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LATTICE BOLTZMANN KINETIC SCHEME FOR ELECTRO-OPTICAL AND MAGNETO-OPTICAL EFFECTS IN FERRONEMATIC LIQUID CRYSTALS

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A new lattice Boltzmann (LB) scheme for ferronematic liquid crystals (FNLCs) is presented. Ferronematics are the colloidal suspension of ferromagnetic nanoparticles in nematic liquid crystals, which have interesting potential applications due to their susceptibility to both the electric field and the magnetic one. We extend the LB model for liquid crystals using our kinetic scheme for magnetic fluids. This model makes it possible to study the coupling effects of electric field and magnetic field in the FNLC efficiently. The LB method is suitable for the numerical investigation of complex fluids such as FNLCs because of its simple algorithm based on the microscopic physics.

Keywords: ferronematic liquid crystals; lattice Boltzmann simulation; kinetic scheme

INTRODUCTION

We present a new lattice Boltzmann (LB) kinetic scheme for studying about electro-optical and magneto-optical effects in Ferronematic liquid crystals (FNLCs). The FNLC [1] is a stable colloidal solution of tiny magnetic particles ($\sim$10 nm diameter) in the nematic liquid crystal (NLC). FNLCs attract much interest from the viewpoints of general physics and of promising applications in the last decades [2–10]. For example, it is known that FNLCs play an important role in the liquid crystal display (LCD). It was verified that FNLCs reduce the magnetic field required to orient the liquid crystal molecules in $1/10^3$ [8–9] and this makes it possible to change

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a pretilt angle of the FNLC by the low magnetic field [10], which is important to improve the response time of the LCD. The FNLC presents a new class of complex fluids because of its magnetic and electric susceptibility. To discuss the properties of such complex fluids numerically, the lattice Boltzmann method [11–16] is a convenient tool due to its simple and stable algorithm based on the microscopic physics.

Several works on liquid crystals have been presented using the lattice Boltzmann method [17–19]. In the recent work [19], they can deal with variation in the magnitude of the nematic order parameter and can simulate the motion of defects, which is a discontinuity in orientation, explicitly. We extend this lattice Boltzmann model in order to simulate the effects of the magnetic field in NLCs with magnetic particles. In NLCs, the orientation by the external electric field is caused by the electric nature of the molecules and the orientation by the magnetic field is caused by moving electric charges, which product magnetic dipoles. On the other hand, in FNLCs the effect of magnetic particles is very important for the orientation by the magnetic field. To investigate these complex properties, we introduce our new lattice Boltzmann algorithm for magnetic fluids [20] to the NLC model [19]. This extension makes it possible to simulate the electro-optical and magneto-optical effects in FNLCs without solving the relaxation equation of magnetization.

We introduce the fundamental equations for FNLCs first and then we present a new idea for solving these equations. The lattice Boltzmann method is a promising scheme for understanding the properties of complex fluids such as FNLCs.

FUNDAMENTAL EQUATIONS

To describe the properties of FNLCs, we consider the three fundamental equations here; the equation of motion of FNLCs, the equation of motion of the tensor order parameter and the relaxation equation of magnetization as follows. The equation of motion of FNLCs is

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t}+(\boldsymbol{u}\cdot\nabla)\boldsymbol{u}\right)=-\nabla P+\eta\nabla^2\boldsymbol{u}+(\boldsymbol{M}\cdot\nabla)\boldsymbol{H}+\frac{1}{2}\nabla\times(\boldsymbol{M}\times\boldsymbol{H})+(\boldsymbol{D}\cdot\nabla)\boldsymbol{E}+\nabla\boldsymbol{S}(F,\boldsymbol{Q}),\tag{1}$$

