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Dynamics of Discs in a Nematic Liquid Crystal

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Abstract

We use hybrid lattice Boltzmann simulations to study the dynamics of discs immersed in a nematic liquid crystal.

In this thesis, a new way of simulating a two-way coupling between a liquid crystal and an immersed object is proposed. It can be used for objects of various geometries and can be expanded to be used for an object of any geometry. Additionally, a simple yet effective model was suggested for calculations of transmitted light through a nematic liquid crystal sample. This model allowed us to clarify the behavior of a ferromagnetic disc in a nematic liquid crystal observed in experiments and incorrectly interpreted at that time.

As a result of this work, a package for an open-source computational fluid dynamics software LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) was created, that was expanded to be used for multiple objects interacting in a nematic liquid crystal, allowing examination of stable structures and studies of particle self-organization.

Our simulations have demonstrated the following: in the absence of external forces and torques, discs with homeotropic (perpendicular) anchoring align with their surface normal parallel to the director of the nematic liquid crystal. In the presence of a weak magnetic field (< 20G, too weak to disturb liquid crystal alignment) a ferromagnetic disc will rotate to equilibrate the elastic torque due to the distortion of the nematic director and the magnetic torque. When the magnetic field rotates the disc so that the angle $\theta$ between normal to the surface of the disc $\hat{a}$ and director of the liquid crystal $\hat{n}$ becomes greater than $\pi/2$, the disc flips around the axis perpendicular to the rotation axis so that the surface normal $\hat{a}$ sweeps through $\pi$ radians, thus resolving the distortion in the liquid crystal. An analysis of this behavior was performed in Chapter 3. In particular, we look at the impact of the disc thickness, and conditions on the edges of the object, on defect creation and the flipping transition. We also analyze the importance of backflow (i.e. coupling of tensor order parameter with velocity field). We also study the same system under the action of fast rotating weak magnetic fields, that demonstrates a different behavior: the disc avoids flipping via creation of two symmetric defects on the sides.

Some results on disc pairs are presented in Chapter 4. Interactions between discs, their motion and final position strongly depend on the distance between them, and the magnitude and angular velocity of the rotating magnetic field. Depending on the initial configuration of the system, different stable structures of discs result. Further work with existing code may be used to predict other stable configurations and periodic structures that might be of interest for applications requiring organization and manipulation of colloidal particles.

Keywords: Liquid Crystals, Lattice Boltzmann, Colloids, Hydrodynamics, Molecular Dynamics
Co-Authorship Statement

All work presented in this thesis was done in collaboration with my supervisor, Dr. Colin Denniston. Parts of Chapter 1, Chapter 2 and 3 of this thesis are based on the published article:

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List of Symbols

Symbols firstly appeared in Chapter 1

\( \hat{n} \)    director of liquid crystal
\( S \)    scalar order parameter of liquid crystal
\( \langle \cdot \rangle \)    coarse grain average
\( \theta_m \)    angle between the director and long axis of \( m^{th} \) molecule
\( P_i \)    Legendre polynomial of order \( i \)
\( Q \)    tensor order parameter of liquid crystal
\( \hat{m} \)    orientation of liquid crystal molecules
\( P \)    measure of the biaxiality
\( \mathcal{F}_{\text{bulk}} \)    bulk free energy
\( F_{\text{bulk}} \)    bulk free energy density
\( F_0 \)    free energy density of the isotropic phase
\( A, \tilde{A}, B, C \)    coefficients of expansion of bulk free energy
\( T_x \)    temperature of coexistence of isotropic and nematic phases
\( T_c \)    temperature of nematic-isotropic phase transition
\( A_0 \)    bulk coefficient
\( \gamma \)    effective temperature or concentration for thermotropic and lyotropic liquid crystals respectively
\( q_{eq} \)    equilibrium bulk value
\( F_{\text{elastic}} \)    elastic free energy
\( K_1, K_2, K_3, K_{13}, K_{24} \)    Frank’s elastic constants
\( L_1, L_2, L_3 \)    elastic constants
Frank’s elastic constant for one elastic constant approximation

$\hat{n}^0$ director orientation at the surface of immersed object

$Q^0$ surface-induced order parameter tensor

$F_{surf}$ surface free energy

$q^0$ set to be equal to equilibrium bulk value

$\alpha_s$ strength of anchoring at the surface

$H^{SC}$ surface conditions molecular field

$F_{MF}$ energy contribution from non-zero magnetic field

$B$ magnetic field

$\mu_0$ magnetic permeability of vacuum

$\Delta\chi^{max}$ maximal magnetic anisotropy

$\chi$ diamagnetic tensor

$B_{crit}$ critical value of magnetic field magnitude for the Freedericksz transition

$\mathcal{F}$ Landau-de Gennes free energy

$u$ bulk fluid velocity

$S(W, Q)$ function responsible for coupling of tensor order parameter with velocity field

$W$ velocity gradient vector

$H$ molecular field

$\Gamma$ rotational diffusion constant

$D$ symmetric part of the velocity gradient tensor

$\Omega$ antisymmetric part of the velocity gradient tensor

$\xi$ aspect ratio of the particles

$H_{bulk}$ bulk molecular field

$H_{elast}$ elastic molecular field

$\rho$ liquid crystal density

$\eta_{iso}$ isotropic viscosity

$\sigma_{\alpha\beta}$ symmetric part of the stress tensor
\( \tau_{\alpha\beta} \) antisymmetric part of the stress tensor

\( \tau_f \) relaxation parameter

\( P_0 \) pressure

\( \varphi_{\text{vr}} \) binary coefficient controlling the coupling between tensor order parameter and velocity field

\( \epsilon_{\parallel}, \epsilon_{\perp} \) dielectric constants parallel and perpendicular to the long axis of liquid crystal molecule

\( \epsilon_{\alpha\beta} \) dielectric constant of a uniaxial nematic

\( \epsilon_a, \epsilon_m \) functions of \( \epsilon_{\parallel} \) and \( \epsilon_{\perp} \)

\( n_o, n_e \) ordinary and extraordinary refractive indexes

\( \theta \) angle defining the orientation of immersed object

**Symbols firstly appeared in Chapter 2**

\( N_{\text{mol}} \) number of particles in gas in a small volume

\( t \) time

\( x_i \) coordinates of \( i^{th} \) particle

\( \mathcal{H} \) Hamiltonian describing the total energy of the system

\( p_i \) momenta of \( i^{th} \) particle

\( f(x, p_1, t) \) particle distribution function

\( m \) mass of a particle

\( \rho e \) energy density

\( \mathbf{F} \) external force

\( \left( \frac{\partial f}{\partial t} \right)_C \) collision operator

\( D_t \) operator, \( D_t = \partial_t + \frac{p_i}{m} \partial_{x_i} + \mathbf{F} \partial_{p_i} \)

\( f_{12}, f_{1'2'} \) two-body particle distribution functions

\( \left| \frac{\partial \sigma}{\partial \Omega} \right| \) differential cross section

\( d\Omega \) element of the solid angle
$f^{eq}$ equilibrium distribution function

$k_B$ Boltzmann constant, $1.38064852(79) \times 10^{-23} J/K$

$T$ temperature of the fluid

$v$ particle velocity

$u$ fluid velocity

$\left. \left( \frac{\partial f}{\partial t} \right) \right|_C^{BGK}$ Bhatnagar – Gross – Krook collision operator

$\Delta x$ (or $dx$) lattice space step

$\Delta t$ (or $dt$) time step

$e_i$ discrete velocity vectors

$f_i^{(0)}, f_i^{(1)}, f_i^{(2)}$ coefficients of expansion of $f_i$ around equilibrium distribution function

$P_{\alpha\beta}$ pressure tensor

$\eta_s$ shear viscosity

$\Lambda_b$ bulk viscosity

$v_c$ ratio of lattice spacing to time step

$v_s$ isentropic speed of sound

$\mathbf{G}_i$ distribution function for tensor order parameter update

$\tau_G$ relaxation parameter for tensor order parameter update

$p_i, \mathbf{M}_i$ additional terms required in lattice Boltzmann method for liquid crystals for recovery of macroscopic equations

$A_s, B_s, C_s, D_s, E_s, \mathbf{J}_s, \mathbf{K}_s, \mathbf{L}_s, \mathbf{N}_s, T_s, \mathbf{R}_s, \mathbf{S}_s$ coefficients of expansions of equilibrium distribution functions $f_i^{eq}$ and $\mathbf{G}_i^{eq}$

$\mathbf{G}_i^{(0)}, \mathbf{G}_i^{(1)}, \mathbf{G}_i^{(2)}$ coefficients of expansion of $\mathbf{G}_i$ around equilibrium distribution function

$\tilde{f}_i^{eq} = f_i^{eq} + \tau f p_i$

$\Upsilon_f 1 - e^{-\Delta t/\tau_f}$

$\Upsilon_G 1 - e^{-\Delta t/\tau_G}$

$\zeta_{\alpha j}$ weight of the trilinear stencil

$\mathbf{v}_n, \mathbf{u}_f$ particle node velocity and velocity of the fluid trilinearly interpolated to the particle node location
\(m_u, m_v\) masses of the particle node and representative fluid mass at the node location, respectively

\(\hat{a}\) surface normal (pointing outward)

\(\sigma^{SC}_{\alpha\beta}\) surface conditions part of the symmetric stress tensor

\(\Delta S_i\) portion of the surface of the colloidal particle represented by node \(i\)

\(\tau^{SC}_{\beta\gamma}\) surface conditions part of the antisymmetric stress tensor

\(\Delta V_i\) volume occupied by \(i^{th}\) object node

\(T_{MF}\) magnetic field torque

\(\mu\) magnetic moment of the disc

**Symbols firstly appeared in Chapter 3**

\(R\) disc radius

\(L\) disc thickness

\(N\) number of nodes

\(l\) size of simulation domain

\(\vartheta_{MF}\) angle of rotation of magnetic field

\(\vartheta_{MF}^{\text{stop}}\) angle of rotation of magnetic field when the rotation stops

\(\tilde{\Gamma}\) torque on the disc from the liquid crustal

\(a\) inter-focal distance

\(C\) capacitance

\(\theta_{crit}\) orientation of the object when it start the flipping motion

\(\beta_{yz}\) angle between the \(z\)-axis and the projection of the surface normal \(\hat{a}\) on the YZ plane

\(\beta = \arccos(\hat{a} \cdot \hat{k})\)

\(\beta_{xy}\) angle between the \(x\)-axis and the projection of the surface normal on the XY plane

\(\varphi^{\text{rot}}\) angle used for analysis of rotation, \(\arccos\left(\frac{\mu \cdot \hat{k}}{|\mu|}\right)\)

\(\hat{k}\) unit vector along \(z\)-axis

\(\bar{A}_{in}^s\) input amplitude of light for \(s^{th}\)
\[ \parallel A^s \parallel \] component of the light along the director

\[ \perp A^s \] component of the light perpendicular to the director

\[ \tilde{A}^s_{\text{out}} \] the output component of the light from the \( s \)th layer

\[ \hat{n}^s \] the director at the point of the \( s \)th layer

\[ \hat{b} \] the projection of the director at the point of the \( s \)th layer on the \( xy \)-plane

\[ q \] equivalent to the scalar order parameter \( S \)

**Symbols firstly appeared in Chapter 4**

\[ V(r) \] Lennard-Jones repulsion potential

\[ \epsilon_{\text{well}} \] depth of the potential well

\[ \sigma_0 \] zero-crossing distance for the potential

\[ r \] distance between centers of mass of the particles

\[ r_c \] cut-off radius

\[ V_s(r) \] soft repulsion potential

\[ A_{sp} \] energy constant for soft repulsion potential
1

Introduction

“Do you know what amazes me more than anything else? The impotence of force to organize anything.”

