alpha\mu}, \tag{A12}$$

where we have again omitted terms proportional to n_μ. Comparison to Eq. (A2) gives

$$\gamma_1 = 2q^2/\Gamma, \tag{A13}$$

$$\gamma_2 = -\frac{2}{3}q(q+2)\xi/\Gamma. \tag{A14}$$

Finally, we consider how the stress tensor maps between the two theories. Using Eqs. (A11) and (A7), the symmetric part (2.7) and the antisymmetric part (2.8) of the Beris-Edwards stress tensor become, respectively,

$$\Gamma\tau_{\alpha\beta} = q^2(n_\alpha N_\beta - N_\alpha n_\beta) - q(q+2)/3\xi(n_\alpha n_\gamma D_{\gamma\beta}$$

$$- D_{\alpha\gamma}n_\gamma n_\beta) \tag{A15}$$

$$\Gamma\sigma_{\alpha\beta} = -\frac{q\xi}{3}(q+2)(n_\beta N_\alpha + n_\alpha N_\beta) + \frac{q\xi^2}{3}(4-q)$$

$$\times(D_{\alpha\gamma}n_\gamma n_\beta + n_\alpha n_\gamma D_{\gamma\beta}) + \frac{2\xi^2}{3}(q-1)^2 D_{\alpha\beta}$$

$$- \frac{8q^2\xi^2}{3}\left(\frac{3}{4} + q - q^2\right)\xi n_\alpha n_\beta D_{\gamma\nu}n_\nu n_\gamma$$

$$+ \text{terms in } \delta_{\alpha\beta}D_{\gamma\nu}n_\nu n_\gamma, \tag{A16}$$

where we have ignored the final distortion term in Eq. (2.7). A comparison of Eq. (A15) and Eqs. (A16)–(A1) gives the

Leslie coefficients (2.10)–(2.15). (These agree with the expressions given by Beris and Edwards in [4] apart for the formula for α_1. However, the formula for α_1 listed in [24] is the same as that calculated here.)

APPENDIX B

We obtain the second-order term (3.24) in the Chapman-Enskog expansion for the equation of motion of the order parameter. Proceeding as in the derivation of Eq. (3.23) but including the second-order term (3.22) gives

$$\partial_t\mathbf{Q} + \partial_\alpha(\mathbf{Q}u_\alpha) - \hat{\mathbf{H}} = \tau_g\{\partial_t^2\mathbf{Q} + 2\partial_\alpha\partial_t(\mathbf{Q}u_\alpha) + \partial_\alpha\partial_\beta(\mathbf{Q}u_\alpha u_\beta)$$

$$- \partial_t\hat{\mathbf{H}} - \partial_\alpha(\hat{\mathbf{H}}u_\alpha)\}, \tag{B1}$$

where we have used the definitions (3.8) and (3.9) to perform the sums over i. Equation (3.23) shows that the first, half the second, and the fourth term in the curly brackets are together of higher order in derivatives and can be eliminated.

We next note that

$$\partial_\alpha\partial_t(\mathbf{Q}u_\alpha) = \partial_\alpha\left(-\frac{\mathbf{Q}}{\rho}(\partial_t\rho)u_\alpha + (\partial_t\mathbf{Q})u_\alpha + \frac{\mathbf{Q}}{\rho}\partial_t(\rho u_\alpha)\right). \tag{B2}$$

The time derivatives can be replaced by spatial derivatives by using Eqs. (3.33), (3.23), and (3.32), respectively. Substituting back into Eq. (B1) and ignoring terms in $\Sigma_i p_i e_{i\alpha} \sim \partial_\beta\tau_{\alpha\beta}$ that contain an extra derivative

$$\partial_t\mathbf{Q} + \partial_\alpha(\mathbf{Q}u_\alpha) - \hat{\mathbf{H}}$$

$$= \tau_g\left\{\partial_\alpha\left(\frac{\mathbf{Q}}{\rho}\right)\partial_\beta(\rho u_\beta)u_\alpha - \partial_\alpha\partial_\beta(\mathbf{Q}u_\beta)u_\alpha + \partial_\alpha(\hat{\mathbf{H}}u_\alpha)\right\}$$

$$- \tau_g\left\{\partial_\alpha\left(\frac{\mathbf{Q}}{\rho}[\partial_\beta(\rho u_\alpha u_\beta) - \partial_\beta\sigma_{\alpha\beta}]\right)\right\}$$

$$+ \partial_\alpha\partial_\beta(\mathbf{Q}u_\alpha u_\beta) - \partial_\alpha(\hat{\mathbf{H}}u_\alpha)\right\}. \tag{B3}$$