where ρ is the fluid density, $\boldsymbol{u}$ is the velocity, t is the time, P is the pressure and η is the viscosity. The parameter $\boldsymbol{M}$ is the local magnetization, which is defined as $\boldsymbol{M}\equiv\rho\boldsymbol{m}$, where $\boldsymbol{m}$ is the magnetic moment. $\boldsymbol{H}$ is the magnetic field, $\boldsymbol{D}$ is the electric displacement and $\boldsymbol{E}$ is the electric field. The relation between $\boldsymbol{D}$ and $\boldsymbol{E}$ is given in Ref. [19]. F is the total free energy [7,21]. By minimizing F with respect to variation of the tensor order parameter $\boldsymbol{Q}$ [22],

we can obtain the equilibrium properties of FNLCs. We adapt the following equation to describe the total free energy F per volume V and surface area S,

$$F = \int_V dV(f_{ibulk} + f_{elastic} + f_{interact} + f_{entropy} + f_{field}) + \int_S dS(f_{surf}), \quad (2)$$

where f_{ibulk}, $f_{elastic}$, $f_{interact}$, $f_{entropy}$, f_{field}, and f_{surf} are the free-energy densities of the immanent bulk, the elasticity, the interaction between nematics and magnetic particles, the mixing entropy and the pinning potential at the surface respectively. Here $\boldsymbol{Q}$ is a traceless symmetric tensor related to a unit vector $\boldsymbol{n}$, which shows the direction of individual molecules, by

$$\boldsymbol{Q}_{\alpha\beta}(\boldsymbol{r}) = \left\langle \boldsymbol{n}_\alpha \boldsymbol{n}_\beta - \frac{1}{3}\delta_{\alpha\beta} \right\rangle, \quad (3)$$

where the angular brackets denotes a statistical average around point $\boldsymbol{r}$. $\delta_{\alpha\beta}$ is the Kronecker delta and Greek indices are used to express Cartesian components of vectors and tensors and the usual summation over repeated indices in the single term of the equation will be assumed. $\boldsymbol{Q}_{\alpha\beta}$ is simply related to the order parameter $q(0 < q < 1)$, which describes the magnitude of the order [22]. Let v_α be the director, which is the unit vector defining the preferred direction of molecular orientation, then

$$v_\alpha \boldsymbol{Q}_{\alpha\beta} v_\beta = \langle \cos^2\theta \rangle - \frac{1}{3} = \frac{2}{3}q, \quad (4)$$

where θ is the angle between the director and the long axis of each molecule. The term $2/3q$ shows the largest eigenvalue of $\boldsymbol{Q}$ and its eigenvector describes the director. The free energy density f_{ibulk} is the immanent surplus bulk free energy density besides the elastic free energy density proposed by de Gennes [7] on the basis of the Landau phase transition theory [23–25]:

$$f_{ibulk} = \frac{A_0}{2}\left(1 - \frac{\gamma}{3}\right) Tr\boldsymbol{Q}^2 - \frac{A_0}{3}\gamma Tr\boldsymbol{Q}^3 + \frac{A_0}{4}\gamma (Tr\boldsymbol{Q}^2)^2. \quad (5)$$

Here, A_0 is the concentration (number/volume) of molecules, γ is the Doi excluded volume parameter [26–27]. For $\gamma = 2.7$ there is a first-order transition from the isotropic to the nematic phase [19]. Tr denotes the trace, which is the sum of the diagonal elements in the square matrix. The Frank elastic free-energy density $f_{elastic}$ [28], which describes the distortions, is accounted,

$$f_{elastic} = \frac{1}{2}L_{11}(\nabla \cdot \boldsymbol{Q})^2 + \frac{1}{2}L_{22}[\boldsymbol{Q} \cdot (\nabla \times \boldsymbol{Q})]^2 + \frac{1}{2}L_{33}[\boldsymbol{Q} \times (\nabla \times \boldsymbol{Q})]^2, \quad (6)$$

where L_{11}, L_{22} and L_{33} are the splay, twist and bend elastic constants, respectively. The free-energy density $f_{interact}$ [29] is

