Generalized lattice Boltzmann algorithm for the flow of a nematic liquid crystal with variable order parameter

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A lattice Boltzmann (LB) scheme is described, which recovers the equations developed by Qian-Sheng for the hydrodynamics of a nematic liquid crystal with a tensor order parameter. The standard mesoscopic LB scalar density is generalized to a tensor quantity and the macroscopic momentum, density, and tensor order parameter are recovered from appropriate moments of this mesoscopic density. A single lattice Boltzmann equation is used with a direction dependent Bhatnagar, Gross, and Krook (BGK) collision term, with additional forcing terms to recover the antisymmetric terms in the stress tensor. A Chapman-Enskog analysis is presented, which demonstrates that the Qian-Sheng scheme is recovered, provided a lattice with sixth-order isotropy is used. The method is validated against analytical results for a number of cases including flow alignment of the order tensor and the Miesowicz viscosities in the presence of an aligning magnetic field. The algorithm accurately recovers the predicted changes in the order parameter in the presence of aligning flow, and magnetic, fields. Preliminary results are given for an extension of the method to model the interface between isotropic and nematic fluids.

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I. INTRODUCTION

The lattice Boltzmann (LB) method has been extensively studied as a mesoscopic method of simulating isotropic fluids (e.g., Refs. [1–4]). The strengths of the method lie in modeling flow in complex geometries (e.g., Ref. [5]) or in multicomponent flow (e.g., Refs. [6,7]). Recently, a number of LB schemes have been developed to represent the flow of anisotropic fluids such as liquid crystals [8,9].

Materials that exhibit liquid crystal phases have anisometric molecules [10,11] and nematic liquid crystals are of particular interest because of their application in display devices. There is also increasing interest in modeling liquid crystal colloids in which colloidal particles are embedded in a nematic phase [12]. The colloidal particles interact through the distortions and defects that they generate in the nematic elastic field. The forces between the particles and the dynamics of their motion is accessible to experiment (cf. Poulin *et al.* [13]). As a consequence of these additional colloidal interactions, the particles rearrange themselves into new structures and the LB method provides a particularly effective way of dealing with the complex boundary conditions in such problems. The method can recover both the nematostatics and nematodynamics of these phases and hence the dynamics of the colloidal phase can be captured and this has been achieved with an earlier LB method developed by the authors [8,14].

Additionally, the colloidal particles may be an isotropic fluid and work is currently in progress to extend the two phase LB algorithms that have been developed for isotropic fluids to describe a mixture in which one of the phases is a nematic liquid crystal. Preliminary results from this work are presented later in the paper and are based on extensions to the method to recover a isotropic-nematic interface following the macroscopic description of Rey [15,16]. The hydrodynamics associated with pair annihilation of line defects is also a matter of current interest and results have been reported using both lattice Boltzmann [17] and conventional solvers [18] of the equations for nematodynamics in the presence of a variable order parameters.

The orientational ordering of the molecules in the nematic phase is characterized by a director field, $n_\alpha(\mathbf{x},t)$, a unit vector that essentially defines the ''average orientation'' of the molecules. However, the nematic ordering is more fully characterized by a traceless and symmetric order tensor $Q_{\alpha\beta}$. In this work, for simplicity, we assume that the director is confined to a two-dimensional plane, and hence that $Q_{\alpha\beta}$ may be written in the form

$$Q_{\alpha\beta}(\mathbf{x},t)=S(2n_\alpha n_\beta-\delta_{\alpha\beta}). \tag{1}$$

The principal eigenvector of $Q_{\alpha\beta}$ is the director and the principal eigenvalue $S(\mathbf{x},t)$ is the scalar order parameter.

The scheme proposed by Care *et al.* [8] to recover the Ericksen, Leslie, and Parodi (ELP) equations [10] used two coupled LB equations. These equations govern the continuum fluid dynamics of an incompressible nematic with an order parameter *S*, which is both position and time *independent*. In the scheme [8], one of the LB equations carried the momentum and the second carried a vector density corresponding to the director field. The Denniston *et al.* [9] scheme is also based on two coupled lattice Boltzmann schemes, one of which carries a momentum density and the second carries a tensor density from which the macroscopic order tensor can be recovered. This latter scheme recovers the Beris-Edwards equations [19] for the flow of a nematic liquid crystal with variable order parameter.

In the work presented in this paper, a third scheme is presented that recovers the Qian-Sheng [20] equations for the flow of a nematic liquid crystal with a variable scalar order parameter. The scheme is based on a single LB equation that governs the evolution of a tensor density and from which both the macroscopic order and momentum evolution equations are recovered. It is worth noting that there have been a number of different derivations of nematodynamics with

variable order parameters with perhaps the earliest results presented by Hess [21] and Olmsted and Goldbart [22]. The recent work by Sonnet, Maffettone, and Virga [23] provides the basis upon which the variety of schemes with a variable order parameter may be compared. The Qian-Sheng equations, such as the Beris-Edwards equations, reduces to the ELP formalism in the limit that the order parameter becomes independent of time and position. There are a number of important differences between the scheme proposed here and that of Denniston. In the scheme described here, the target equations are those of Qian-Sheng rather than Beris-Edwards, there is a single Boltzmann equation, the equilibrium distribution function is isotropic (as is expected on physical grounds), and the scheme is able to recover the full tensorial coupling of the order tensor to the velocity gradient tensor, from a single lattice distribution function.

The target macroscopic equations of the Qian-Sheng scheme are summarized in Sec. II, the proposed scheme is described in Sec. III, and a Chapman Enskog analysis of the scheme is presented in Sec. IV. A number of analytical results are developed from the Qian-Sheng equations in Sec. V, which provide the basis for validation of the LB algorithm in Sec. VI A. Preliminary results for a nematic-isotropic interface are presented in Sec. VI B and the conclusions are presented in Sec. VII.