– Napoleon Bonaparte

During the transition from solid to liquid some substances demonstrate an intermediate stable phase that has some properties of liquids and some of crystalline solids. Because of this the material was named a “liquid crystal” (or, often, a mesogen). Like liquids, mesogens have an ability to flow and like crystals, they have long-range orientation order (meaning that particles of a liquid crystal on average tend to be along some preferred direction). It is exactly these two main properties of liquid crystals that make possible all the various applications and devices without which we cannot imagine our life today: TV’s, PC’s, phones’ and tablets’ screens, liquid crystal thermometers, various tools for medical industry, and other electro-optical devices. Liquid crystals have also provided methods for templating porous materials and synthesis of nano-particles of desired shapes for further use in various fields, and much more [3].

1.1 Liquid Crystals

1.1.1 History of Liquid Crystals

Liquid crystals were discovered at the end of the 19th century, but it took the scientific community a lot of time to accept the existence of a new state of matter and even more time to understand how it could be used.

Liquid crystals were discovered accidentally, not by a physicist, but by a Professor of Botany and Technical Microscopy, Friedrich Reinitzer in 1888 [4]. During his experiments on cholesterol derivatives he observed two melting points of cholesteryl benzonate, at 145.5°C and 178.5°C. Surprised, he repeated experiments with further derivative, cholesteryl acetate, and made similar observations [5]. Reinitzer contacted Otto Lehman, a German physicist, who was able to perform more precise experiments using the polarizing microscope with a hot stage (hot-stage systems have heating elements beneath and above the sample that uniformly can heat or cool the sample). As a result of these experiments, in 1889 Lehman published an article “Über fließende Kristalle” [6] on the
subject of “flowing crystals”, as Lehmann called them, that became the first publication on liquid crystal phenomena. However, the scientific community rejected the existence of liquid crystals at that time – “Soft crystals definitely do exist, flowing crystals may exist, but liquid crystals definitely cannot exist”, – said Gustav Tammann, a German physicist and chemist, in 1905 at the annual convention of the German Bunsen Society in Karlsruhe [4]. Many other members of the scientific community agreed with him at that time. Liquid crystals remained unpopular among scientists for the first half of 20th century and even in 1960s there were only a few facilities for liquid crystal research [7].

Nevertheless, the development of a theoretical basis continued. In the 1920–30s a number of important works were published. The first one [8], written by Georges Friedel, explained smectic and nematic crystalline structures and introduced a classification for various types of liquid crystals. In 1933, Carl Wilhelm Oseen suggested a theory to describe the elastic properties of liquid crystals. Another significant contribution was made by Russian physicist Vsevlad Freedericksz who described the effect of electrical and magnetic fields on the alignment of liquid crystal molecules. Freedericksz’s theory became the foundation stone of the idea of liquid crystal displays (LCD).

By the 1950s interest in liquid crystals was decaying since nobody could find any practical applications for them [4]. This changed in 1958 when, finally, the first application of liquid crystals, namely the use of liquid crystals to determine temperature, was conceived by James Fergason. This invention, resulted in many publications and patents (see [9] and [10] for example), brought back the interest in liquid crystals.

The theory continued to develop by works of Maier & Saupe (1959-60) [11, 12] and Pierre-Gilles de Gennes (1971) [13, 14] who proposed theories to describe liquid crystals that explained phase transitions and the dependence of particle order on temperature. Along with theory development, further experiments in the field discovered new liquid crystal phenomenon that led to a number of applications of great importance, including, of course, liquid crystal displays: the first prototype was made in 1968 by Heilmeyer [15], and was followed by various improvements and related discoveries [16–20].

More than 125 years have now passed since the discovery of liquid crystals and still new inventions and applications are revealed one after another, meaning that research on the subject of liquid crystals has to be continued.

1.1.2 Types of Liquid Crystals

There are certain structural features that are often found in the molecules of the substances that have a liquid crystal phase (see the details on the effects of various molecular features on the nematic phase in [21]). For example, a substance that has flat segments such as benzene rings is likely to have a liquid crystal phase [22], as, for example, the nematic liquid crystal 4-cyano-4’-pentylbiphenyl (5CB) that has two aromatic rings (see fig.1.1 a and b). Molecules of liquid crystals materials also often have strong dipoles and easily polarizable groups [23].

Another important property is anisotropy of the molecules, i.e. they have to be non-spherically symmetric in shape. Thus, one of the existing liquid crystal classifications is based on the form of the molecules. If liquid crystal molecules are rod-like in form, then this liquid crystal is called calamatic (like 5CB). If the molecules are of disc-shaped form
1.1. Liquid Crystals

Figure 1.1: In a) and b): the chemical structure and chemical representation of 5CB nematic liquid crystal. In c) the chemical structure and geometric forms of benzene hexaalkonoates is shown.

It is a discotic liquid crystal (for example, benzene hexaalkonoates, the first discotic liquid crystals discovered; they were detected by Sivaramakrishna Chandrasekhar [24] and are shown on figure 1.1 c). Liquid crystals with board-like molecules are called sanidic liquid crystals [22]. There are also recently discovered classes of liquid crystal materials consisting of bent-core molecules (or banana-shaped molecules) [25], tapered molecules (pear-shaped ones) [26] and other more exotic shapes [27–30] that have a lot of promising applications and have raised a lot of interest [31–33]; even mixtures of particles of different shapes can produce a liquid crystal phase [34].

Calamatic and discotic liquid crystalline phases are usually stable in certain temperature ranges; liquid crystals whose stability depends on temperature are called thermotropic liquid crystals. Substances that can form liquid crystals phase when mixed with certain solvents, with the concentration being responsible for the stability of liquid crystal phase, are called lyotropic liquid crystals. For example, 5CB nematic liquid crystal that is used throughout this work as the main reference, is a thermotropic liquid crystal; DDAB (dimethyldioctadecylammonium bromide) is an example of a lyotropic one.

Based on the orientation order, there are nematic (or nematogens), smectic (also smectogens) and cholesterics (or chiral nematic) liquid crystals (see fig. 1.2). The first and most simple ones, nematics, are characterized by long-range orientation order, i.e. the long axes of the molecules tend to align along one preferred direction that is often called a director and denoted by \( \hat{n} \). The centers of mass of liquid crystal molecules do not demonstrate any translational order. These properties imply there is no physical difference between \( \hat{n} \) and \(-\hat{n}\), since molecules of a nematic can rotate along their long axis showing no preference between two ends of the molecules. That property has to
Figure 1.2: Types of liquid crystals: schematic representation of most common structures.
be incorporated into both theoretical and numerical models. Mesogens of disk-shaped molecules can also have a layer-like organization known as the discotic nematic phase. If these molecules pack into stacks of discs, the phase is called a discotic columnar phase.

The cholesteric phase is similar to the nematic phase in having long-range orientation order and demonstrating no long-range position order, but the director varies periodically (usually) from one layer to another by rotating about a direction perpendicular to the nematic director. This type of liquid crystal is commonly characterized by the distance measured along the axis of the twist over which the director rotates through a full circle. This distance is called the pitch of the cholesteric [23] and is an important parameter in optical applications. One can also think of nematics as a cholesterics with an infinite pitch.

The most important difference between nematics and smectics is some positional order and, thus, tendency to align themselves in layers or planes in addition to orientational ordering. For example, the director of smectic A is perpendicular to the smectic plane, and there is no particular positional order in the layer. At the same time, the director of a smectic C is at a constant tilt with respect to the line perpendicular to all layers.

There are also uniaxial and biaxial types of liquid crystals. The second ones have an additional symmetry axis (for example, when molecules are of rectangular shape).

This study focuses on nematic rod-like liquid crystal materials and takes the commonly known 4-cyano-4'-pentylbiphenyl (5CB) liquid crystal as the main example. Its molecules are between 20 Å and 40 Å long and around 5 Å wide; 5CB undergoes the phase transition from crystalline to nematic at 18°C and then to the isotropic state at 35°C [35].

1.1.3 Mathematical Description

1.1.3.1 Order Parameter

For a quantitative measure of the level of order in liquid crystals, it is common to introduce a scalar order parameter. In the liquid, disordered state it has to be equal to 0; for a perfectly ordered “crystal” structure it should be 1. One of the simplest expressions that satisfy these conditions was firstly introduced by Tsvetkov [36]:

\[ S = \frac{1}{2} \langle 3 \cos^2 \theta_m - 1 \rangle, \]  

(1.1)

where \( \langle \rangle \) denotes statistical average. This is a weighted average of molecular orientation angles \( \theta_m \) (angle between the director and long axis of a molecule as shown in fig. 1.3). When the material is in an ordered phase, all molecules are exactly along the director, i.e. \( \theta_m = 0 \) for each molecule and \( \langle \cos^2 \theta_m \rangle = 1 \), implying \( S = 1 \). In an isotropic fluid, since there is no preferred direction, \( \langle \cos^2 \theta_m \rangle = 1/3 \), which leads to \( S = 0 \).

The right-hand side of equation (1.1) is, in fact, the second order Legendre polynomial, \( P_2(\cos \theta_m) \). When higher accuracy is required, one can use higher order Legendre polynomials but only the even ones, \( P_{2n}(\cos \theta_m) \), since the odd ones would not contribute due to the equivalence of \( \hat{n} \) and \( -\hat{n} \). Thus, a scalar order parameter of the form (1.1) fits to describe quantitatively the order in a uniaxial liquid crystal.
However, a scalar order parameter of this form requires a priori knowledge of the overall director orientation that may not be known. Also, it can be used for a liquid crystal that contains only cylindrically symmetric molecules (i.e. cylindric form) and would not work properly for biaxial molecules (2 axes of symmetry); for details of the order parameter for biaxial nematics, one can refer to [37–39].

An alternative is to describe the level of order in terms of a local tensor order parameter $\mathbf{Q}$ that is related to the orientation of constituent molecules $\mathbf{\hat{m}}$ by

$$Q_{\alpha\beta} = \langle m_{\alpha}m_{\beta} - \frac{1}{3}\delta_{\alpha\beta} \rangle,$$

where angular brackets denote a coarse-grain average and the Greek indices here and elsewhere are used to represent Cartesian components, and the usual summation over repeated indexes will be assumed. $\mathbf{Q}$ is a traceless symmetric 3x3 matrix that has 3 orthogonal eigenvectors with 3 real eigenvalues: the principle eigenvalue, $\frac{2}{3}S$, where $S$ is the scalar order parameter, describes the magnitude of order along the corresponding eigenvector $\mathbf{\hat{n}}$, being the director [14, 39]. Thus, $\mathbf{Q}$ is still equal to zero matrix for the isotropic phase and has non-zero components for the liquid crystal phase. $\mathbf{Q}$ can be written as

$$\mathbf{Q} = \begin{pmatrix} 2S/3 & 0 & 0 \\ 0 & -S/3 + P & 0 \\ 0 & 0 & -S/3 - P \end{pmatrix},$$

where $P$ is a measure of the biaxiality (a tensor order parameter of this form is suitable for describing biaxial liquid crystals), and when $P = 0$ this equation would describe a uniaxial nematic.