$$f_{interact} = -2(U_{particle}\phi/d)(\boldsymbol{Q}\cdot\boldsymbol{M})^2, \tag{7}$$

where $U_{particle}$ is the anchoring energy on the particle surface. The longitudinal director trapping is given on the magnetic particle surface. The filling factor ϕ is the volume fraction of the magnetic particle and d is the particle diameter. The free-energy density $f_{entropy}$ [1] is

$$f_{entropy} = \frac{\phi k_B T}{V}\ln\phi, \tag{8}$$

k_B is the Boltzmann constant, and T is the temperature, V is the volume of the sample. The field free-energy density is composed of the magnetic term and the electric term,

$$f_{field} = -M_S\phi(\boldsymbol{M}\cdot\boldsymbol{H}) - \frac{\Delta\varepsilon}{8\pi}(\boldsymbol{E}\cdot\boldsymbol{Q})^2, \tag{9}$$

where $\Delta\varepsilon = \varepsilon_{\parallel} - \varepsilon_{\perp}$ is the dielectric anisotropy due to the quasistatic electric field, M_S is the saturation magnetization of the magnetic particle. The surface free-energy density on the surface of nematics is

$$f_{surf} = \int_{S_0}\frac{U_0}{2}(\boldsymbol{Q}\times\boldsymbol{Q}_0)^2 dS_0 + \int_{S_D}\frac{U_D}{2}(\boldsymbol{Q}\times\boldsymbol{Q}_0)^2 dS_D, \tag{10}$$

where S_0 and S_D are the area of the surface given on bottom (z = 0) and upper (z = D) ferronematic cell plane. Similarly U_0 and U_D are the nematic anchoring energies U_Z given on bottom and upper. This means that a director at the surface prefers to lie along the direction of the eigenvector of $\boldsymbol{Q}_0$ corresponding to the largest eigenvalue $2/3q$ [22].

$\boldsymbol{S}(F,\boldsymbol{Q})$ is the stress tensor given by [25,30]

$$\boldsymbol{S} = -3\boldsymbol{h} + \boldsymbol{h}\cdot\boldsymbol{Q} - \boldsymbol{Q}\cdot\boldsymbol{h} - \nabla Q_{\alpha\beta}\cdot\frac{\delta F}{\delta\nabla Q_{\alpha\beta}}, \tag{11}$$

where δF represents the variation of F and $\boldsymbol{h}$ is called the molecular field [25,30], which provides the driving motion and is related to the derivative of the free energy by

$$\boldsymbol{h} = -\frac{\delta F}{\delta\boldsymbol{Q}} + \frac{\boldsymbol{I}}{3}Tr\frac{\delta F}{\delta\boldsymbol{Q}}, \tag{12}$$

where $\boldsymbol{I}$ is the identity tensor.

The Beris-Edwards equation of motion for the nematic tensor order parameter [25–27,30–34] is

$$\frac{\partial \boldsymbol{Q}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{Q} = (\xi \boldsymbol{W}^{(s)} + \boldsymbol{W}^{(a)})\left(\boldsymbol{Q} + \frac{\boldsymbol{I}}{3}\right) + \left(\boldsymbol{Q} + \frac{\boldsymbol{I}}{3}\right)(\xi \boldsymbol{W}^{(s)} - \boldsymbol{W}^{(a)}) - 2\xi\left(\boldsymbol{Q} + \frac{\boldsymbol{I}}{3}\right) Tr(\boldsymbol{Q}\boldsymbol{W}) + \Gamma\left(-\frac{\delta F}{\delta \boldsymbol{Q}} + \frac{\boldsymbol{I}}{3} Tr\frac{\delta F}{\delta \boldsymbol{Q}}\right), \tag{13}$$

where ξ is a constant, which depends on the molecular details of a liquid crystal [19]. $\boldsymbol{W}$ is the velocity gradient tensor defined by $W_{\alpha\beta} = \partial_\beta \boldsymbol{u}_\alpha$. $\boldsymbol{W}^{(s)}$ and $\boldsymbol{W}^{(a)}$ are the symmetric part and the anti-symmetric part of $\boldsymbol{W}$ respectively. Γ is a collective rotational diffusion constant [18,26–27,30,33].