II. QIAN-SHENG FORMALISM

In this section we summarize the target macroscopic equations for the LB method. The two governing equations of the Qian scheme are the momentum evolution equation

$$\rho D_t u_\beta = \partial_\beta(-P\delta_{\alpha\beta}+\sigma^d_{\alpha\beta}+\sigma^f_{\alpha\beta}+\sigma'_{\alpha\beta}) \tag{2}$$

and the order tensor evolution equation

$$J\ddot{Q}_{\alpha\beta}=h_{\alpha\beta}+h'_{\alpha\beta}-\lambda\delta_{\alpha\beta}-\varepsilon_{\alpha\beta\gamma}\lambda_\gamma. \tag{3}$$

It is shown by Qian that in the limit of constant order parameter, the solutions of these equations are identical to those obtained from the ELP equations. Throughout this work we use the repeated index notation for summations over Cartesian indices. In the above equations, $D_t=\partial_t+u_\mu\partial_\mu$ is the convective derivative, P is the pressure, $\sigma^d_{\alpha\beta}$ is the distortion stress tensor given by

$$\sigma^d_{\alpha\beta}=-\frac{\partial F_{LdG}}{\partial(\partial_\alpha Q_{\mu\nu})}\partial_\beta Q_{\mu\nu}, \tag{4}$$

and $\sigma^f_{\alpha\beta}$ is the stress tensor associated with an externally applied field. In the current work we only consider an externally applied magnetic field for which the stress tensor is given by Landau and Lifshitz [24]

$$\sigma^f_{\alpha\beta}=-\frac{1}{4\pi}\left(H_\alpha H_\beta-\frac{1}{2}H^2\delta_{\alpha\beta}\right). \tag{5}$$

The viscous stress tensor $\sigma'_{\alpha\beta}$ is given by

$$\sigma'_{\alpha\beta}=\beta_1 Q_{\alpha\beta}Q_{\mu\nu}A_{\mu\nu}+\beta_4 A_{\alpha\beta}+\beta_5 Q_{\alpha\mu}A_{\mu\beta}+\beta_6 Q_{\beta\mu}A_{\mu\alpha}+\tfrac{1}{2}\mu_2 N_{\alpha\beta}-\mu_1 Q_{\alpha\mu}N_{\mu\beta}+\mu_1 Q_{\beta\mu}N_{\mu\alpha}, \tag{6}$$

where $A_{\alpha\beta}=\frac{1}{2}(\partial_\alpha u_\beta+\partial_\beta u_\alpha)$ is the symmetric velocity gradient tensor. The elastic molecular field is given by

$$h_{\alpha\beta}=-\frac{\partial F_{LdG}}{\partial Q_{\alpha\beta}}+\partial_\mu\frac{\partial F_{LdG}}{\partial(\partial_\mu Q_{\alpha\beta})}, \tag{7}$$

where, in the current work, the Landau–de Gennes free energy is assumed to be of the form

$$F_{LdG}=\tfrac{1}{2}(\alpha_F Q^2_{\mu\nu}+L_1 Q^2_{\mu\nu,\tau}+L_2 Q_{\mu\nu,\nu}Q_{\mu\tau,\tau})-\beta_F Q_{\mu\nu}Q_{\nu\tau}Q_{\tau\mu}+\gamma_F(Q^2_{\mu\nu})^2, \tag{8}$$

where $Q_{\alpha\beta,\gamma}\equiv\partial_\gamma(Q_{\alpha\beta})$. Using this form of the free energy and the definition of the molecular field, Eq. (7), we find

$$h_{\alpha\beta}=L_1\partial^2_\mu Q_{\alpha\beta}+L_2\partial_\beta\partial_\mu Q_{\alpha\mu}-\alpha_F Q_{\alpha\beta}+3\beta_F Q_{\alpha\mu}Q_{\beta\mu}-4\gamma_F Q_{\alpha\beta}Q^2_{\mu\nu}. \tag{9}$$

The quantities λ and λ_α in Eq. (3) are Lagrange multipliers that impose the constraints on the elastic molecular field, which arise because the order tensor $Q_{\alpha\beta}$ is symmetric and traceless. For a three-dimensional system they have the values

$$\lambda=\tfrac{1}{3}(h_{\mu\mu}-\tfrac{1}{2}\mu_2 A_{\mu\mu}),\quad \lambda_\alpha=\tfrac{1}{2}\varepsilon_{\alpha\mu\nu}h_{\mu\nu}. \tag{10}$$

The term $A_{\mu\mu}$ in the first of Eqs. (10) does not appear in the Qian-Sheng equations, but is necessary in order to correct for the slight compressibility of the LB fluid. In the presence of an external magnetic field, the free energy is assumed to be augmented by a term of the form

$$F_H=-\tfrac{1}{2}(\chi_\parallel-\chi_\perp)Q_{\alpha\beta}H_\alpha H_\beta, \tag{11}$$

which gives an additional term in the molecular field of the form

$$h^H_{\alpha\beta}=\tfrac{1}{2}\chi_a H_\alpha H_\beta, \tag{12}$$

where $\chi_a=\chi_\parallel-\chi_\perp$ is the anisotropy in the susceptibility. The viscous molecular field $h'_{\alpha\beta}$ is given by

$$-h'_{\alpha\beta}=\tfrac{1}{2}\mu_2 A_{\alpha\beta}+\mu_1 N_{\alpha\beta}, \tag{13}$$

where $N_{\alpha\beta}$ is the corotational derivative defined by

$$N_{\alpha\beta}=\partial_t Q_{\alpha\beta}+u_\mu\partial_\mu Q_{\alpha\beta}-\varepsilon_{\alpha\mu\nu}\omega_\mu Q_{\nu\beta}-\varepsilon_{\beta\mu\nu}\omega_\mu Q_{\nu\alpha}, \tag{14}$$

where the vorticity $\underline{\omega}=\frac{1}{2}(\nabla\times\underline{u})$.

In order to develop a lattice Boltzmann scheme we rearrange Eq. (6) by substituting from Eq. (14) for the corotational derivative $N_{\alpha\beta}$ and obtain the form

$$\sigma'_{\alpha\beta}=\beta_1 Q_{\alpha\beta}Q_{\mu\nu}A_{\mu\nu}+\left(\beta_4-\frac{(\mu_2)^2}{2\mu_1}\right)A_{\alpha\beta}+\left(\beta_5+\frac{1}{2}\mu_2\right)Q_{\alpha\mu}A_{\mu\beta}+\left(\beta_6-\frac{1}{2}\mu_2\right)Q_{\beta\mu}A_{\mu\alpha}+\frac{\mu_2}{2\mu_1}(h_{\alpha\beta}-\delta_{\alpha\beta}\lambda-\varepsilon_{\alpha\beta\mu}\lambda_\mu)+Q_{\beta\mu}h_{\mu\alpha}-Q_{\alpha\mu}h_{\mu\beta}\varepsilon_{\mu\beta\nu}Q_{\alpha\mu}\lambda_\nu-\varepsilon_{\mu\alpha\nu}Q_{\beta\mu}\lambda_\nu. \quad (15)$$

Equation (3) for the order tensor evolution can be cast in the form

$$D_t Q_{\alpha\beta}=-\frac{\mu_2}{2\mu_1}A_{\alpha\beta}+\frac{1}{\mu_1}h_{\alpha\beta}+\epsilon_{\alpha\mu\nu}\omega_\mu Q_{\nu\beta}+\epsilon_{\beta\mu\nu}\omega_\mu Q_{\nu\alpha}-\frac{1}{\mu_1}(\delta_{\alpha\beta}\lambda+\varepsilon_{\alpha\beta\mu}\lambda_\mu), \quad (16)$$

where we have set the inertial density of the fluid, J, to zero. Equations (15) and (16) are the expressions recovered by the LB scheme proposed below. After each time step, the macroscopic density, momentum, and the order tensor are recovered from the LB tensor density. The gradients of the order tensor are then used to construct the molecular field through Eq. (9) and this modifies the dynamics through appropriate forcing terms in the LB equation.

