Lattice Boltzmann simulations of liquid crystal devices

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I. INTRODUCTION

In this work we study the switching hydrodynamic behavior of nematic liquid cristal cells and multistable devices by using a lattice Boltzmann (LB) algorithm to perform the simulations.

Liquid crystal are ubiquitous in applications ranging from laptop displays to skincare products and pharmaceutical delivery systems. For these systems the flow properties are important and the hydrodynamics plays a crucial role. Moreover in many of these applications it is important to study the dynamical behavior in presence of an applied electric field. Due to the flexibility of the LB algorithm, our simulations, which include correctly hydrodynamics and complicated boundary conditions, are the ideal tool to study the switching hydrodynamics of liquid crystal devices. In particular we analyse multi-domain hybridly aligned nematic cells, which are important technologically but not studied so far [1], with multistable behavior, whose main characteristic consists in the possibility to consume power less than a monostable device, in consequence of a non continuous application of an electric field to work.

The prototype liquid crystal device is the "twisted nematic display", commonly employed in the construction of flat panel monitors. In these devices the molecules are forced to align along two boundary planes, a few microns apart from each other. The alignment directions are mutually perpendicular and the "off" state produced is the twisted one. To take the system in the "on" state an electric field needs to be applied perpendicular to the boundary planes. The main problems (relevant for our work) with these devices are, firstly the constant application of an electric field for the whole time the device is in the "on" state and secondly the "viewing angle problem", i.e. the limitation of the range of viewing angles of common twisted nematic displays. These two issues are solved with physical and technological solutions. The viewing angle can be enhanced by building multi-domain devices with the consequence of the inevitable creation of disclination lines between regions of different twist [2]. On the other hand, a multistable device can solve the problem of having a constant field to keep the system in the "on" state [3].

In the present work we use LB simulations to study the switching hydrodynamics of multistable multi-domain devices. The main results is that a simple 2-domain nematic cell shows a bistable behavior in absence any flexoelectric field and with planar boundaries. The director field is hybridly aligned to the boundaries: perpendicular on one plane and parallel on the other one. Moreover the planar anchoring is such that different stripes of splay-bend deformation are present (Fig.1). With this configuration, two metastable states with competing free-energy can be observed: one in which there are stripes with alternating splay-bend directions with defects in between, and another one in which the device becomes a single domain. The way in which the electric field is switched on and off is fundamental for the final metastable state.

II. THE MODEL

The dynamics of a nematic liquid crystal cell is described by the continuity, the Navier-Stokes and the convection-diffusion equations, that, expressed in terms of the total density ρ and the order parameter $\mathbf{Q}$, take the form

$$\partial_t\rho + \partial_\alpha(\rho u_\alpha) = 0, \tag{1}$$

$$\begin{aligned}\rho(\partial_t + u_\beta\partial_\beta)u_\alpha &= \partial_\beta(\Pi_{\alpha\beta}) + \eta\partial_\beta(\partial_\alpha u_\beta + \partial_\beta u_\alpha \\ &+ (1 - 3\partial_\rho P_0)\partial_\gamma u_\gamma \delta_{\alpha\beta}),\end{aligned} \tag{2}$$

$$(\partial_t + \vec{u}\cdot\nabla)\mathbf{Q} - \mathbf{S}(\mathbf{W},\mathbf{Q}) = \Gamma\mathbf{H}, \tag{3}$$