The relaxation equation of magnetization [35] is

$$\frac{\partial \boldsymbol{M}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{M} = \Omega \times \boldsymbol{M} - \frac{1}{\tau_m}(\boldsymbol{M} - \boldsymbol{M}_0) - \frac{1}{6\eta\phi}\boldsymbol{M} \times (\boldsymbol{M} \times \boldsymbol{H}), \tag{14}$$

where $\boldsymbol{\Omega}$ is the local angular velocity of the fluid, τ_m stands for the Brownian time of rotational particle diffusion since the particles are assumed to be rigid magnetic dipoles whose reorientation is possible only with rotation of the particles themselves. $\boldsymbol{M}_0$ is the magnetization at the equilibrium in a stationary field.

LATTICE BOLTZMANN SOLVER

In the standard LB method, we need the three procedures to solve (1), (13) and (14). However by applying our new LB model for magnetic fluids to these fundamental equations of FNLCs, we can solve (1) and (14) at once. This method deals with FNLCs as rodlike liquid-crystal molecules in magnetic fluids.

We present the following new LB equation of motion based on our LB model for magnetic fluids [20]. This model can deal with the effects of magnetic moments efficiently. We assume the temperature is constant and choose a 6-velocity isothermal model on a hexagonal lattice for simplicity. The LB equation of motion is

$$\begin{aligned} &f_{a\sigma}(\boldsymbol{x}, t) - (1-p) f_{a\sigma}(\boldsymbol{x} - \boldsymbol{e}_a \Delta t, t - \Delta t) - p f_{a\sigma}(\boldsymbol{x} - \boldsymbol{e}_\sigma \Delta t, t - \Delta t) \\ &= \frac{\Delta t}{2}\{(1-p) C_{f_{a\sigma}}(\boldsymbol{x} - \boldsymbol{e}_a \Delta t, t - \Delta t, \{f_{a\sigma}\}) \\ &\quad + p C_{f_{a\sigma}}(\boldsymbol{x} - \boldsymbol{e}_\sigma \Delta t, t - \Delta t, \{f_{a\sigma}\}) \\ &\quad + (1-p) C_{f_{a\sigma}}(\boldsymbol{x}, t\{f^*_{a\sigma}\}) + p C_{f_{a\sigma}}(\boldsymbol{x}, t, \{f^*_{a\sigma}\})\}, \end{aligned} \tag{15}$$

where $f_{a\sigma}$ is the velocity distribution function associated with a lattice vector $\boldsymbol{e}_a$ and $\boldsymbol{e}_\sigma$. This equation represents free streaming in a lattice step Δt with velocity $\boldsymbol{e}_a$ and $\boldsymbol{e}_\sigma$ and a collision step, which is the relaxation process towards the equilibrium. The parameter p is the given streaming

ratio, which represents the fraction of $f_{a\sigma}$ that propagates along σ direction. This streaming procedure makes it possible to deal with the magnetic force efficiently. Here the velocity along the a direction is $\boldsymbol{e}_a = (\cos[2\pi(a-1)/6], \sin[2\pi(a-1)/6])$ with $a = 1, \ldots, 6$. The parameter σ with $\sigma = 1, 2$ is defined relative to a in the following manner: $\sigma = 1$ corresponds to the direction $a+1$ (mod 6) and $\sigma = 2$ to $a-1$ (mod 6). Then we can write the local microscopic velocity $v_{a\sigma}$ and the microscopic magnetic moment $\boldsymbol{m}_{a\sigma}$,

$$\boldsymbol{v}_{a\sigma} \equiv (1-p)\boldsymbol{e}_a + p\boldsymbol{e}_\sigma, \tag{16}$$

$$\boldsymbol{m}_{a\sigma} \equiv r\boldsymbol{e}_a + q\boldsymbol{e}_\sigma. \tag{17}$$