III. THE LATTICE BOLTZMANN ALGORITHM

In order to recover both the momentum evolution Eq. (2) and the order tensor evolution Eq. (3) within a lattice Boltzmann scheme, the scalar density of a standard lattice Boltzmann scheme, $f_i(\underline{r},t)$, is replaced by a tensor density $g_{i\alpha\beta}(\underline{r},t)$, where i is the normal velocity index and α and β label either a two- or three-dimensional Cartesian basis. One can think of the tensor density as carrying information about the ordering of that population of the fluid ''element'' on the velocity link i, associated with a particular position and time. Hence the densities of a standard LB scheme have been generalized to carry information about the order associated with the fluid in addition to the density and momentum.

The density $g_{i\alpha\beta}(\underline{r},t)$ is assumed to have the following moments:

$$\rho=\sum_i g_{i\mu\mu}, \quad (17)$$

$$\rho u_\alpha=\sum_i c_{i\alpha}g_{i\mu\mu}, \quad (18)$$

$$\rho S_{\alpha\beta}=\sum_i g_{i\alpha\beta}, \quad (19)$$

where $S_{\alpha\beta}$ is an order matrix with unit trace, which is related to $Q_{\alpha\beta}$ by

$$S_{\alpha\beta}=\tfrac{1}{2}(Q_{\alpha\beta}+\delta_{\alpha\beta}), \quad (20)$$

which in two dimensions is related to $Q_{\alpha\beta}$ by Eq. (20). The LB algorithm governing the evolution of $g_{i\alpha\beta}$ is taken to be of the form

$$g_{i\alpha\beta}(\underline{r}+\delta\underline{c}_i,t+\delta)=g_{i\alpha\beta}(\underline{r},t)+\sum_j g^{(neq)}_{j\mu\nu}(\underline{r},t)M_{i\alpha\beta j\mu\nu}+\phi_{i\alpha\beta}+\chi_{i\alpha\beta}, \quad (21)$$

where $\phi_{i\alpha\beta}$ and $\chi_{i\alpha\beta}$ are the forcing terms for the momentum and order, respectively, and there is an implicit summation over repeated Cartesian indices. The nonequilibrium distribution function is given by

$$g^{(neq)}_{i\alpha\beta}=g_{i\alpha\beta}-g^{(0)}_{i\alpha\beta}, \quad (22)$$

where the equilibrium distribution function $g^{(0)}_{i\alpha\beta}$ is taken to be of the form

$$g^{(0)}_{i\alpha\beta}=S_{\alpha\beta}f^{(0)}_i. \quad (23)$$

The distribution function $f^{(0)}_i$ is assumed to be second order in the velocity u_α and is determined in the usual way, by the requirements

$$\rho=\sum_i f^{(0)}_i, \quad \rho u_\alpha=\sum_i c_{i\alpha}f^{(0)}_i, \quad (24)$$

and Galilean invariance in the form

$$\sum_i c_{i\alpha}c_{i\beta}g^{(0)}_{i\alpha\beta}=c_s^2\rho\delta_{\alpha\beta}+\rho u_\alpha u_\beta. \quad (25)$$

Hence, we have

$$\sum_i g^{(0)}_{i\alpha\beta}=\rho S_{\alpha\beta}, \quad \sum_i c_{i\alpha}g^{(0)}_{i\alpha\beta}=\rho S_{\alpha\beta}u_\alpha. \quad (26)$$

In Sec. IV, it is shown that in order to recover the required tensor coupling of the order tensor to the velocity gradient tensor it is necessary to have sixth order isotropy of the velocity tensors. In this work, the required isotropy is achieved by using a two-dimensional hexagonal lattice with three speeds and coordination number 13 (D2Q13) for which the velocity vectors $\mathbf{c}_p$ are given by

$$\mathbf{c}_0=\{0,0\},$$
$$\mathbf{c}_1=c\{\pm1,0\},c\{\pm1/2,\pm\sqrt{3}/2\},$$
$$\mathbf{c}_2=c\{0,\pm\sqrt{3}\},c\{\pm3/2,\pm\sqrt{3}/2\}, \quad (27)$$

the subscripts 0, 1, and 2 being associated with particles with velocity 0, c, and $\sqrt{3}c$, respectively. Imposing conditions (24) and (25) leads to the result

$$g^{(0)}_{i\alpha\beta}=\rho S_{\alpha\beta}t_i\left[1+\frac{1}{c_s^2}u_\alpha c_{i\alpha}+\frac{1}{2c_s^2}u_\alpha u_\beta\left(\frac{c_{i\alpha}c_{i\beta}}{c_s^2}-\delta_{\alpha\beta}\right)\right], \quad (28)$$

where, in D2Q13, $t_0=11/25$, $t_1=9/100$, and $t_2=1/300$ and the velocity of sound $c_s=(3/10)^{1/2}$. The collision operator is taken to be of the form

$$M_{i\alpha\beta j\mu\nu}=\delta_{\alpha\mu}\delta_{\beta\nu}\left[-\frac{\delta_{i,j}}{\tau_j}+\frac{\delta_{i0}}{\tau_j}+\frac{t_i c_{i\varepsilon}c_{j\varepsilon}}{c_s^2}\left(\frac{1}{\tau_j}-2\right)\right], \tag{29}$$

where the *direction dependent* relaxation parameter is defined to be

$$\tau_i=\tau_0(1+\eta_0 c_{i\mu}c_{i\nu}\delta_{\mu\nu}+\eta_2 c_{i\mu}c_{i\nu}Q_{\mu\nu}). \tag{30}$$