1.1.3.2 Topological Defects

The equilibrium state of liquid crystals implies all particles being more-or-less along the director $\mathbf{\hat{n}}$. However, boundary conditions, or external forces such as electrical/magnetic
1.1. Liquid Crystals

Figure 1.4: Defects in liquid crystals. Here dashed lines correspond to the director field and $s$ is the type of the defect.

fields, or addition of an inclusion may cause an abrupt change in the orientation of particles and, thus, create areas where the director is locally undefined (this corresponds to a singularity in the director field). These areas are called defects. Defects cost some energy and their stability depends on the Frank Free Energy [40] which will be discussed in the next section.

There are two types of defects in the uniaxial nematic phase: point defects and line defects (often refer to as disclinations). Both can be classified with a number $s$ that corresponds to the multiple of $2\pi$ by which the director rotates when going in a closed loop counter-clockwise around the defect [14]. This number is negative when the rotation goes clockwise. Some examples of defects with different $s$ number are shown on fig. 1.4. Defects of opposites signs can cancel each other (if they are close enough to affect each other). Point defects can occur, for example, in liquid crystal droplets [41] and in capillaries [42].

In this work we are more interested in the second type of defects – line defects, where the orientation of the director is undefined along a curve. They often appear to balance anchoring requirements on the surface of an inclusion with the far-field director of liquid crystal (this will be discussed in more detail in sec. 1.1.3.3 and sec. 1.1.4). Since line defects allow the creation of stable colloidal structures [43–45] (as will be discussed in sec.1.1.4), their formation and behavior are of special interest in liquid crystal studies. However, it is very hard to locate a defect and analyze its behavior in 3D sample in experiments. Numerical simulations provide opportunities for this analysis and help to
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1.1.3.3 Free Energy Description

In this work we use a theory of Landau and de Gennes [14] to calculate bulk free energy $F_{bulk}$. This theory assumes that the free energy density $F_{bulk}$ is an analytical function of the tensor order parameter $Q$ and the free energy density can be expanded in a power series, since the system is assumed to be near the transition point and, thus, $Q$ is small:

$$F_{bulk} = F_0 + \frac{1}{2} A Q_{\alpha\beta} Q_{\alpha\beta} - B Q_{\alpha\beta} Q_{\beta\gamma} Q_{\gamma\alpha} + C (Q_{\alpha\beta} Q_{\beta\alpha})^2,$$  \hspace{1cm} (1.3)

where $F_0$ is the free energy density of the isotropic phase. In general, coefficients $A$, $B$ and $C$ depend on pressure $P$ and temperature $T$. In a fully aligned uniaxial nematic, substituting $Q$ in terms of the scalar order parameter $S$, would lead to the following approximation of the bulk free energy:

$$F_{bulk} = F_0 + \frac{1}{2} A S^2 - \frac{1}{3} B S^3 + \frac{4}{6} C S^4.$$  \hspace{1cm} (1.4)

One can find values of $S$ that minimizes the above expression by taking the derivative of the bulk free energy with respect to $S$ and setting it equal to 0:

$$A S - B S^2 + \frac{8}{3} C S^3 = 0.$$  \hspace{1cm} (1.5)

This equation is satisfied when $S = 0$, i.e. the liquid is in isotropic phase, and by

$$S = \frac{3 B + \sqrt{9 B^2 - 96 A C}}{16 C}.$$  \hspace{1cm} (1.6)

The value of $S$ given by eq. (1.6) is called the equilibrium bulk value or equilibrium order parameter [14,46].

If one would need to explicitly include the temperature dependence into eq. (1.4), the simplest and most common way would be to include the temperature dependence only in the coefficient $A$

$$F_{bulk} = F_0 + \frac{1}{2} \tilde{A} (T - T_c) S^2 - \frac{1}{3} B S^3 + \frac{4}{6} C S^4.$$  \hspace{1cm} (1.7)

Here $T_c$ is a critical temperature for transition. An example of a first order phase transition for a simplified case when $\tilde{A} = B = C = 1$ is shown in fig. 1.5: when the temperature is higher than the temperature $T^*$, the free energy of the medium is minimized by an isotropic phase ($S = 0$); when the temperature is equal to $T^*$ nematic and isotropic phases coexist together; for $T_c$ that is slightly lower than $T^*$, the free energy is at its minimum in the nematic phase.

Since in this work we are not interested in the isotropic to nematic transition but rather will stay in the nematic phase at all times, we fixed constants $A, B, C$ and set them in a way to guarantee the nematic phase [47]:

$$A = A_0 (1 - \frac{\gamma}{3}), \quad B = A_0 \frac{\gamma}{3}, \quad C = A_0 \frac{\gamma}{4}.$$
1.1. Liquid Crystals

Figure 1.5: Phase transition in a liquid crystal. For $T > T^*$, $T^*$ is slightly higher than $T_c$, the system is in isotropic phase; for $T = T^*$ two phases co-exist; for $T < T_c < T^*$ the energy in minimized by being in nematic phase. Here $\tilde{A} = B = C = 1$ for simplicity.

that substituted into eq. (1.6) would give the following equilibrium bulk value that we label as $q_{eq}$:

$$S = \frac{1}{4} \left( 1 + 3 \sqrt{1 - \frac{8}{3} \gamma} \right).$$  \hfill (1.8)

Here $A_0$ is constant and $\gamma > \frac{8}{3} \approx 2.7$ corresponds to the nematic phase [47] (tuning $\gamma$ means changing the temperature of the fluid and concentration of liquid crystal molecules in the solvent; with $\gamma < 2.7$ system has only one minimum – at isotropic state with $S = 0$; when $\gamma > 2.7$ the second minimum $S = q_{eq}$ appears and set the tensor order parameter in eq. (1.3) equal to equilibrium $Q$ and, thus, the system with such $\gamma$ (or temperature and concentration) would be in the nematic state).

Substituting these expressions in eq. (1.4) would give:

$$F_{\text{bulk}} = \frac{A_0}{2} (1 - \frac{\gamma}{3}) Q_{\alpha\beta}^2 - \frac{A_0 \gamma}{3} Q_{\alpha\beta} Q_{\alpha\gamma} Q_{\gamma\alpha} + \frac{A_0 \gamma}{4} (Q_{\alpha\beta}^2)^2. \hfill (1.9)$$

The total bulk free energy can be obtained by integrating over the volume of liquid crystal:

$$F_{\text{bulk}} = \int_V F_{\text{bulk}} dV.$$

We also need to include the energy associated with local distortions. According to the Frank-Oseen free energy theory [14,23,48], these local distortions can be a result of
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Figure 1.6: Twist, bend and splay deformations in liquid crystals.

either twist, splay or bend in the orientation of liquid crystal molecules (see fig.1.6) or a mix of them. Then the elastic energy $F_{\text{elastic}}$ has the form

$$F_{\text{elastic}} = \frac{1}{2}K_1(\nabla \cdot \hat{n})^2 + \frac{1}{2}K_2(\hat{n} \cdot \nabla \times \hat{n})^2 + \frac{1}{2}K_3((\hat{n} \cdot \nabla)\hat{n})^2,$$

(1.10)

where $K_1$, $K_2$ and $K_3$ are Frank’s splay, twist and bend constants respectively. There are also mixed elastic constants for the splay-bend and saddle-splay deformations often denoted as $K_{13}$ and $K_{24}$ that some authors have used recently [49–51], but their effects are primarily limited to the surface of the nematic liquid crystals [52] and due to this reason we neglect them in our work. One can generalize (1.10) in terms of the tensor order parameter:

$$F_{\text{elastic}} = \frac{L_1}{2} (\partial_\alpha Q_{\beta\gamma})^2 + \frac{L_2}{2} (\partial_\alpha Q_{\alpha\gamma})(\partial_\alpha Q_{\beta\gamma}) + \frac{L_3}{2} Q_{\alpha\beta}(\partial_\alpha Q_{\gamma\delta})(\partial_\beta Q_{\gamma\delta}).$$

(1.11)

Here the $L_i$ describe the elastic properties of the chosen liquid crystal and $\alpha$ corresponds to cartesian coordinates $x$, $y$, $z$. For a uniaxial nematic, the $L_i$ can be mapped to the Frank elastic constants through [53]

$$L_1 = \frac{3K_2 - K_1 + K_3}{6q_{eq}^2}, \quad L_2 = \frac{K_1 - K_2}{q_{eq}^2}, \quad L_3 = \frac{K_3 - K_1}{2q_{eq}^2},$$

(1.12)

where $q_{eq} = \frac{1}{4}(1 + 3\sqrt{1 - \frac{8}{3\gamma}})$ is the equilibrium bulk value. In the one elastic constant approximation, i.e. when $K_1 = K_2 = K_3 = K$, equivalent to $L_1 > 0, L_2 = L_3 = 0$, the elastic free energy simplifies to

$$F_{\text{elastic}} = \frac{L_1}{2} (\partial_\alpha Q_{\beta\gamma})^2 \text{ with } L_1 = \frac{K}{2q_{eq}^2}.$$

The presence of an object in a liquid crystal can deform the director field and lead to a different equilibrium state. The molecular alignment at surfaces can propagate over
1.1. Liquid Crystals

Figure 1.7: Variety of surface anchoring: planar, homeotropic (perpendicular), delegate planar anchoring and tilted homeotropic anchoring.

significant distances and has a noticeable effect on the liquid crystal and any particle immersed in it. This effect is called surface anchoring [54] and was firstly reported in 1913 by Mauguin, who observed it for a mica substrate [55]. Depending on the type of surface and/or chemical treatment performed on the object, one can get homeotropic, planar, tilted or more complicated orientations of liquid crystal molecules on the surface (see fig. 1.7). Pierre Chatelain in 1944 mentioned the effect of treatment of the surface on liquid crystal anchoring in his work [56]. Even such simple actions like rubbing the surface with paper or velvet makes a difference and plays an important role in production of devices that use liquid crystals [4].

The preferred orientation of the director at a surface is often called an easy axis; we denote it by \( \hat{n}^0 \) here. Mathematically this can be represented by a surface-induced order parameter tensor, \( Q^0 \), that has the form \( Q^0_{\alpha\beta} = q^0(n^0_\alpha n^0_\beta - \frac{1}{3}\delta_{\alpha\beta}) \), where \( q^0 \) is set to the equilibrium bulk value. The director field on the surface of the object, \( Q^0 \), is imposed by adding a surface term \( F_{surf} \) to the free energy of the system [57,58]:

\[
F_{surf} = \frac{1}{2} \alpha_s(Q_{\alpha\beta} - Q^0_{\alpha\beta})^2, \tag{1.13}
\]

where \( \alpha_s > 0 \) (for homeotropic anchoring) defines the strength of pinning (for strong pinning \( Q \approx Q^0 \) on the surface). Such a quadratic pinning term penalizes all deviations of particle orientation on the surface from the desired vector \( \hat{n}^0 \).