with ρ and $\vec{u}$ density and velocity field, respectively. η and Γ are the shear viscosity and the collective rotational diffusion constant, respectively. An explicit expression for the stress tensor is $\Pi_{\alpha\beta} = P_0\delta_{\alpha\beta} + 2\xi(Q_{\alpha\beta} + 1/3\delta_{\alpha\beta})Q_{\gamma\epsilon}H_{\gamma\epsilon} - \xi H_{\alpha\gamma}(Q_{\gamma\beta} + 1/3\delta_{\gamma\beta}) - \xi(Q_{\alpha\gamma} + 1/3\delta_{\alpha\gamma})H_{\gamma\beta} - \partial_\alpha Q_{\gamma\nu}\delta f/\delta\partial_\beta Q_{\gamma\nu} + Q_{\alpha\gamma}H_{\gamma\beta} - H_{\alpha\gamma}Q_{\gamma\beta}$ where P_0 is a constant and ξ is a constant that depends on the molecular details of a given liquid crystal. In the Eq. (3) the first term on the right hand side is the material derivative describing the time dependence of a quantity advected by a fluid with velocity $\vec{u}$ [4]. This is generalized for rod-like molecules by a second term $\mathbf{S}(\mathbf{W},\mathbf{Q}) = (\xi\mathbf{D} + \mathbf{\Omega})(\mathbf{Q} + \mathbf{I}/3) + (\mathbf{Q} + \mathbf{I}/3)(\xi\mathbf{D} - \mathbf{\Omega}) - 2\xi(\mathbf{Q} + \mathbf{I}/3)\mathrm{Tr}(\mathbf{QW})$, where Tr denotes the tensorial trace and $\mathbf{D} = (\mathbf{W} + \mathbf{W}^T)/2$ and $\mathbf{\Omega} = (\mathbf{W} - \mathbf{W}^T)/2$ are the symmetric part and the anti-symmetric part respectively of the velocity gradient tensor $W_{\alpha\beta} = \partial_\beta u_\alpha$.

The equilibrium properties of the system are fixed by the bulk free energy density

$$f = \frac{A_0\gamma}{3} Q_{\alpha\beta} Q_{\beta\gamma} Q_{\gamma\alpha} + \frac{A_0}{4} (Q^2_{\alpha\beta})^2 + \frac{K}{2} (\partial_\gamma Q_{\alpha\beta})^2 + \frac{\epsilon}{2} Q_{\alpha\beta} \mathbf{E}_\alpha \mathbf{E}_\beta \tag{4}$$

where A_0 is a constant and γ controls the magnitude of the ordering. (Greek indices denote Cartesian components and summation over repeated indices is implied.) The third term in the Eq. (4) is related to the free-energy cost of distorsions, with K elastic constant in the one-constant approximation, while the last term is related to the electric field contribution $\mathbf{E}$. A surface free energy density contribution is given by

$$f_s = \frac{1}{2} W_0 (Q_{\alpha\beta} - Q^0_{\alpha\beta})^2. \tag{5}$$

The parameter W_0 controls the strenght of the anchoring while $Q^0_{\alpha\beta}$ is the order parameter defined on the surfaces.

To solve numerically the Eqs. (1)-(3) we use an hybrid approach, in which the LB scheme solves Eqs. (1) and (2) and a finite difference scheme solves Eq. (3) [5]. The order parameter and the velocity field are updated at every time steps via these algorithms. The LB requires as an input the order parameter field and, on the other hand, the LB algorithm updates the velocity field which is required by finite difference scheme to further evolve the dynamics of the order parameter. The advantages to this approach are, firstly, related to the possibility to perform simulations of large systems with a memory requirements smaller than those required using a full lattice Botzmann approach. Secondly, the absence of error term arising in the Chapman-Enskog expansion used in the lattice Boltzmann approach, gives better analytical results.

III. RESULTS

In this section we present numerical results obtained for a quasi-2D device which exploits hybrid alignment to yield a bistable response. The hybrid alignment is a “conflict” anchoring on the walls: parallel on one plane and perpendicular on the other plane. In particular we simulate a system in which the director on the parallel plane has a pretilt of 10 degrees. The dynamical schedule with which the electric field is switched on and off is fundamental to observe the bistability.

In Fig.1 the director profile and the corresponding free energy are shown. We start from a two-domain nematic cell, in which two stripes with a splay-bend deformation, alternatively clockwise and anticlockwise, are observed. Almost in the middle of the cell, as a consequence of the two-domain structure, there is a defect of topological charge $-1/2$. After the switching on and off the electric field along the x-direction, the device becomes a single domain with a clockwise deformation. The last step is to switch on and off the electric field along the y-direction, allowing the system to recover a two-domain structure, with the defect almost in the middle of the cell. The bistability can also be observed from the free energy plots; the two-domain structures show the same value of the free energy at equilibrium -10.52, while in the one-domain structure the value of the free energy is -10.66. The simulation results are obtained on a lattice size $L_x \times L_y = 40 \times 40$, with elastic constant $K = 0.08$ and different values of electric field, from $|\vec{E}| = 0.01$ to $|\vec{E}| = 0.1$ in simulation units. The bistable behavior is observed with and without hydrodynamics with the same dynamical schedule for the electric field. Moreover we study the system for different lattice sizes and various values of pretilt, showing that different values can affect the bistability guiding the system to one-domain final states rather than two-domain states. The main results of this study is in the possibility to observe a bistable behavior for a very simple two-domain nematic cell with planar boundaries and without a flexoelectric field.