This collision operator may be seen more transparently after performing the contraction with the nonequilibrium distribution function as in Eq. (21)

$$\sum_{j\mu\nu} M_{i\alpha\beta j\mu\nu}g_{j\mu\nu}^{(neq)}=-\frac{g_{i\alpha\beta}^{(neq)}}{\tau_i}+\delta m_{i\alpha\beta}+\delta p_{i\alpha\beta}, \tag{31}$$

where

$$\delta m_{i\alpha\beta}=\delta_{i0}\sum_j \frac{g_{j\alpha\beta}^{(neq)}}{\tau_j} \tag{32}$$

is a correction to conserve mass. The term

$$\delta p_{i\alpha\beta}=\frac{t_i c_{i\varepsilon}}{c_s^2}\sum_j c_{j\varepsilon}g_{j\alpha\beta}^{(neq)}\left(\frac{1}{\tau_j}-2\right) \tag{33}$$

includes a term in $1/\tau_j$, which is a correction to conserve momentum and a term associated with a factor -2, which is explained at the end of Sec. IV A. The collision operator is essentially a lattice Bhatnagar-Gross-Krook (LBGK) collision operator (e.g., Ref. [2]) with a relaxation time that is direction dependent. When written in the matrix form, the collision operator is seen to lie between a conventional LBGK operator and a linearized lattice Boltzmann scheme (e.g., Ref. [25]) although the usual circulant properties of the matrix associated with an isotropic fluid are destroyed by the direction dependent scattering in the method presented here.

The momentum forcing term is given by

$$\phi_{i\alpha\beta}=t_i S_{\alpha\beta}c_{i\mu}\partial_\nu F_{\nu\mu}, \tag{34}$$

where

$$F_{\alpha\beta}=-\frac{1}{c_s^2}\left(-\frac{\mu_2(h_{\alpha\beta}-\varepsilon_{\alpha\beta\mu}\lambda_\mu)}{2\mu_1}+Q_{\alpha\mu}(h_{\mu\beta}-\varepsilon_{\mu\beta\nu}\lambda_\nu)\right.$$
$$\left.-Q_{\beta\mu}(h_{\mu\alpha}-\varepsilon_{\mu\alpha\nu}\lambda_\nu)-\sigma_{\alpha\beta}^d-\sigma_{\alpha\beta}^f\right) \tag{35}$$

and the angular forcing term is given by

$$\chi_{i\alpha\beta}=t_i\rho[(\varepsilon_{\alpha\nu\mu}Q_{\beta\mu}+\varepsilon_{\beta\nu\mu}Q_{\alpha\mu})\omega_\nu]-\frac{t_i\rho}{2\mu_1}[\mu_2 A_{\alpha\beta}-2h_{\alpha\beta}$$
$$+2\delta_{\alpha\beta}\lambda+2\varepsilon_{\alpha\beta\mu}\lambda_\mu]. \tag{36}$$

IV. ANALYSIS OF THE ALGORITHM

A. Chapman-Enskog expansion

In this section the key results of the Chapman-Enskog analysis are given, which demonstrate how the scheme described in Sec. II can be recovered from the LB algorithm described in Sec. III. We follow a standard Chapman-Enskog analysis [2] and expand the density and the time derivatives in the form

$$g_{i\alpha\beta}=\sum_{n=0}^{\infty}\delta^n g_{i\alpha\beta}^{(n)}, \tag{37}$$

$$\partial_t=\sum_{n=0}^{\infty}\delta^n\partial_{t,n}. \tag{38}$$

We assume for the purposes of the following analysis that the forcing terms $\phi_{i\alpha\beta}$ and $\chi_{i\alpha\beta}$ can both be introduced at order $O(\delta^2)$ since both include gradient terms in both the velocity and director field (cf. Ref. [8]). The choice is supported by the agreement of the Chapman-Enskog analysis with the measured simulation data; however the assumption relies upon assumptions implicit in LB hydrodynamics in general. Accordingly, it requires more careful analysis, which will be undertaken in a later work.

The Chapman-Enskog expansion gives to $O(\delta)$

$$\partial_{t,0}g_{i\alpha\beta}^{(0)}+c_{i\mu}\partial_\mu g_{i\alpha\beta}^{(0)}=\sum_j g_{j\mu\nu}^{(1)}M_{i\alpha\beta j\mu\nu} \tag{39}$$

and to $O(\delta^2)$

$$\partial_{t,1}g_{i\alpha\beta}^{(0)}+(\partial_{t,0}+c_{i\mu}\partial_\mu)\left(g_{i\alpha\beta}^{(1)}+\frac{1}{2}\sum_j g_{j\mu\nu}^{(1)}M_{i\alpha\beta j\mu\nu}\right)$$
$$=\sum_j g_{j\mu\nu}^{(2)}M_{i\alpha\beta j\mu\nu}+\phi_{i\alpha\beta}+\chi_{i\alpha\beta}. \tag{40}$$

We now take moments of Eqs. (39) and (40) in order to recover the macroscopic equations to which the algorithm is equivalent. If we sum the two equations over index i, take the trace of the distribution density, and sum the resulting equations, we recover

$$(\partial_{t,0}+\partial_{t,1})\rho+\partial_\mu(\rho u_\mu)=0, \tag{41}$$

which is the continuity equation to second order. If we multiply Eqs. (39) and (37) by $c_{i\nu}$, sum over index i, take the trace of the distribution density, and sum the resulting equations, we recover

$$(\partial_{t,0}+\partial_{t,1})(\rho u_\alpha)+\partial_\mu\left(\Pi_{\alpha\mu}^{(0)}+\Pi_{\alpha\mu}^{(1)}+\frac{1}{2}\Omega_{\alpha\mu}^{(1)}\right)=c_s^2\partial_\mu F_{\mu\alpha}, \tag{42}$$

where

$$\Pi_{\alpha\beta}^{(n)}=\sum_i c_{i\alpha}c_{i\beta}g_{i\mu\mu}^{(n)} \tag{43}$$

and

$$\Omega^{(n)}_{\alpha\beta}=\sum_{ij}\ g^{(n)}_{j\mu\nu}c_{i\alpha}c_{i\beta}M_{i\kappa\kappa j\mu\nu}. \tag{44}$$

Further progress can be made by noting that, to $O(u)$, the lowest-order equation (39) can be written in the form

$$t_i\left(\frac{c_{i\mu}c_{i\nu}}{c_s^2}-\delta_{\mu\nu}\right)\partial_\mu(\rho S_{\alpha\beta}u_\nu)=\sum_j\ g^{(1)}_{j\mu\nu}M_{i\alpha\beta j\mu\nu}. \tag{45}$$