In the famous book by de Gennes and Prost [14], a vector field, called the molecular field with analogy to magnetism, was introduced and determined through the derivative of the free energy with respect to the order parameter. The meaning of this term is the
following: in equilibrium, the director has to be at each point parallel to the molecular field. Thus, the molecular field drives the orientation of the particles to the equilibrium configuration. For the energy term $F_{surf}$ the corresponding molecular field that requires particles to be along $\hat{n}^0$ is (similarly to eq. (1.20)):

$$H^{SC} = \alpha_s(Q - Q^0).$$

(1.14)

Since $F_{surf}$ is only added at the surface, $H^{SC}$ is also determined only at the surface of the object (otherwise, it would impose the alignment $\hat{n}^0$ on the particles far away from the surface).

The surface anchoring often becomes the reason for a creation of a point defect in a liquid crystal due to a conflict between the required orientation of liquid crystal molecules on the surface of an immersed object and a far-field director. One of the most common and well studied [59, 59–61] point defects that appears due to putting a particle into a liquid crystal are hedgehogs (or satellite defects, shown in fig. 1.8, a), resulting from parallel anchoring on the surface of a spherical particle, and boojums (in fig. 1.8, b), that appear due to parallel alignment of liquid crystal molecules on the surface of a spherical particle.

We will also have a magnetic field acting on our system. Because liquid crystal molecules can be aligned by magnetic and electric fields (if they are strong enough), in principle one has to include a term that would reflect the effect of external fields. The existence of these effects was firstly observed by Freedericksz [62], who applied an electrical field to a liquid crystal sample squeezed between two parallel glass planes (see fig. 1.9). Using for example ref. [63], we can write down the free energy density $F_{MF}$ due to the presence of a magnetic field $\mathbf{B}$:

$$F_{MF} = -\frac{1}{3} \mu_0 \Delta \chi^{max} B_\alpha Q_{\alpha\beta} B_\beta - \frac{1}{6} \mu_0 \chi_{\gamma\gamma},$$

(1.15)

Figure 1.8: Point defects in a liquid crystal resulted from surface conditions on an immersed spherical particle: hedgehog (perpendicular anchoring on the surface) and boojums (parallel anchoring).
with $\chi$ being the diamagnetic tensor, $\Delta \chi^{max}$ being maximal anisotropy and $\mu_0$ is the magnetic permeability of vacuum. However, in our simulations the magnetic field $B$ is tiny ($< 20G$), and is much less than a critical value for the Freedericksz transition when the director aligns with the magnetic field [14] ($B_{crit} = 3500G$ for a 5CB slab with 10$\mu$m thickness [57], 700G for a 100$\mu$m thin cell [64]). Thus, $F_{MF}$ is negligibly small and we do not include it in our calculations (situation corresponds to fig.1.9 a) case).

To sum up, the equilibrium properties of the liquid crystal can be described by a Landau-de Gennes free energy [14] of the form

$$F = \int_V dV \{F_{bulk} + F_{elastic} + F_{MF}\} + \int_{\partial V} dS F_{surf},$$

where $F_{bulk}$ is determined by eqn. (1.9), $F_{elastic}$ is given by eqn. (1.11), $F_{MF}$ is from eqn. (1.15) and $F_{surf}$ comes from eqn. (1.13).

### 1.1.3.4 Equations of motion

Due to the long-range orientation order in liquid crystals, their hydrodynamic properties and flow regimes are more complicated compared to those of simple isotropic fluids. Flow and order affect each other. For example, change in the alignment may induce flow [14], while flow may disturb the alignment of particles, as shown in fig. 1.10. This two-way interaction has to be included into equations of motion.

The first theory of nematodynamics that contained backflow was developed by Ericksen, Leslie and Parodi (ELP) [65, 66] in the 1960s. This theory used a macroscopic
Figure 1.10: Flow induced reorientation of liquid crystal molecules. In a) a simple shear flow is presented: conditions on the walls create the boundary layer with no effect from the flow, but the particles of middle part becomes tilted and align themselves with the flow. In b) is schematic representation of liquid crystal molecule reorientation under Poiseuille flow: boundary layers can be seen again near the walls, but the flow geometry now creates an adjustment layer in the middle.

approach and was based on the dynamics of the director $\hat{n}$ and assumed constant order parameter. Because the director at the defect core is biaxial \cite{67,68} and the tensor order parameter near it changes abruptly, this theory would not work correctly for the hydrodynamics of defects \cite{69,70}.

Another theory was suggested by Beris and Edwards \cite{53,71}. It does not have the problems described above, since the hydrodynamic description is based on the tensor order parameter and was selected in this research for this reason. According to Beris – Edwards theory, the order parameter $Q$ evolves according to the convection-diffusion-like equation

$$\frac{\partial}{\partial t} + u \cdot \nabla Q - S(W, Q) = \Gamma H,$$  \hspace{1cm} (1.17)

where $u$ is the bulk fluid velocity, $H$ is the molecular field, and $\Gamma$ is a rotational diffusion constant. The first term on the left-hand side of this equation is the material derivative that describes the time dependence. The second term appears in the equation because the particles of the liquid crystal are usually of rod-like form and, therefore, the order parameter distribution can be both stretched and rotated by the flow gradients. $S(W, Q)$ has the form

$$S(W, Q) = \left( \xi D + \Omega \right) \left( Q + \frac{1}{3} I \right) + \left( Q + \frac{1}{3} I \right) \left( \xi D - \Omega \right) - 2\xi \left( Q + \frac{1}{3} I \right) Tr(QW),$$  \hspace{1cm} (1.18)

where $D$ and $\Omega$ are symmetric and antisymmetric parts of the velocity gradient tensor.
\[ W_{\alpha\beta} = \partial_{\beta} u_{\alpha} \] accordingly:
\[
D = \frac{1}{2} (W + W^T), \quad \Omega = \frac{1}{2} (W - W^T) \tag{1.19}
\]
and \(\xi\) is a constant that depends on the molecular details of the liquid crystal (i.e. aspect ratio of the particles). The term on the right-hand side of (1.17) describes the relaxation of the tensor order parameter towards the minimum of the free energy. The molecular field \(H\), related to the variational derivative of the free energy, provides the driving force
\[
H = -\frac{\delta F}{\delta Q} + \frac{1}{3} \text{Tr}(\frac{\delta F}{\delta Q}) = H_{\text{bulk}} + H_{\text{elast}}, \tag{1.20}
\]
where, based on corresponding energy expressions [72],
\[
H_{\text{bulk}} = -A_0(1 - \frac{\gamma}{3})Q + A_0\gamma(Q^2 - \frac{1}{3} \text{Tr}Q^2) - A_0\gamma Q\text{Tr}Q^2,
\]
\[
H_{\text{elast}} = L_1(\partial_\gamma Q_{\alpha\beta}) + L_2 \left[ \frac{1}{2}(\partial_\beta \partial_\gamma Q_{\gamma\beta} + \partial_\gamma \partial_\beta Q_{\gamma\alpha}) - \frac{1}{3} \delta_{\alpha\beta} \partial_\gamma \partial_\varepsilon Q_{\gamma\varepsilon} \right] + \frac{1}{2} L_3 \left[ \partial_\gamma(Q_{\gamma\varepsilon} \partial_\varepsilon Q_{\alpha\beta}) - (\partial_\alpha Q_{\gamma\varepsilon}) (\partial_\beta Q_{\gamma\varepsilon}) + \frac{1}{3} \delta_{\alpha\beta} (\partial_\eta Q_{\gamma\varepsilon})^2 \right]. \tag{1.21}
\]

Liquid crystals also obey the continuity equation
\[
(\partial_t \rho + \partial_\alpha \rho u_\alpha) = 0, \tag{1.22}
\]
and Navier-Stokes equations
\[
\rho \partial_t u_\alpha + \rho u_\beta \partial_\beta u_\alpha = \partial_\beta \tau_{\alpha\beta} + \partial_\beta \sigma_{\alpha\beta} + \eta_{\text{iso}} [\partial_\gamma (\partial_\alpha u_\beta + \partial_\beta u_\alpha)], \tag{1.23}
\]
where \(\rho\) is the density and \(u\) is the velocity, \(\eta_{\text{iso}} = \rho \tau_f / 3\) is the isotropic viscosity. Here the stress tensor has not only a symmetric part
\[
\sigma_{\alpha\beta} = -P_0 \delta_{\alpha\beta} - \varphi_{\nu \nu} \left[ \xi H_{\alpha\gamma}(Q_{\gamma\beta} + \frac{1}{3} \delta_{\gamma\beta}) \right.
- \xi(Q_{\alpha\gamma} + \frac{1}{3} \delta_{\alpha\gamma}) H_{\gamma\beta} + 2\xi(Q_{\alpha\beta} + \frac{1}{3} \delta_{\alpha\beta}) Q_{\gamma\varepsilon} H_{\gamma\varepsilon}
\left. - \partial_\beta Q_{\gamma\nu} \frac{\delta F}{\delta \partial_\alpha Q_{\gamma\nu}} \right], \tag{1.24}
\]
but also an antisymmetric part \(\tau_{\alpha\beta}\)
\[
\tau_{\alpha\beta} = \varphi_{\nu \nu} \left[ Q_{\alpha\gamma} H_{\gamma\beta} - H_{\alpha\gamma} Q_{\gamma\beta} \right] \tag{1.25}
\]
due to the ability of liquid crystals to transmit torque.

Hydrodynamic motion of the nematic liquid crystal as a result of director reorientation is often called the backflow effect or just backflow (in other words, backflow means that the flow of the medium is prompted by the reorientation of the director). Mathematically, backflow means that in the stress tensor we have components related to the tensor order parameter; removing those terms would result in a stress tensor of an isotropic liquid again. In eq. (1.24) and eqn. (1.25) the presence of backflow effects are determined by variable $\varphi_{vr}$: when $\varphi_{vr}$ is equal to 1, we have coupling between the tensor order parameter and the flow, when it is set to 0 we switch it off. In Chapter 3 two different cases are examined: with backflow effects being switched off; and with backflow taken into account. For each simulation there is a specification in the text and/or picture what case is being examined. The purpose of investigating both cases is to determine when the backflow can be neglected or not in this type of simulations and examine the effects of backflow on disc’s dynamics, i.e. determine which forces drive the motion. The general importance of backflow effect are reported in, for example, [73].