Although the parameters r, q and p are unrelated, a connection between r and q is set by the dynamical requirements for the proper equilibrium function in the collision term [20]:

$$r = -\boldsymbol{q}\frac{1+p}{2-p}. \tag{18}$$

The parameter $f^*_{a\sigma}$ is first order approximations to $f_{a\sigma}(\boldsymbol{x}, t)$. Discretizing in this way, which is similar to a predictor-corrector scheme, means that lattice viscosity terms are eliminated and the stability is improved [19]. The collision operator $C_{f_{a\sigma}}$ is taken to have the form of a single relaxation time with the forcing term $\mathrm{p}_{a\sigma}$

$$C_{f_{a\sigma}} = -\frac{1}{\tau_f}(f_{a\sigma} - f^{eq}_{a\sigma} + \mathrm{p}_{a\sigma}), \tag{19}$$

where $f^{eq}_{a\sigma}$ is the equilibrium distribution function and τ_f is the single relaxation time toward the equilibrium. Physical variables are defined as moments of the velocity distribution function and $f^{eq}_{a\sigma}$ is constrained as follows:

$$\rho \equiv f_0 + \sum_{a,\sigma} f_{a\sigma} = f^{eq}_0 + \sum_{a,\sigma} f^{eq}_{a\sigma}, \tag{20}$$

$$\rho\boldsymbol{u} \equiv \sum_{a,\sigma} \boldsymbol{v}_{a\sigma} f_{a\sigma} = \sum_{a,\sigma} \boldsymbol{v}_{a\sigma} f^{eq}_{a\sigma}, \tag{21}$$

$$\rho\boldsymbol{m} \equiv \sum_{a,\sigma} \boldsymbol{m}_{a\sigma} f_{a\sigma} = \sum_{a,\sigma} \boldsymbol{m}_{a\sigma} f^{eq}_{a\sigma}. \tag{22}$$

The moments of $\mathrm{p}_{a\sigma}$ is

$$\sum_{a,\sigma} \mathrm{p}_{a\sigma} = 0, \tag{23}$$

$$\sum_{a,\sigma} \mathrm{p}_{a\sigma} v_{a\sigma} = (\boldsymbol{D}\cdot\nabla)\boldsymbol{E} + \nabla S(\boldsymbol{F}, \boldsymbol{Q}), \tag{24}$$

where f_0 represents the stopped distribution function, which is introduced in order to avoid undesirable dependence of the pressure on the velocity [14–15]. The equilibrium distribution function and the forcing term are chosen in a similar manner to Ref. [19,20] satisfying conditions (20)–(24). Taking the continuum limit of (15) and performing a Chapman-Enskog expansion [37] leads to the equation of motion of FNLCs and the relaxation equation of magnetization. This means that we can get the hydrodynamic properties by solving (15) without solving (14) directly.

In order to solve (13), the following lattice Boltzmann equation has been presented [17–19]:

$$\boldsymbol{G_a}(\boldsymbol{x},t)-\boldsymbol{G_a}(\boldsymbol{x}-\boldsymbol{e_a}\Delta t,t-\Delta t)=\frac{\Delta t}{2}\Big[C_{\boldsymbol{G_a}}(\boldsymbol{x}-\boldsymbol{e_a}\Delta t,t-\Delta t,\{\boldsymbol{G_a}\}) + C_{\boldsymbol{G_a}}\big(x,t,\{\boldsymbol{G_a^*}\}\big)\Big], \tag{25}$$