Substituting into Eq. (44), this yields the result

$$\Omega^{(1)}_{\alpha\beta}=\sum_i\ t_ic_{i\alpha}c_{i\beta}\left(\frac{c_{i\mu}c_{i\nu}}{c_s^2}-\delta_{\mu\nu}\right)\partial_\mu(\rho u_\nu), \tag{46}$$

where the unit trace property of $S_{\alpha\beta}$ has been used. In order to obtain an expression for $\Pi^{(1)}_{\alpha\beta}$, we use Eqs. (31) and (45) to give, to first order in the velocity,

$$g^{(1)}_{i\alpha\beta}=-\tau_i\left[t_i\left(\frac{c_{i\mu}c_{i\nu}}{c_s^2}-\delta_{\mu\nu}\right)\partial_\mu(\rho S_{\alpha\beta}u_\nu)-\delta m_{i\alpha\beta}-\delta p_{i\alpha\beta}\right], \tag{47}$$

where we have made the approximation, correct to $O(\delta^2)$, that $g^{(neq)}_{i\alpha\beta}\simeq g^{(1)}_{i\alpha\beta}$. Term $\delta m_{i\alpha}$ does not contribute to $\Pi^{(1)}_{\alpha\beta}$, as can be seen from Eq. (43), since it is included in the rest mass. It can further be shown that the contribution from the term $\delta p_{i\alpha\beta}$ is essentially zero. We, therefore, find

$$\Pi^{(1)}_{\alpha\beta}=-\tau_0\sum_i\ t_ic_{i\alpha}c_{i\beta}(1+\eta_0c_{i\mu}c_{i\nu}\delta_{\mu\nu}+\eta_2c_{i\mu}c_{i\nu}Q_{\mu\nu})\times\left[\left(\frac{c_{i\tau}c_{i\varepsilon}}{c_s^2}-\delta_{\tau\varepsilon}\right)\partial_\tau(\rho u_\varepsilon)\right], \tag{48}$$

where we have substituted for the anisotropic relaxation parameter τ_i. Assuming that the velocity tensors

$$E^{(n)}_{\alpha_1\cdots\alpha_n}=\sum_i\ t_ic_{i\alpha_1}\cdots c_{i\alpha_n} \tag{49}$$

are isotropic up to sixth order, we recover the required form of the tensor coupling between the order tensor and the velocity gradient tensor.

Using these results it can be shown that, apart from the term associated with β_1, the required momentum evolution equation (2) is recovered when Eq. (35) is used as the momentum forcing term. The term in β_1 could be recovered by including a fourth-order velocity product in the anisotropic relaxation parameter but this would require the velocity tensors to be isotropic to eighth order. However, for simplicity, the term in β_1 is omitted in the results presented in this paper.

The order tensor evolution equation is recovered from Eqs. (39) and (40) by summing over index i and adding the two resulting equations to give

$$\partial_{t,0}(\rho Q_{\alpha\beta})+\partial_{t,1}(\rho Q_{\alpha\beta})+\partial_\gamma(\rho Q_{\alpha\beta}u_\gamma)=\sum_i\ \chi_{i\alpha\beta}. \tag{50}$$

Equation (50) combined with the forcing term (36) gives the required evolution equation (3). However, in order to obtain the result (50) it is necessary to suppress a contribution of the form

$$\partial_\gamma\left(\sum_i\ c_{i\gamma}g^{(1)}_{i\alpha\beta}\right) \tag{51}$$

at second order in the Chapman-Enskog analysis and this is achieved using the term associated with the factor -2 in Eq. (33).

The term (51) arises because conservation of mass and momentum alone are insufficient to constrain all the first-order elements of the distribution function. This arises because in order to recover the required macroscopic equations, the form of the equilibrium distribution function must satisfy Eqs. (26). However, the limitations on the definitions of the moments of the distribution function lead to the result

$$\sum_i\ c_{i\gamma}g_{i\alpha\beta}\neq\rho S_{\alpha\beta}u_\gamma \tag{52}$$

and, as a consequence, the argument of the derivative in Eq. (51) is nonzero.

B. Choice of LB parameters

The following correspondence is found between the parameters of the LB algorithm and the parameters of the target scheme:

$$\beta_4=\frac{\mu_2^2}{4\mu_1}-\rho c_s^2(1-2\tau_0\zeta),$$

$$\beta_5=-\frac{\mu_2}{2}+\eta_2\rho\tau_0c_s^2,$$

$$\beta_6=\frac{\mu_2}{2}+\eta_2\rho\tau_0c_s^2, \tag{53}$$

where parameter $\zeta=1+\eta_0(1+d/4)$ with d being the dimensionality of the LB scheme, which is taken to be 2 for the results presented in Sec. VI. The viscosity set $\{\beta_4,\beta_5,\mu_1,\mu_2\}$ of the Qian scheme is recovered from the parameter set $\{\tau_0,\eta_0,\eta_2,\mu_1,\mu_2\}$ of the LB algorithm. We note from Qian [20] that $\beta_6-\beta_5=\mu_2$ and this is seen to be consistent with the last two of Eqs. (53). There is one free parameter in the LB scheme since we require to recover only four Qian parameters from five LB parameters. The free parameter is taken to be η_0 which is adjusted to place the LB scheme in a stable region of its parameter space, as is explained below.

Equations (53) can be inverted to give

$$\eta_2 = -\frac{4\mu_1\zeta(2\beta_5+\mu_2)}{\mu_2^2-4\mu_1(\beta_4+\rho c_s^2)},$$

$$\tau_0 = \frac{4\beta_4+4\rho c_s^2-\dfrac{\mu_2^2}{\mu_1}}{8\rho c_s^2\zeta}. \tag{54}$$

In the absence of any anisotropic terms, the last expression in Eq. (54) becomes $\beta_4/\rho = c_s^2(1-2\tau_0)$, which is equivalent to the standard result for the kinematic viscosity in an LBGK scheme. The relationship between the Qian parameters $\{\beta_4,\beta_5,\mu_1,\mu_2\}$ and the standard Leslie coefficients is given in Sec. V.

We now establish an approximate criterion for the stability of the LB algorithm by considering a system that is evolving towards a uniform density and velocity distribution at all points. The algorithm involves repeated application of the collision operator $M_{i\alpha\beta j\mu\nu} \equiv \underline{\underline{M}}$ and ignoring forcing terms, the nonequilibrium part of the distribution function is transformed at each time step according to the symbolic equation

$$\underline{g}^{(neq)} \rightarrow (\underline{\underline{1}}+\underline{\underline{M}})\underline{g}^{(neq)}. \tag{55}$$

In order for the nonequilibrium part to decay to zero under successive applications of Eq. (55), it is necessary that

$$-1 < (\underline{\underline{1}}+\underline{\underline{M}})_{i\alpha\beta j\mu\nu} < 1 \tag{56}$$

for all choices of indices. This equation may be recast as the stability criteria

$$-2 < M_{(Diag)} < 0, \quad |M_{(OffDiag)}| < 1. \tag{57}$$

However, it should be remembered that the matrix $\underline{\underline{M}}$ is a function of position, as a consequence of its dependence on the order tensor through the anisotropic relaxation parameter τ_i. Hence, in a given simulation, conditions (57) cannot be guaranteed under all flow conditions. The criteria have been achieved in the implementation of the algorithm described in Sec. VI by explicit evaluation of all the nonzero elements of the collision matrix prior to running the algorithm and after making appropriate assumptions about the ordering in the system. Parameter η_0 is then chosen to ensure that conditions (57) are satisfied for all possible values of the director and scalar order parameter.