1.1.4 Colloids in Liquid Crystals

In the 1990s a novel class of composite materials was discovered examining suspensions of colloidal particles in liquid crystals [74–81]. Their properties arise because of the existence of unique long-range interactions between colloidal particles in a liquid crystal medium that are not present in isotropic fluids. These interactions have their origin in the coupling between colloidal particles and the orientation of liquid crystal molecules. When an inclusion is added to the liquid crystal, interactions at the particle surface impose boundary conditions on the orientation of the liquid crystal molecules close to the particle surface, leading to a distortion of the director field and, possibly defects, thus increasing the elastic energy of the medium [77, 78, 82]. The particles can share regions of distortion and defects to lower the energy [1, 83]. This can result in a short range attraction between particles which may be different in character from the long-range forces. This provides opportunities for organization and manipulation of colloids and leads to strategies for formation of self-assembled structures and ways of fabricating metamaterials [43, 44, 78, 79, 84–87]. For example, defect lines allow creation of stable colloidal structures [43] and provide self-assembling techniques [44, 45] to bind colloidal particles together. One common example of a line defect is a saturn ring [88, 89] (fig. 1.11, a), when a circular defect line is formed due to a conflict between perpendicular surface anchoring and far field director. Saturn rings can be arranged into a longer defect line to create a stable structure of spherical particles [90]. Another example of a defect line that encourages organization of colloidal particles is “handles”, observed in cholesteric liquid crystals [1] (see fig. 1.11,b). A strong planar anchoring on the surface of a spherical particle generates two handles near the surface of the particle, and when a group of such particles comes close together, they share the distortion areas and, as a result, defect line chains are created that keep the particles together (fig. 1.11, c). Such structures of self-assembling particles have potential applications in photonic, optoelectronic, as well as in chemical and biological sensing [87,91–96].
1.1. Liquid Crystals

Figure 1.11: Line defect in a liquid crystal: a) saturn ring (appears due to perpendicular anchoring on the surface of a spherical particle); b) schematic representation of the “handles” formed on the surface of a spherical particle immersed in a cholesteric liquid crystal observed in numerical simulations by F. Mackay et al. [1]; c) when multiple spheres with handles are joint together, configuration transforms into a defect-bounded chain [1].

1.1.5 Optical properties

One of the most important properties of liquid crystals for optical applications is birefringence (i.e. the refractive index depends on the propagation direction of light). Due to the anisotropy of the molecules (see fig. 1.12, a), dielectric susceptibility is also anisotropic and has two components, along the long axis of the molecule, $\epsilon_\parallel$, and $\epsilon_\perp$ perpendicular to it. The dielectric constant of a uniaxial nematic depends on the tensor order parameter,
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Figure 1.12: Birefringence of liquid crystals. In a): anisotropy in molecule geometry leads to dielectric anisotropy and two refractive indexes. In b): the light enters a liquid crystal sample and divides into ordinary and extraordinary rays.

\[ \epsilon_{\parallel} - \epsilon_{\perp} > 0, \]
\[ n_e - n_o > 0 \]

Correspondingly, there are two different refractive indexes, ordinary \( n_o = \sqrt{\epsilon_{\perp}} \) and extraordinary \( n_e = \sqrt{\epsilon_{\parallel}} \). Thus, when the light enters a liquid crystal sample, it gets divided into a fast ordinary ray and slow extraordinary ray (fig. 1.12, b) and, hence, the polarization state of the output ray is different too. The phase shift may be tuned by the thickness of the sample.

Liquid crystal birefringence made possible a lot of optical devices, including liquid crystal displays (LCD). The main idea of a LCD is the following. As was mentioned in section 1.1.3.3, rubbing of the glass with a cotton or velvet cloth orients the liquid crystal molecules along the direction of rubbing. This property was used in creation of twisted nematic cells – small blocks filled with nematic with glass top and bottoms, treated to produce planar anchoring on both surfaces but at right angles to each other (see fig. 1.13). Thus, the molecules in the middle of the sample have rotated by 90° going from bottom to top to satisfy conditions on both walls (fig. 1.13a). When an electrical field is applied to the cell (fig. 1.13b), it aligns the molecules along itself (if \( \epsilon_{\parallel} - \epsilon_{\perp} > 0 \)), due to molecular and dielectric anisotropy of liquid crystals (Freedericksz transition). If now we would put the cell in between two crossed polarizers, we may control the rotation of the polarization in liquid crystal and, thus, outgoing intensity of light through tuning the strength of electrical field: zero electric field would rotate the initial direction of light and let it through the second polarizer; a strong electric field would prevent rotation and the light would be stopped by the second polarizer (see fig. 1.13).
Figure 1.13: Twisted nematic cell (schematically). In a): polarized via polarizer 1 light enters liquid crystal medium; conditions on the walls make molecules twist and, thus, light beam got rotated and able to pass through polarizer 2. In b): electrical field orients the particles, preventing the rotation of the molecules; polarization of the input beam now stayed unchanged and the light can not get through the second polarizer.

Another interesting optical effect helped to create temperature sensitive devices. LC thermometers and mood rings, for example, do exist due to chiral nematics’ ability to selectively reflect light of wavelengths equal to the length of the pitch, i.e. the desired color of reflected light can be achieved by making the cholesteric pitch length equal to the wavelength of light in the visible spectrum (that can be done by tuning the temperature of the system) [98]. For more details on optical properties of liquid crystals one may
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Although liquid crystals have been in production for quite a long time now, there still exist some difficulties in manufacturing liquid crystal devices. For instance, the rubbed polymer technique for setting surface anchoring is still widely used in the production of devices with liquid crystals, meaning that fiber residues may appear and lead to inclusions and impurities, that would affect the optical properties and intensity of transmitted light. The response time of a LCD is another direction of liquid crystal research and optical studies. Thus, control over optical properties and the ability to predict the optical image are very important. There are a number of methods that allow the calculation of the outgoing intensity of light thought the liquid crystal sample for LCDs. For example, one popular method uses Jones calculus [23, 99], but it is applicable only for a defect-free liquid crystal and would not work in case of any inclusions. In this work we suggest a simple, yet effective, method to calculate the outgoing intensity of transmitted light that takes into account the orientation of each molecule group and allow for a particle inclusion. This will be discussed in section 3.2.2.5 of the thesis.

1.2 Research Motivation

Liquid crystals are used in a range of different applications, including those that involve submerging colloidal particles into a liquid crystal. The behavior of spherical particles immersed in mesogens are well-studied both experimentally and numerically. Motion of aspherical particles is less explored, and at the same time is more complicated since changes in the orientation may cause a reorientation of liquid crystal molecules and, thus, alter the elastic energy of the system, as was discussed in sec. 1.1.4.

The group of Robert Leheny from Johns Hopkins University performed a series of experiments on ferromagnetic rod- and disc-shaped particles in a nematic [2,100–102] to understand more fully the behavior of aspherical inclusions in liquid crystals and explore how a distortion in the liquid crystal can be controlled through the orientation of the particle.

In the experiments on thin rod particles [100–102] the group studied static and dynamic properties of ferromagnetic cylindrical particles with parallel anchoring on the surface immersed in nematic liquid crystal under the action of weak magnetic fields. During the experiments, they observed the following behavior: at equilibrium, rods oriented themselves with their long axis parallel to the director of the liquid crystal to avoid any distortion (fig. 1.14a); any change in particle orientation would mean that the director field around the particle had to be distorted in order to satisfy both surface conditions and the far-field director of the liquid crystal. Thus, when the weak magnetic field, initially aligned along the long axis of the wire, changed its orientation, making the wire follow it, a distortion area appeared around the wire (fig. 1.14b). With increase of the angle of rotation of the wire (θ) the distortion enlarged too, leading to an increase in the energy of the system. Since for the a uniaxial nematic there is no difference between +\( \hat{n} \) and −\( \hat{n} \), the elastic torque from the liquid crystal distortion should be symmetric across θ = π/2. However, when the wire rotated by that angle, this symmetry got broken and the distortion around the particle continued to increase (fig. 1.14c). Only when the
1.2. Research Motivation

Figure 1.14: The motion of the wire observed in experiments (top view, schematically). The wire is colored in turquoise, red arrow corresponds to the magnetic moment $\hat{\mu}$ of the wire and green arrow track the direction of magnetic field. Blue arrow shows the direction of spinning.

The wire was rotated by $\pi$ from its initial orientation, the wire precessed around its long axis by $180^\circ$ (fig. 1.14d) and, then continued rotation but with less twisted director field (fig. 1.14e), finally reached a distortion-free configuration shown in fig. 1.14f.

However, a different behavior was observed for disc-shaped particles with perpendicular anchoring on the surface under similar conditions (i.e. the particle was immersed in a uniaxial nematic liquid crystal and a weak magnetic field was acting on the system) [2]. In equilibrium, the disc aligned itself in a way to avoid any distortion in the system, i.e. surface normal $\hat{a}$ is parallel to the director $\hat{n}$ (see fig. 1.15a). When the magnetic
field changed its orientation, it forced the disc to rotate after it. Rotation of the disc was accompanied by a distortion in the liquid crystal director field that arose from the liquid crystal molecules orientation on the disc surface due to chemical treatment of the particle (fig. 1.15b). When the disc rotated by more than 90° from its original position, the configuration became unstable and before the disc rotated by 180° it flipped about the axis perpendicular to the axis of rotation, as shown in fig. 1.16 and schematically drawn in fig. 1.15,c. Thus, the release of distortion for the disc happened much earlier then for the wire. Results of polarization microscopy from this experiment are shown in fig. 1.16 [2]: the top row shows the optical microscopy images, and the bottom row schematic diagrams of corresponding disc orientation are given. One can note a darker area around the disc, bounded by a circular edge, that appeared during the flipping motion; it firstly enlarged and then shrank back to the surface of the disc. Finally, the disc ended in a distortion-free configuration (shown schematically in fig. 1.15d), where the magnetic moment was aligned with the magnetic field.

A behavior such as precession of the wire along its long axis or flipping of the disc is very hard to see and explain using only polarization microscopy, and numerical simulations, where one may track the behaviour of the particle in details, are very useful. Previous numerical simulations [57] performed on a ferromagnetic wire immersed in a nematic liquid crystal under the action of weak rotating magnetic fields in a setup similar to the experiments described above, was not aiming to simulate the spinning behavior, but rather simulated a rotation of the wire in a static limit. Moreover, in these simulations the wire moved along a predetermined path (compared to a free moving particle). In this work, however, we describe a method that allows the particle in a liquid crystal to

![Figure 1.15](image)

Figure 1.15: The motion of the disc observed in experiments (top view, schematically, where the disc is seen edge-on). Disc is shown in orange, green arrow represents the direction of the magnetic field, red arrow corresponds to the magnetic moment of the disc. a) Original position of the disc. b) The disc follows the rotation of the magnetic field, director field is distorted to satisfy both a far field director and conditions on the surface of the disc. c) The disc rotated by more then 90°, director field is highly distorted and the disc flips (shown by blue arrow). d) Final, distortion-free configuration.
move freely (i.e. the motion of the object is not predefined by the user): the motion is
determined only by forces that arise due to the coupling between the liquid crystal and
the particle, and is also affected by external forces, such as magnetic fields, acting on the
system. None of the previous numerical simulations have allowed a free-moving particle.

When we started this work, we were curious about what drives the flipping behavior
and especially interested in explanations of a peculiar loop around the disc seen in the
experiments and interpreted by the Robert Leheny’s group as a disclination loop [2] (we
will show that this loop was interpreted incorrectly).

After all, we defined the following aims for this research:

- simulate and explain the peculiar flipping behavior observed in the experiments
described above,
- analyze the behavior of disc-shaped inclusions in nematic liquid crystals,
- investigate ways to control the director field and its distortion via orientation of
the disc particle,
- look for potential ways of self-organization of disc particles in a nematic liquid
crystal.