Rearranging the derivatives this simplifies to

$$\partial_t\mathbf{Q} + \partial_\alpha(\mathbf{Q}u_\alpha) - \hat{\mathbf{H}} = -\tau_g\left\{\partial_\alpha\left(\frac{\mathbf{Q}}{\rho}\partial_\alpha P_0\right)\right\}. \tag{B4}$$

[1] P. G. de Gennes and J. Prost, *The Physics of Liquid Crystals*, 2nd ed. (Clarendon Press, Oxford, 1993).

[2] A. D. Rey and T. Tsuji, Macromol. Theory Simul. **7**, 623 (1998); T. Tsuji and A. Rey, Phys. Rev. E **57**, 5609 (1998); J. Non-Newtonian Fluid Mech. **73**, 127 (1997).

[3] P. T. Mather, A. Romo-Uribe, C. D. Han, and S. S. Kim, Macromolecules **30**, 7977 (1997).

[4] A. N. Beris and B. J. Edwards, *Thermodynamics of Flowing Systems* (Oxford University Press, Oxford, 1994).

[5] J. L. Ericksen, Phys. Fluids **9**, 1205 (1966).

[6] F. M. Leslie, Arch. Ration. Mech. Anal. **28**, 265 (1968).

[7] J.-I. Fukuda, Eur. Phys. J. B **1**, 173 (1998).

[8] S. Chen and G. D. Doolen, Annu. Rev. Fluid Mech. **30**, 329 (1998).

[9] M. R. Swift, E. Orlandini, W. R. Osborn, and J. M. Yeomans, Phys. Rev. E **54**, 5041 (1996).

[10] J. M. Yeomans, Annu. Rev. Comput. Phys. **VII**, 61 (1999).

[11] A. Lamura, G. Gonnella, and J. M. Yeomans, Europhys. Lett. **45**, 314 (1999).

[12] O. Theissen and G. Gompper, Eur. Phys. J. B **11**, 91 (1999).

[13] C. Care, I. Halliday, and K. Good (private communication).

[14] R. G. Larson, *Constitutive Equations for Polymer Melts and*

Solutions, Butterworths series in Chemical Engineering (Butterworth, Washington, D.C., 1988).

[15] M. Doi, J. Polym. Sci., Polym. Phys. Ed. **19**, 229 (1981); N. Kuzuu and M. Doi, J. Phys. Soc. Jpn. **52**, 3486 (1983); M. Doi, Faraday Symp. Chem. Soc. **18**, 49 (1983); M. Doi and S. F. Edwards, *The Theory of Polymer Dynamics* (Clarendon Press, Oxford, 1989).

[16] P. D. Olmsted and P. M. Goldbart, Phys. Rev. A **46**, 4966 (1992).

[17] P. D. Olmsted and C.-Y. David Lu, Phys. Rev. E **56**, 55 (1997); **60**, 4397 (1999).

[18] S. Sarman and D. J. Evans, J. Chem. Phys. **99**, 9021 (1993).

[19] A. J. Wagner, Europhys. Lett. **44**, 144 (1998).

[20] I. V. Karlin, A. Ferrante, and H. C. Ottinger, Europhys. Lett. **47**, 182 (1999).

[21] S. Chapman and T. Cowling, *The Mathematical Theory of Non-uniform Gases*, 3rd ed. (Cambridge University Press, Cambridge, 1990).

[22] C. Denniston, E. Orlandini, and J. M. Yeomans, Theor. Comp. Polym. Sci. (to be published).

[23] C. Denniston, E. Orlandini, and J. M. Yeomans (unpublished).

[24] A. N. Beris, B. J. Edwards, and M. Grmela, J. Non-Newtonian Fluid Mech. **35**, 51 (1990).