V. ANALYTICAL RESULTS FROM THE QIAN FORMALISM

In this section we quote without detailed proof some analytical results that can be derived from the Qian formalism and that will be used in Sec. VI to validate the algorithm. Further discussion of the results and their significance is being prepared for a future publication. The results quoted in Sec. VI have been derived for a system in which the director is confined to lie in a two-dimensional plane and the order tensor for such a system may be written in the form

$$Q_{\alpha\beta} = S(2n_\alpha n_\beta - \delta_{\alpha\beta}), \tag{58}$$

where the time and position dependent quantities S and n_α are the order parameter and director. If form (58) is substituted into the free energy expression (8) and all the time and spatial derivatives are removed, we find that the equilibrium Landau–de Gennes free energy in the presence of a uniform magnetic field is given by

$$F_{LdG}^{(equ)} = \alpha_F S_H^2 + 4\gamma S_H^4 - \tfrac{1}{2} S_H \chi_a H_\alpha^2, \tag{59}$$

where it is assumed that the director is parallel to the magnetic field. The equilibrium order parameter, which minimizes Eq. (59), has the form

$$S_H = S_+ + S_- \tag{60}$$

with

$$S_\pm = \frac{1}{12}\left(\frac{27\chi_a H^2}{\gamma} \pm 3\sqrt{3}\sqrt{\frac{8\alpha_F^3+27\gamma\chi_a^2H^4}{\gamma^3}}\right)^{1/3}, \tag{61}$$

where the free energy parameter α will be negative in the nematic phase and we choose the real solutions of S_0. In the limit $H \rightarrow 0$, we have

$$S_0 = \frac{1}{2}\sqrt{\frac{-\alpha_F}{2\gamma}}, \tag{62}$$

which is the equilibrium order parameter that effectively minimizes the Landau–de Gennes free energy in the absence of director gradients. Using Eq. (58) with S set to S_0, we may follow the arguments given in Appendix B of Qian to determine the relationship between the Leslie coefficients of a material and the viscosity coefficients used in the Qian scheme. It is found for a system with the order tensor given by Eq. (58)

$$\beta_1 = \alpha_1/(4S_0^2), \quad \beta_4 = (1/2)(2\alpha_4+\alpha_5+\alpha_6)$$

$$\beta_5 = \alpha_5/(2S_0), \quad \beta_6 = \alpha_6/(2S_0)$$

$$\mu_1 = (\alpha_3-\alpha_2)/(8S_0^2), \quad \mu_2 = (\alpha_2+\alpha_3)/(2S_0), \tag{63}$$

where S_0 is the order parameter defined by Eq. (62). In simple shear flow between two parallel plates and in the absence of any external field, Eq. (3) for the evolution of the order tensor can be solved to find the steady state value of the angle of orientation and the order parameter. In the center of the flow, remote from the walls, the gradients in the order tensor may be ignored and the director is found to lie at an angle θ with respect to the flow velocity, where

$$\cos(2\theta) = -\frac{4S\mu_1}{\mu_2} \tag{64}$$

and this is directly equivalent to the result found for the ELP equations, $\cos(2\theta) = -\gamma_1/\gamma_2$ [10]. The order parameter is also modified in shear flow and is given by the solution of the cubic equation

$$ax^3+bx^2+cx+d=0, \tag{65}$$

where $x=S^2$ and

$$a=1024\gamma^2, \quad b=256\alpha\gamma$$

$$c=16[\alpha^2+(\mu_1\partial_y u_x)^2], \quad d=-(\mu_2\partial_y u_x)^2. \tag{66}$$

This equation may be solved and to first order in the velocity gradient the order parameter is found to be

$$S=S_0+\frac{\sqrt{\mu_2^2-16S_0^2\mu_1^2}}{8|\alpha_F|}|\partial_y u_x| \tag{67}$$

and hence the order parameter increases as a consequence of flow alignment. Finally we consider the Miesowicz viscosities in a system with a variable order parameter. The stress tensor evolution equation can be solved for a simple shear flow in the presence of a strongly aligning external field. If the director is given by $\{n_x,n_y\}$, the associated Miesowicz viscosity η_{eff} is given by

$$\eta_{eff}=\frac{1}{4S_0^2}\{S_0^2[2\alpha_4+\alpha_5+\alpha_6]+S^2[\alpha_3-\alpha_2+4\alpha_1 n_x^2 n_y^2]$$
$$+SS_0[\alpha_6(2n_x^2-1)+(\alpha_2+\alpha_3)(n_x^2-n_y^2)$$
$$+\alpha_5(2n_y^2-1)]\}, \tag{68}$$

where S is the order parameter in the flow and S_0 is the equilibrium value of the order parameter defined in Eq. (62). In the limit that the order parameter is fixed (i.e., $S=S_0$), Eq. (68) reduces to the standard results

$$\eta_{par}=\tfrac{1}{2}(\alpha_4+\alpha_3+\alpha_6),$$

$$\eta_{perp}=\tfrac{1}{2}(\alpha_4-\alpha_2+\alpha_5), \tag{69}$$

where η_{par} and η_{perp} correspond to the director being aligned parallel, $\mathbf{n}=\{1,0\}$ and perpendicular, $\mathbf{n}=\{0,1\}$, to the flow. In the presence of both a velocity gradient and a strong aligning field, the change in the order parameter is dominated by the aligning field and is hence given to a good approximation by Eqs. (60) and (61).

VI. RESULTS

In this section we first present results that validate the proposed scheme and conclude by presenting some preliminary results in which the scheme is extended to recover a nematic-isotropic interface.

A. Validation results

A number of simulations were undertaken in order to validate the method described in the preceding section. All the results were obtained using a D2Q13 lattice.