To do this, we first need to modify the previous simulation algorithm to include dynamics
of the inclusion, that will be discussed in the next chapter.

1.3 Thesis Outline

The main properties of liquid crystals are described in this introductory chapter.
In this thesis we describe and then use a numerical method to simulate the behavior of disc-shaped inclusions immersed in a nematic liquid crystal. We start the explanations of the numerical method in Chapter 2, where we give details of the hybrid lattice Boltzmann method we used for simulations and explain our contribution allowing free motion of inclusions in the simulation.

Chapter 3 discusses the dynamics of a single disc inclusion in a nematic liquid crystal under the action of magnetic fields of different magnitude and angular velocity. This chapter also describes our method to predict the light transmission through a liquid crystal sample with a particle submerged in it.

The numerical method is expanded in Chapter 4 to allow particle interactions in the medium and give some results on the behavior of disc pairs under the action of weak slowly rotating magnetic fields.

Then we end with conclusion and discussions of potential future directions of this work.
In the past, there were only two approaches in science: theoretical and experimental. With the beginning of the (super)computer era numerical approaches started to gain momentum. Since then numerical simulations helped to develop a lot of new theories and check the existing ones without performing expensive experiments. Computational Fluid Dynamics (CFD) methods appeared, that allow not only cheaper and faster ways to study fluid flows, but also allow investigations of phenomena unapproachable analytically such as oceans or weather. As computers evolved, CFD methods changed too, offering more and more algorithms to study fluids. Originally, there were two groups of simulation approaches: macroscopic and microscopic.

Macroscopic methods, often also called top-down or continuum methods [103], treats the fluid as a continuum and try to numerically solve macroscopic Navier-Stokes equations. This can be done in a number of ways, the most common of those are the Finite Difference Method (FDM), Finite Element Method (FEM), and Finite Volume Method (FVM) [104–106].

Microscopic or atomistic models fall in the group of bottom-up approaches. The method keeps track of the motion and collisions of individual atoms or molecules in the simulation and then uses averaging to get macroscopic parameters of the fluid. The classic Molecular Dynamics method (MD) [107] and Monte Carlo methods [108] are examples of a microscopic approach. Though these types of models give full details at the molecular level, it either requires a lot of computational resources [109] and/or is limited in time and system size (usually to the nano scale) because the number of atoms to track is very large and the complexity of interactions makes computation expensive. Since in soft matter studies, and in this research in particular, long times and big system scales are of interest, molecular dynamics methods are not the best fit for the task.

To fill in the gap between micro- and macroscopic methods a number of mesoscopic methods were developed in the past decades. Mesoscopic methods are based on the idea of coarse-graining, when each particle represents a cluster of atoms or molecules and the system is simplified to catch the behavior of interest but ignore minor, uninteresting details. For example, one can decrease the degrees of freedom by simplifying a group of...
Chapter 2. Numerical Method

Atoms in a molecule and replacing them by a single particle, ignoring some intermolecular interactions, and thus decreasing the number of particles to track and of interactions to calculate.

Particles in coarse-gained models can be either “hard” [110, 111] or “soft” [112, 113]. “Hard” particles have a strong “hard-core” repulsion at short scales; “soft” particles can also interact on short scales but typically allow some overlap. Later, in chapter 4, we give more details on how to implement a particle repulsion for purposes of this research.

Mesoscopic methods can also be subdivided into on-lattice and off-lattice groups. In off-lattice methods particles move stochastically in continuous space, while in on-lattice algorithms particles are occupying sites on a grid (which simplifies the calculations since positions of particles are fixed and known). Dissipative Particle Dynamics (DPD) [114], Smoothed Particles Hydrodynamics (SPH) [115, 116], and Multiple Particle Collision Dynamics (MPCD) [117, 118], are examples of off-lattice algorithms.

The Lattice Boltzmann Method (LB) and Lattice Gas Automata (LGA) are examples of mesoscopic on-lattice methods. The LB method can be used to simulate suspensions of colloidal particles in fluids [119], porous media [120], multiphase flows [121] and is also applicable for simulations of magnetohydrodynamics [122–124], quantum mechanics [125, 126] and in superconductor studies [127]. The details of the LB method, that was used throughout this work, and the main ideas of LGA are given below.

2.1 Lattice Boltzmann Method and its Historical Origin

The lattice Boltzmann method has its historical origin in Cellular Automata (CA) [128] introduced in the 1940s by Stanislaw Ulam and John von Neumann. CA consists of a simple grid where each node has a finite number of states (“on” and “off” for example) plus a set of rules to update states. At the beginning of the simulation, the initial state of each cell is defined. At each time step, a set of rules determine the new state for each cell based on the cell’s current state and the states of its neighbors [129]. An example of a one-dimensional cellular automata is demonstrated in fig.2.1. CA can be used to qualitatively describe different fractal growths, such as growth of biological organisms, patterns of sea shells and snowflakes, predator-prey dynamics and evolution, and is also used in cryptography.

The main problem of the CA is creation of additional non-physical invariants (they depend on the properties of a particular CA, such as the rule set). For a two dimensional binary CA the additional non-physical invariant can be, for example, the ratio of the number of cells in state 0 to the number of cells in state 1 [130]. Such invariants have no correlation with the real world. Moreover, even if invariants of a CA are known, it is hard to analyze how they would affect the evolution of the CA and to what deviations from the hydrodynamic behavior they would lead to in the macroscopic limit [129].

The first (simplest and unsuccessful) lattice-gas cellular automata (LGCA) – a CA for simulation of gas and fluid flows – was suggested in 1973 by Hardy, Pomeau and de Pazzis [129,131] and therefore named the HPP model after them. HPP is a two-
2.1. Lattice Boltzmann Method and its Historical Origin

dimensional LGCA model over a square lattice. According to HPP, at each node there can be no more than one particle at a time (Pauli exclusion principle); the presence of a particle at the node is determined by a boolean variable – it is 0 if there is no particle, and 1 if a particle is located at a selected node. A particle can move in one of four directions (called lattice velocity vectors) that would move it to the next location on the lattice. At the beginning of the simulation an initial configuration is set up, then a loop of application of the rule set and the movement of the particles follows (see sec. 2.2.4 for more details). For HPP with its two dimensional square lattice, collision rules are as follows: if particles comes from opposite directions, a head-on collision rotates particles velocities by 90° if required cells are empty; in all other cases the collision step does not change positions of the particles. There are also some additional details (such as sub-grids) that we will leave out of this discussion because of their irrelevance to the development of the lattice Boltzmann method.

However, HPP does not lead to Navier-Stokes equations in the macroscopic limit because of a lack of rotational symmetry originating from the choice of the lattice being square [129]. In 1986 this problem was pointed out and HPP was updated by Frisch, Hasslacher and Pomeau who replaced the square lattice with a hexagonal one. A new model was named using the first letters of the authors names – FHP. It had hexagonal symmetry (i.e. invariant under rotations by 60°) and gave Navier-Stokes equations in the macroscopic limit [129]. Due to the new lattice, collision rules became a little more

![Rule set](image1)

![Initial state](image2)

![First step](image3)

Figure 2.1: Example of a one dimensional cellular automata: a set of rules (corresponds to so-called “rule 90” with periodic boundary conditions), initial state and the first step.
Chapter 2. Numerical Method

Figure 2.2: Examples of the sets of velocity vectors for two and three dimensional lattices.

complicated and contained 2 head-on collisions.

Later different, more suitable lattices were found and a classification named $DnQm$ was introduced. Here $n$ stands for the number of dimensions and $m$ is equal to the number of possible lattice velocities. Some of them are represented in fig. 2.2. In this work the D3Q15 model (implying 3D simulation with 15 discrete velocity vectors on a cubic lattice) was used as shown on fig. 2.2.

FHP became the basis for numerous lattice-gas methods, including the lattice Boltzmann method [132,133]. The idea of using a method based on a Lattice Boltzmann Equation originates from McNamara & Zanetti (1988) [134]. Comparing lattice Boltzmann methods with its ancestors and CFD alternatives, we can see the following major positives and negatives [135]:

+ the nature of the particle density in the FHP is discrete (due to use of a boolean variable to determine if a particle is at the node): at each node, any of the allowed discrete velocities may be taken by just one or no particles; this results in statistical noise [136]; the LB method replaces them by a set of distribution functions that now describe the probability of finding a particle at the node and moving in each of the possible directions and, thus, gets rid of this noise;

+ the LB method inherited the simplicity of boundary condition implementation (for example, to implement bounce-back boundary conditions, i.e. no-slip, on the walls one need to reverse the distribution functions at the boundary node; thus, all particles are streamed back to where they came from; see, for instance, [137] for more details on the implementation of boundary conditions);

+ from the computational point of view, the LGA methods family and the LB method are easy to parallelize allowing significant speed up of the simulation;

+ computation in LB and LGA methods requires only local data (compared to some CFD solvers);

+ LB methods as well as LGA methods avoid direct calculation of the nonlinear convective term $\mathbf{u} \cdot \nabla \mathbf{u}$ from Navier-Stokes equations;
2.2 From Boltzmann Equation to Lattice Boltzmann Method

2.2.1 Boltzmann Equation

Let us start with \( N_{\text{mol}} \) identical gas particles (since Boltzmann equation originally was derived for rare gases) moving in three dimensional space. If the mass of each particle is \( m \), coordinates and momenta of the \( i \)th particle are \( x_i \) and \( p_i \), the motion of each particle can be described by Hamilton’s equations:

\[
\frac{dx_i}{dt} = \frac{\partial \mathcal{H}}{\partial p_i}, \tag{2.1}
\]

\[
\frac{dp_i}{dt} = -\frac{\partial \mathcal{H}}{\partial x_i}, \tag{2.2}
\]

where \( \mathcal{H}(x_1, ..., x_{N_{\text{mol}}}; p_1, ..., p_{N_{\text{mol}}}) \) is the Hamiltonian, describing the total energy of the system. If now we would decide to describe the motion of \( 1 \mu m^3 \) of air at standard conditions using these equations, we would be required to solve a system of size \( 6N_{\text{mol}} \), where \( N_{\text{mol}} \) is the number of molecules in this volume, \( N_{\text{mol}} = 2.6 \times 10^7 \). Solution of such enormous systems of equations is beyond the ability of current computers.

Since we are not interested in the properties of the individual particles, but rather want to know macroscopic properties of the system, we can switch to a statistical description of particles collective behavior. For that, let us introduce a function \( f(x, p_1, t) \), called the particle distribution function (PDF). This function describes the probability density for finding a particle with momentum \( p_1 \) at location \( x \) at the moment of time \( t \). Thus, the number of particles in a small volume \( d^3x \) (i.e. in the range \( [x, x + d^3x] \)) with momentum in the range \( [p_1, p_1 + d^3p_1] \) at time \( t \) can be described via \( f(x, p_1, t)d^3xd^3p_1 \). Macroscopic properties of the system such as mass density, momentum density, and energy density are defined via the moments of the distribution function \( f \):

- LGA and LB methods are inefficient for steady state problems as you have to evolve in time;
- the LB method has troubles with high Mach number flows because the method uses expansions based on a small Mach number assumption (expansions of equilibrium distribution function in particular, as will be discussed in the next section);
- LB is memory extensive, because the method has to track all the distribution functions in addition to physical parameters of the fluid.