where $\boldsymbol{G_a}$ is the distribution function of the symmetric traceless tensors associated with a lattice vector $\boldsymbol{e_a}$. $\boldsymbol{G_a^*}$ is set the first order approximation to $\boldsymbol{G_a}$. The collision operator is taken to have the form with a forcing term K_a,

$$C_{G_a}=-\frac{1}{\tau_g}(\boldsymbol{G}_a-\boldsymbol{G}_a^{eq}+K_{\mathrm{a}}), \tag{26}$$

where $\boldsymbol{G_a^{eq}}$ is the equilibrium distribution function and τ_g is the single relaxation time toward the equilibrium. Physical variable is

$$\boldsymbol{Q}=\sum_a \boldsymbol{G}_a. \tag{27}$$

In the hexagonal model, $\boldsymbol{G_a^{eq}}$ is constrained by

$$\sum_a \boldsymbol{G_a^{eq}}=\boldsymbol{Q}, \tag{28}$$

$$\sum_a \boldsymbol{G_a^{eq}}\boldsymbol{e_a}=\boldsymbol{Q}\boldsymbol{u}. \tag{29}$$

This ensures that the order parameter is conveyed with the flow. The evolution of the order parameter is most conveniently modeled by choosing

$$\sum_a \boldsymbol{K}_a=\Gamma\boldsymbol{h}(\boldsymbol{Q})+(\xi\boldsymbol{W}^{(s)}+\boldsymbol{W}^{(a)})\left(\boldsymbol{Q}+\frac{\boldsymbol{I}}{3}\right)+\left(\boldsymbol{Q}+\frac{\boldsymbol{I}}{3}\right)(\xi\boldsymbol{W}^{(s)}-{}^{(a)}) - 2\xi\left(\boldsymbol{Q}+\frac{\boldsymbol{I}}{3}\right)Tr(\boldsymbol{Q}\boldsymbol{W}), \tag{30}$$

$$\sum_a \boldsymbol{K}_a\boldsymbol{e}_a=\left(\sum_a \boldsymbol{K}_a\right)\boldsymbol{u}, \tag{31}$$

which ensures that the fluid minimizes its free energy at equilibrium [19]. Conditions (27)–(31) can be satisfied as is usual in lattice Boltzmann schemes by writing the equilibrium distribution function and the forcing term as polynomial expansions in the velocity [16,18,19,36]. By taking the continuum limit of (25) and performing a Chapman-Enskog expansion (37), the equations of motion of the tensor order parameter is recovered. Therefore we can get the tensor order parameter by solving (25).

Equations (15) and (25) are the discretized equations of (1), (13) and (14) by the LB kinetic scheme. We can get the answers of these continuum equations easily by solving (15) and (25), which are the so-called LB equations.

DISCUSSION

We have proposed a new idea of lattice Boltzmann algorithm in order to investigate the FNLC hydrodynamics by introducing our magnetic-fluid model (20) into a NLC model (19). This idea makes it possible to study hydrodynamic properties of FNLCs without solving the relaxation equation of magnetization.

This FNLC model can deal with variation in the magnitude of the nematic order parameter and can simulate the motion of defects explicitly under the influence of magnetic particles. This is a convenient model, which is suitable for investigation of electro-optical and magneto-optical effects in FNLCs. These effects have played an important role in an application of the LCD device. Moreover the magnetic fluid, in itself, is thought as an attractive candidate for flat panel display devices (38). It has been reported that a thin magnetic-fluid film can be operated very fast and provides a very high contrast ratio (39). We think that FNLCs have rich possibility as a LCD device.

Many directions for further research on FNLCs using this model are expected. For example, new bistable displays or multidomain nematics with magnetic particles, which exploit defect properties, are investigated explicitly and efficiently by using our model. This scheme will be a powerful numerical tool for these complex problems. Moreover, adjustment of boundary conditions is easy because of the simple algorithm and parallel computing is possible due to locality in the model. The lattice Boltzmann method based on simple microscopic physics is a convenient scheme for complex-hydrodynamic simulations.

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