In the absence of flow and in the presence of periodic boundary conditions, the order parameter is found to be consistent with the value predicted by Eq. (62) to machine accuracy. If an external magnetic field is applied through the introduction of a molecular field term of form (12), it is found that the director becomes fully aligned with the external field and that the order parameter follows Eq. (60) with an accuracy of better than 0.1%. These two results confirm that the free energy correctly controls the dynamical equations through the associated molecular field. In principle, therefore, the effects of temperature could be introduced into the model through the coefficients in the Landau–de Gennes free energy.

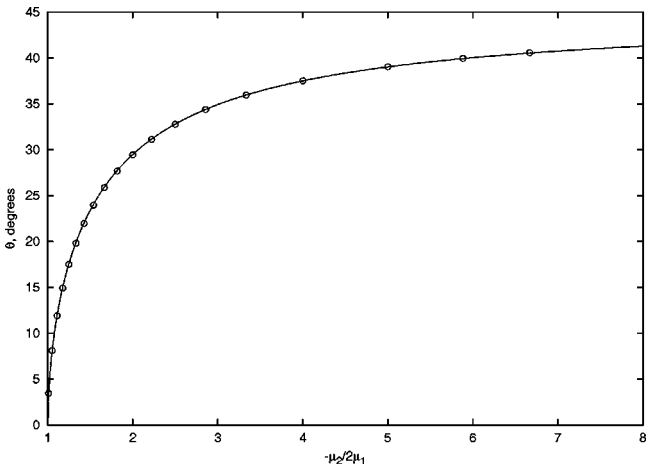

FIG. 1. Director orientation θ in a shear flow as a function of μ_2/μ_1. The continuous curve is $\cos(2\theta)=-4S\mu_1/\mu_2$.

The angle of alignment of the director in a shear flow in the absence of an external magnetic field is given by Eq. (64). In order to test that the technique recovered this result, simulations were run with the free energy parameters ($\alpha_F=-0.0512$, $\beta_F=0$, $\gamma_F=0.01$), chosen to give an equilibrium order parameter of 0.8 and the parameters ($L_1=0.001$, $L_2=0$) selected to give nematic elastic behavior equivalent to the one constant approximation. The LB parameters were chosen to be ($\tau_0=1.1000$, $\eta_0=0.3036$, $\eta_2=0.1565$, $\mu_1=0.3823$, $\mu_2=-1.261$, $\rho=1.8$). If the order parameter S_0 is assumed to be 0.8, these values recover the viscosity ratios ($\alpha_2/\alpha_4=-0.9556$, $\alpha_3/\alpha_4=-0.0144$, $\alpha_5/\alpha_4=0.5565$, $\alpha_6/\alpha_4=-0.4135$), which are consistent with methoxy-benzylidene butyl-aniline (MBBA) at 25 °C [26].

With this choice of parameters, the angle of rotation of the director is predicted to be 7° and this is recovered to an accuracy of less than 1%. The parameters were then adjusted to give a range of values of the angle of alignment (with S_0 set at 0.5) and the results are shown in Fig. 1. The continuous curve in the figure is a fit to Eq. (64) generated with the value of the order parameter taken from the simulation data. The change in the order parameter predicted by Eq. (67) is also recovered to within less than 0.3%.

As a final test of the algorithm, the Miesowicz viscosities were measured for simulations in which the director orientation was controlled by a strong magnetic field. Using the parameters appropriate for MBBA the expected ratio of the viscosities with the director aligned parallel and perpendicular to the direction of flow is 5.03 and this value was recovered with an error of 0.1%. The expected form of the vis-

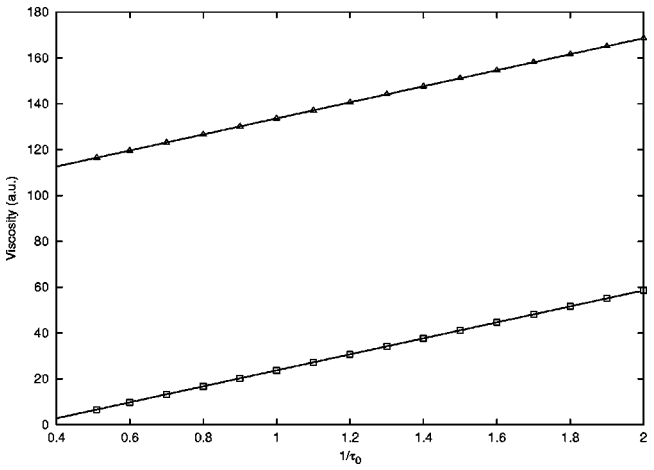

FIG. 2. Viscosity in shear flow as a function of $1/\tau_0$. The upper (lower) line is for director perpendicular (parallel) to the flow direction.

cosity is given by Eq. (68) and it can be shown that this implies that the viscosity should be a linear function of $1/\tau_0$. Figure 2 shows that the expected linearity is observed within the simulations; the slope to intercept ratio for each curve is in error by less than 0.2%.

B. Isotropic-nematic interface

In this section we give a brief summary of a method that the authors are developing to model a nematic-isotropic interface. Preliminary results are presented, but a more detailed study will be given in a forthcoming publication. Experimental results have been reported [27] for the distortion of isotropic droplets embedded in a nematic matrix under the application of a strong electric field and this is a target problem for future studies.

The lattice Boltzmann method has particular advantages in the description of the interface between two isotropic fluids [6,7]. In a recent paper, [28], the authors proposed a method of obtaining a surface tension at the interface between two isotropic fluids by introducing a forcing term on the mixed (surface) sites which is dependent on the surface curvature; the segregation of the two fluids is maintained by the technique of Gunstensen [29]. The method [28] significantly reduces the microcurrents that are an artifact observed in most LB interface schemes.

It is possible to combine the technique described in the earlier sections of this paper with the interface scheme [28] to recover a nematic-isotropic interface based on the continuum description proposed by Rey [15,16]. The lattice is populated by an isotropic density f_i and a nematic density $g_{i\alpha\beta}$ which give the corresponding macroscopic densities ρ^I and ρ^N. A surface unit normal k_α is constructed from the gradient of the nematic density at mixed sites, $\phi_\alpha = \partial_\alpha(\rho^N/\rho)$. The surface normal is used to calculate an elastic surface molecular field

$$\mathbf{h}^S_{\alpha\beta} = -Wk_\alpha k_\beta - L_1 k_\mu \partial_\mu Q_{\alpha\beta} - L_2 k_\alpha \partial_\mu Q_{\mu\beta} \tag{70}$$

and an elastic surface stress tensor

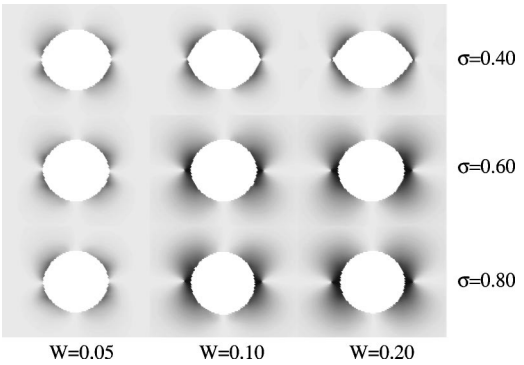

FIG. 3. Droplet of isotropic fluid embedded in a nematic matrix for different values of the surface tension parameter σ and anchoring energy W.