To sum up, although the LB method has its hardships, it has a lot of positive sides. Researchers are successively working on overcoming problems and limitations the method currently has, and popularity of the LB method continues to increase.
\[ \rho = m \int f \, dv, \]  
\[ \rho u_\alpha = m \int f v_\alpha \, dv, \]  
\[ \rho e = m \int f \frac{v^2}{2} \, dv, \]

where \( v = \frac{p}{m} \), \( \rho \) is fluid density, \( u_\alpha \) is fluid velocity, and \( \rho e \) is the energy density.

If there are no particle collisions and an external (not due to other particles) force \( F \) acts on the system, at time \( t + \Delta t \) the number of particles in the initial unit phase-space volume \( d^3x d^3p_1 \) would become:

\[ f \left( x + \frac{p_1}{m} \Delta t, p_1 + F \Delta t, t + \Delta t \right) d^3x d^3p_1, \]

where we used the fact that the phase space volume element \( d^3x d^3p_1 \) is constant.

However, since collisions do occur, they can change the particle distribution function, and hence the number of particles in \( d^3x d^3p_1 \):

\[ \Delta N_{mol} = \left( \frac{\partial f}{\partial t} \right) \bigg|_C \Delta t d^3x d^3p_1 = \left[ f \left( x + \frac{p_1}{m} \Delta t, p_1 + F \Delta t, t + \Delta t \right) - f \left( x, p_1, t \right) \right] d^3x d^3p_1, \]

where \( \left( \frac{\partial f}{\partial t} \right) \bigg|_C \) is a collision operator. Dividing both parts of eq. (2.7) by \( d^3x d^3p_1 \Delta t \) we would get:

\[ \left( \frac{\partial f}{\partial t} \right) \bigg|_C = \frac{\partial f}{\partial t} + \left( \frac{\partial f}{\partial x} \frac{dx}{dt} + \frac{\partial f}{\partial y} \frac{dy}{dt} + \frac{\partial f}{\partial z} \frac{dz}{dt} \right) + \left( \frac{\partial f}{\partial p_x} \frac{dp_x}{dt} + \frac{\partial f}{\partial p_y} \frac{dp_y}{dt} + \frac{\partial f}{\partial p_z} \frac{dp_z}{dt} \right) \]
\[ = \frac{\partial f}{\partial t} + \left( \frac{\partial f}{\partial x} \frac{dx}{dt} + \frac{\partial f}{\partial p_1} \frac{dp_1}{dt} \right) = \frac{\partial f}{\partial t} + \frac{p_1}{m} \frac{\partial f}{\partial x} + F \frac{\partial f}{\partial p_1} = D_t f, \]

where at the last step we have introduced an operator \( D_t = \partial_t + \frac{p_1}{m} \partial_x + F \partial_{p_1} \).

Since the full derivation of this equation is quite complex, we will provide only a heuristic explanation on the matter of the collision term. One can find more details in, for example, [138]. That leads to the following form of the collision operator:

\[ \left( \frac{\partial f}{\partial t} \right) \bigg|_C = \frac{1}{m} \int |p_2 - p_1| (f_{1'2'} - f_{12}) \left| \frac{d\sigma}{d\Omega} \right| d^2\Omega dp_2, \]

where \( d\Omega \) is an element of the solid angle and \( \left| \frac{d\sigma}{d\Omega} \right| \) is a differential cross section. The last value characterizes the probability of detecting particles at a given solid angle after scattering from collision. In this equation \( f_{12} \) and \( f_{1'2'} \) are two-body distribution functions. Function \( f_{12} = f_{12}(x, p_1, p_2, t) \) describes the probability to find a particle at position \( x \) with momentum \( p_1 \) together with a particle at the same position with momentum \( p_2 \) at the same time \( t \); \( f_{1'2'} = f_{1'2'}(x, p_1', p_2', t) \) measures the probability
that particles appeared suddenly at position $x$ as a result of another collision between particles which have moments $p_1'$ and $p_2'$. Thus, $f_{1'2'}$ describes the increase in the number of particles scattered into the unit phase space element, while $f_{12}$ corresponds to the loss of particles that scattered out from it.

The next important assumption that is necessary for simplifying the expression for the collision term is the so called molecular chaos assumption, that states that particles are uncorrelated before the collision and allows us to replace the two-body distributions by the product of single-body distributions, $f_{12} = f_1 f_2$ and $f_{1'2'} = f_{1'} f_{2'}$ (i.e. particles are uncorrelated prior to the collision and, thus, distributions after the collision depends only on that particular collision and does not contain any information on the previous ones).

Finally, the Boltzmann equation is:

$$
\left[ \frac{\partial}{\partial t} + \frac{p_1}{m} \frac{\partial}{\partial x} + F \frac{\partial}{\partial p_1} \right] f(x, p_1, t) = \frac{1}{m} \int |p_2 - p_1| (f_{1'2'} - f_{1f_2}) \frac{d\sigma}{d\Omega} d^2\Omega dp_2.
$$

The left-hand side of eq. (2.10), often referred to as streaming, describes the motion of a single particle distribution under the action of external forces $F$. The right-hand side of the equation, referring to collision effects, describes how the probability of finding a particle with position $x$ and momentum $p_1$ would be changed in case of a collision with a particle that has momentum $p_2$ (corresponds to the term with $f_{1f_2}$), and increased by the incoming particles from other collisions (corresponds to the integral of the term with $f_{1'f_2'}$)

### 2.2.2 Equilibrium Distribution Function

A situation, when the number of particles that leaves a given phase space volume $d^3x d^3p$ is equal to the number of particles that enter it (that in the case of the lattice Boltzmann method with discretized velocities also implies the conservation of momentum), is called the local equilibrium and implies that

$$
\left( \frac{\partial f}{\partial t} \right) \bigg|_C \equiv 0.
$$

A distribution function $f^{eq}$ that satisfies this condition is called the local equilibrium distribution function. Using eq. (2.9) for the collision operator, the last equation can be rewritten as

$$
f_{1'}^{eq} f_{2'}^{eq} = f_1^{eq} f_2^{eq}.
$$

Taking the logarithm of the both sides would lead to

$$
\ln f_{1'}^{eq} + \ln f_{2'}^{eq} = \ln f_1^{eq} + \ln f_2^{eq}.
$$

Thus, $\ln f^{eq}$ is an additive collision invariant and stays unchanged during the collision. There are five quantities that are conserved during a binary elastic collision: mass (or particle number), three components of the momentum, and energy. Therefore, $\ln f^{eq}$ can be expressed in terms of these five parameters:
\[ \ln f^{eq} = A + B_\alpha p_\alpha + \frac{C}{2m} p^2, \]  
(2.14)

where \( \alpha \) corresponds to cartesian coordinates \( x, y, z \), and summation over repeated indexes is assumed. One can express the unknown interpolation coefficients \( A, B_\alpha, \) and \( C \) in terms of the conserved macroscopic moments

\[ m \int f^{eq} dv = \rho, \]  
(2.15)

\[ m \int f^{eq} v_\alpha dv = \rho u_\alpha, \]  
(2.16)

\[ m \int \frac{f^{eq} v^2}{2} dv = \rho e, \]  
(2.17)

where, as before, \( v = \frac{p}{m} \), \( \rho \) is fluid density, \( u_\alpha \) is fluid velocity, and \( \rho e \) is the energy density, and come up with the following expression for the equilibrium distribution function:

\[ f^{eq} = \rho \left( \frac{m}{2\pi k_B T} \right)^{3/2} \exp \left[ -\frac{m(v - u)^2}{2k_B T} \right], \]  
(2.18)

where \( T \) is the temperature of the fluid, \( k_B \) is the Boltzmann constant. This distribution is called the Maxwell-Boltzmann equilibrium distribution function and describes the local equilibrium.

### 2.2.3 Bhatnagar – Gross – Krook Collision Operator

For simulations of gases and fluid, eq. (2.10) is quite complicated to work with, and the right-hand side of the equation is often replaced by simpler collision terms. One of the most common replacements, that conserves mass, momentum and energy, is the Bhatnagar – Gross – Krook (BGK) collision operator [139] based on linearization of the collision integral from eq. (2.10):

\[ \left( \frac{\partial f}{\partial t} \right)^{BGK}_C = \frac{f - f^{eq}}{\tau_f}. \]  
(2.19)

The above equation is an approximation of the collision term by using a single relaxation time towards local equilibrium, where \( \tau_f \) is the relaxation time. With the BGK approximation, eq. (2.10) becomes:

\[ \frac{\partial f}{\partial t} + \frac{P_1}{m} \partial_x f + F \partial_p f = \frac{1}{\tau_f} \left( f - f^{eq} \right). \]  
(2.20)

The Boltzmann equation with this collision operator (for simplicity referred to as LBE BGK), discretized in space, time and velocity space, leads to the Navier – Stokes equations in the macroscopic limit and, therefore, is suitable for simulations of gases and fluids.
2.2. From Boltzmann Equation to Lattice Boltzmann Method

Figure 2.3: Streaming and collision steps in the lattice Boltzmann method. Thickness of the arrows corresponds to the magnitude of $f_i$ along the given velocity direction $e_i$. In a): the distribution function at the beginning of the step. In b): the distribution function got changed due to the collision. In c): streaming step.

2.2.4 Discretized Lattice Boltzmann Equation

In order to solve the LBE BGK eq. (2.20) on the grid, it has to be discretized. After a standard discretization in space with step $\Delta x$ and time step $\Delta t$, the phase space $d^3x d^3p = md^3x d^3v$ also has to be discretized in velocity space. As was mentioned before, there exist a lot of one-, two- and three-dimensional velocity schemes where the number of possible directions starts at 2 (D1Q2) and grows (D3Q15, shown in fig. 2.2, and D3Q19 are two of the most popular three dimensional schemes).

After discretization, eq. (2.20) becomes:

$$f_i(\mathbf{x} + e_i \Delta t, t + \Delta t) - f_i(\mathbf{x}, t) = -\frac{\Delta t}{\tau_f} \left( f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t) \right),$$

(2.21)

where $e_i$ are discrete velocity vectors of the chosen velocity model. The distribution functions $f_i$ and $f_i^{eq}$ have to be discretized as well. Eq. (2.21) is accompanied by a set of discretized equations similar to (2.3)-(2.4):

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

(2.22)

and similar relations act as constraints on $f_i^{eq}$.

Usually in LBE BGK algorithm the update of the state happens in two steps - streaming and collision. The collision step corresponds to the right-hand side of eq. (2.21), where all calculations related to the collisions between particles are performed. The left-hand side of this equation updates the distribution functions $f_i$ and therefore moves the particle distributions, as represented in fig. 2.3. This division of an update is done for simplicity: for example, when one wants to implement the bounce-back boundary conditions, which requires reversing some of $f_i$, it is much easier to do this reversing after the collision, but before the streaming part.
2.2.5 Recovery of Macroscopic Equations from LBE BGK

2.2.5.1 Continuity equation

Let us start with the standard lattice-Boltzmann BGK equation with no external forces acting on the system:

\[ f_i(x + e_i \Delta t, t + \Delta t) - f_i(x, t) = -\frac{\Delta t}{\tau_f} \left( f_i(x, t) - f_i^{eq}(x, t) \right). \]  \hspace{1cm} (2.23)

Using a Taylor series expansion of the first term on the left-hand side of this equation, it can be rewritten as:

\[ \Delta t D_i f_i + \frac{\Delta t^2}{2} D^2_i f_i = -\frac{1}{\tau_f} (f_i - f_i^{eq}), \] \hspace{1cm} (2.24)

where the operator \( D_i = (\partial + e_i \partial_\alpha) \) is introduced similar to what was done in eq. (2.8) and the arguments of the distribution functions were omitted for simplicity.