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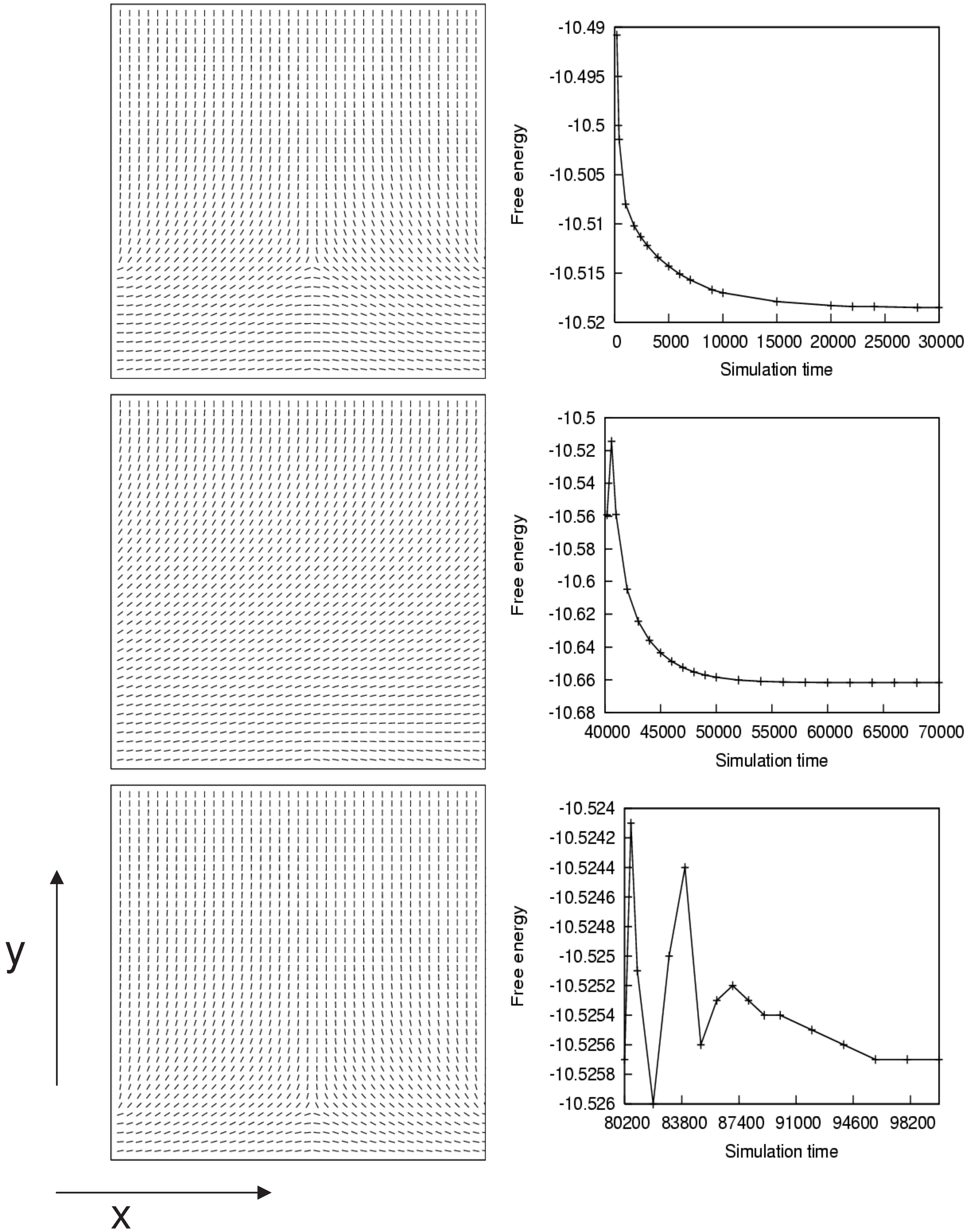

FIG. 1: On the left of the panel the director profile and on the right the corresponding free energy, both taken at consecutive times. The walls of the lattice, of size $L_x \times L_y = 40 \times 40$, are placed at the top and bottom of each snaphot of the director profile.