$$\sigma^S_{\alpha\beta} = \sigma(\delta_{\alpha\beta} - k_\alpha k_\beta) + W[\delta_{\alpha\beta} Q_{\mu\nu} k_\mu k_\nu + Q_{\mu\nu} k_\mu k_\nu k_\alpha k_\beta - 2Q_{\alpha\mu} k_\mu k_\beta], \tag{71}$$

where σ controls the strength of the surface tension, W controls the anchoring energy and $\{L_1, L_2\}$ control the elastic constants of the nematic. Results (70) and (71) follow from a surface free energy density equivalent to that proposed by Rapini [30].

In order to generate an isotropic-nematic interface, the forcing introduced in Ref. [28] is adapted to give a forcing for the nematic surface densities of the form

$$\phi^N_{i\alpha\beta} = \frac{\rho^N}{\rho} S_{\alpha\beta} \phi^S_i \tag{72}$$

and, for the isotropic surface densities,

$$\phi^I_i = \frac{\rho^I}{\rho} \phi^S_i, \tag{73}$$

where

$$\phi^S_i = \frac{1}{c_s^2} t_i c_{i\mu} |\phi| \partial^S_\nu \sigma^S_{\nu\mu} \tag{74}$$

with the surface gradient defined by

$$\partial^S_\alpha = (\delta_{\alpha\beta} - k_\alpha k_\beta) \partial_\beta. \tag{75}$$

The angular forcing term, Eq. (36), is also modified on the surface sites to include a contribution from the surface molecular field

$$\chi_{i\alpha\beta} = t_i \rho^N \left\{ (\varepsilon_{\alpha\nu\mu} Q_{\beta\mu} + \varepsilon_{\beta\nu\mu} Q_{\alpha\mu}) \omega_\nu - \frac{1}{2\mu_1} [\mu_2 A_{\alpha\beta} - 2(h_{\alpha\beta} + |\phi| h^S_{\alpha\beta}) + 2\delta_{\alpha\beta}\lambda + 2\varepsilon_{\alpha\beta\mu}\lambda_\mu] \right\}. \tag{76}$$

The segregation of the two fluids is achieved using the method of Gunstensen [29], but it is important to note that the surface tension inducing perturbation used by Gunstensen is replaced by the forcing described above.

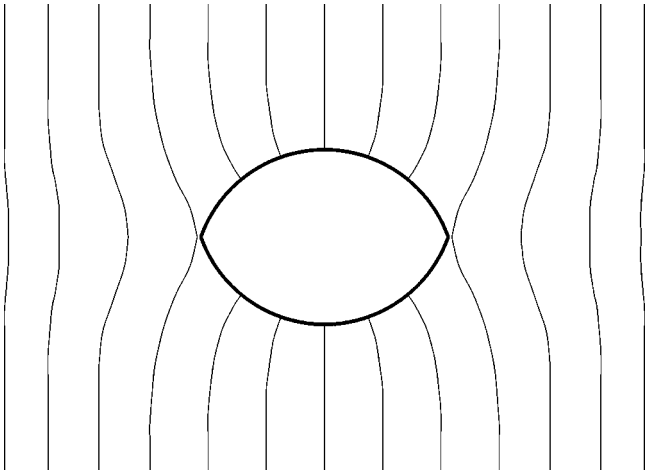

FIG. 4. Sketch of director field for $W=0.2$, $\sigma=0.4$.

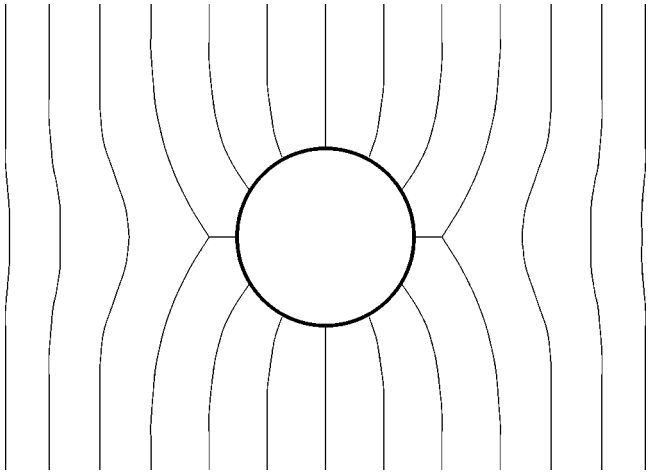

FIG. 5. Sketch of director field for $W=0.2$, $\sigma=0.8$.

Figure 3 illustrates the effect of modifying the surface tension parameter σ and the anchoring energy W. The picture is a collage of nine separate simulations with the specified values for σ and W. In all the simulations, $L_1=10^{-4}$ and $L_2=0$. Each simulation was run to steady state on a 200 $\times 200$ grid with the droplet being initialized as a disk with a diameter of 48 sites. Periodic boundary conditions were imposed with the additional constraint that the director was aligned perpendicular to the top and bottom surfaces. The gray scale is used to represent the direction of the director as seen experimentally through crossed polarizers; white (black) corresponds to the director aligned vertically (horizontally).

It can be seen that as the surface tension parameter σ is reduced and the anchoring strength W is increased, the nematic field significantly distorts the droplet. It can further be seen that as the surface tension and anchoring strength are increased, satellite defects form on each side of the droplet. Figures 4 and 5 are sketches of the director field associated with these two cases.

VII. CONCLUSIONS

In this paper we have presented a generalized lattice Boltzmann scheme which recovers the tensor order parameter equations for a nematic liquid crystal proposed by Qian and Sheng [20]. The generalized method is based on a single tensor density from which all the macroscopic quantities can be recovered. A Chapman-Enskog analysis demonstrates that the algorithm recovers the target macroscopic equations and test simulations demonstrate that the method correctly recovers the evolution of the director, the order parameter, and the velocity gradients in the presence of shear and magnetic fields. Preliminary results have been presented for an extension of the scheme to model a mixture of a isotropic and nematic fluids.

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