According to the Chapman – Enskog theory, one expands the probability distribution function \( f_i \) around the equilibrium distribution function \( f_i^{(0)} \). Because we assume small changes from the equilibrium configuration, the velocity is small (relative to the speed of sound), and gradients are small as well. Since the system will approach the equilibrium state in time, we use \( \Delta t \) as an expansion parameter [140]:

\[ f_i = f_i^{(0)} + \Delta t f_i^{(1)} + \Delta t^2 f_i^{(2)} + \mathcal{O}(\Delta t^3). \] \hspace{1cm} (2.25)

Using expressions for the moments of the equilibrium distribution function, and grouping terms of the same orders of \( \Delta t \), we would get:

\[ f_i^{(0)} = f_i^{eq}, \quad D_i f_i^{(0)} = -\frac{f_i^{(1)}}{\tau_f}, \quad D_i f_i^{(1)} + \frac{1}{2} D^2_i f_i^{(0)} = -\frac{f_i^{(0)}}{\tau_f}. \] \hspace{1cm} (2.26)

Using eqns. (2.26), we can rewrite eq. (2.24):

\[ f_i = f_i^{eq} - \tau_f D_i f_i^{eq} + \tau_f \left( \tau_f - \frac{\Delta t}{2} \right) D^2_i f_i^{eq} + \mathcal{O}(\Delta t^3). \] \hspace{1cm} (2.27)

Summing this equation over \( i \), i.e. over the lattice vectors, and using again the equations for the moments of the equilibrium distribution function \( f_i^{eq} \), and neglecting terms of orders \( \Delta t^3 \) and higher, eq. (2.27) will lead to [141]:

\[ \partial_t \rho + \partial_\alpha (\rho u_\alpha) = \left( \tau_f - \frac{\Delta t}{2} \right) \left[ \partial_t (\rho u_\alpha) + \partial_\beta \sum_i e_{i\alpha} e_{i\beta} f_i^{eq} \right] + \mathcal{O}(\Delta t^3). \] \hspace{1cm} (2.28)

In order to calculate the term in the square brackets, we multiply both sides of eq. (2.27) by \( e_{i\alpha} \), perform the summation over the velocity vectors again and leave only terms of order \( \Delta t \); after these actions we will get that this term is equal to \( 0 + \mathcal{O}(\partial^2) \).
2.2. From Boltzmann Equation to Lattice Boltzmann Method

\[ \partial_t (\rho u_\alpha) + \partial_\beta \sum_i e_{i\alpha} e_{i\beta} f_i^{eq} = \left( \tau_f - \frac{\Delta t}{2} \right) \partial_t \left[ \partial_t (\rho u_\alpha) + \partial_\gamma \sum_i e_{i\alpha} e_{i\gamma} f_i^{eq} \right] + \left( \tau_f - \frac{\Delta t}{2} \right) \partial_\beta \left[ \partial_t \left( \rho u_\alpha \right) + \partial_\gamma \sum_i e_{i\alpha} e_{i\gamma} f_i^{eq} \right], \]

(2.29)

Substituting this result into equation eq. (2.28) would finally lead to the continuity equation up to third order of accuracy:

\[ \partial_t \rho + \partial_\alpha (\rho u_\alpha) = 0 + \mathcal{O}(\partial^3). \]

(2.30)

\[ \rho \]

2.2.5.2 Navier-Stokes equations

In order to reproduce the Navier-Stokes equation for the fluid, we start with substitution of eq. (2.30) into the right-hand side of eq. (2.29) and again use the moments of the equilibrium distribution function to get:

\[ \partial_t (\rho u_\alpha) + \partial_\beta (\rho u_\alpha u_\beta) + \partial_\beta P_{\alpha\beta} = \left( \tau_f - \frac{\Delta t}{2} \right) \partial_t \delta_{\alpha\beta} \left( \frac{\rho}{3} (u_\alpha \delta_{\alpha\beta} + u_\beta \delta_{\alpha\gamma} + u_\gamma \delta_{\alpha\beta}) \right) + \partial_t (-\sigma_{\alpha\beta} + \rho u_\alpha u_\beta). \]

(2.32)

If we use \( P_{\alpha\beta} = -P_0 \delta_{\alpha\beta} \), then

\[ \frac{\partial P_{\alpha\beta}}{\partial t} = -\frac{\partial P_0}{\partial t} \delta_{\alpha\beta} = -\frac{\partial P_0}{\partial t} \delta_{\alpha\beta}. \]

(2.33)

If the fluid is incompressible, we can rewrite this equation using eq. (2.31) to get:

\[ \partial_t P_{\alpha\beta} = \rho (\partial_\rho P_0)(\partial_\gamma u_\gamma) \delta_{\alpha\beta}. \]

(2.34)

Next, using the terms of \( \mathcal{O}(\partial) \) from eq.(2.32), we can write:

\[ \partial_t (\rho u_\alpha u_\beta) = \partial_t (\rho u_\alpha) u_\beta + u_\alpha \partial_t (\rho u_\beta) = -\partial_\gamma (\rho u_\alpha) u_\gamma u_\beta - u_\alpha \partial_\gamma (\rho u_\beta) u_\gamma. \]

(2.35)

However, this term can be neglected because it is third order in velocity. Collecting all the results together, we would finally get the Navier – Stokes equations for incompressible fluids [141]:

\[ \partial_t (\rho u_\alpha) + \partial_\beta (\rho u_\alpha u_\beta) = -\partial_\beta P_{\alpha\beta} + \frac{\rho}{3} \left( \tau_f - \frac{\Delta t}{2} \right) \partial_\beta \delta_{\alpha\beta} \left( 1 - 3 \partial_\rho P_0 \partial_\gamma u_\gamma + \partial_\beta u_\alpha + \partial_\alpha u_\beta \right). \]

(2.36)

In this case the shear viscosity is \( \eta_s = \frac{\rho (\tau_f - \Delta t/2)}{3} v_c^2 \) and bulk viscosity is determined as \( \Lambda_b = \eta_s \left( \frac{5}{3} - \frac{3}{v_c^2} \partial_\rho P_0 \right) \), where \( v_c = \frac{\Delta x}{\Delta t} \). Typically we will take \( P_0 = \rho v_s^2 \), where \( v_s \) is the isentropic speed of sound. In this case \( \Lambda_b = \eta_s \left( \frac{5}{3} - \frac{3}{v_c^2} v_s^2 \right) \).
2.3 Lattice-Boltzmann Method for Liquid Crystals With Immersed Particle

2.3.1 Liquid Crystal Hydrodynamics

Originally, the lattice Boltzmann method, described in sec. 2.2, was made for simple isotropic fluids and reproduced Navier-Stokes equations and the continuity equation on a discrete grid using a finite difference scheme based on the linearized lattice Boltzmann equation with the BGK collision operator as described above. The lattice Boltzmann method suitable for simulation of liquid crystals behavior within the Beris-Edwards formalism was firstly introduced by Denniston et al. [142]. The main idea is to recover Beris-Edwards equations by introducing a second Boltzmann-like equation which is responsible for evolution of a tensor order parameter $Q$.

2.3.1.1 Lattice Boltzmann method for three-dimensional LC hydrodynamics

As for simple isotropic fluids, we require a set of distribution functions existing on mesh sites. At each site we define a scalar partial distribution function $f_i = f_i(x, t)$, that would be “responsible” for evaluation of density and velocity. However, for liquid crystals, which have an antisymmetric part of the stress tensor, an additional term $p_i$ has to be added to the right-hand side of eq. (2.21), i.e.

$$f_i(x + e_i \Delta t, t + \Delta t) - f_i(x, t) = -\frac{\Delta t}{\tau_f} \left( f_i(x, t) - f_i^{eq}(x, t) \right) + p_i,$$  (2.37)

that leads to extra constraints to impose the antisymmetric part of the stress tensor in addition to equations eqns. (2.22) for the moments:

$$\rho = \sum_i f_i, \quad \rho u_\alpha = \sum_i f_i e_{i\alpha},$$  (2.38)

$$\sum_i p_i = 0, \quad \sum_i p_i e_{i\alpha} = \partial_\beta \tau_{\alpha\beta}, \quad \sum_i p_i e_{i\alpha} e_{i\beta} = 0,$$  (2.39)

Liquid crystals also have the tensor order parameter $Q$ that, according to the algorithm of Denniston et al. [142], is evaluated via the equation already mentioned in sec. 1.1.3.4:

$$(\partial_t + u \cdot \nabla)Q - S(W, Q) = \Gamma H.$$  (2.40)

Therefore, for liquid crystal hydrodynamics we also need another set of distribution functions — symmetric traceless tensors $G_i$ with a similar meaning to $f_i$ to evaluate the tensor order parameter $Q$. Then eq. (2.40), after discretization and introduction of the density functions $G_i$ and relaxation time $\tau_G$, becomes

$$(\partial_t + e_i \cdot \nabla)G_i = -\frac{1}{\tau_G} (G_i - G_i^{eq}) + M_i.$$  (2.41)
or

\[ G_i(x + e_i \Delta t, t + \Delta t) - G_i(x, t) = -\frac{\Delta t}{\tau_G} \left(G_i(x, t) - G_i^{eq}(x, t)\right) + M_i. \]  (2.42)

that is similar to eq. (2.37). The additional term \( M_i \) has the following constraints in order to recover the macroscopic equations:

\[ \sum_i M_i = \hat{H} = S(W, Q) + \Gamma H, \quad \sum_i M_i e_{i\alpha} = \left(\sum_i M_i\right) u_\alpha, \]  (2.43)

and distribution functions \( G_i \) also satisfy

\[ \sum_i G_i = Q. \]  (2.44)

Equilibrium distribution functions have to be discretized as well. For \( f_i^{eq} \), determined via eq. (2.18), this can be done using the Taylor series expansion of the exponential with respect to velocity. Similarly, equilibrium distribution functions \( G_i^{eq} \) and forcing terms \( p_i \) and \( M_i \) can be expanded and approximated with the following expressions, assuming low velocities (i.e. small Mach numbers):

\[ f_i^{eq} = A_s + B_s \rho \alpha e_{i\alpha} + C_s u_\alpha + D_s u_\alpha \epsilon_{i\alpha} e_{i\beta} + E_s \epsilon_{i\alpha} e_{i\beta}, \]
\[ G_i^{eq} = J_s + K_s \rho \alpha e_{i\alpha} + L_s u_\alpha + N_s \epsilon_{i\alpha} e_{i\beta}, \]  (2.45)

\[ p_i = T_s \partial_\beta \tau_{\alpha\beta} e_{i\alpha}, \]
\[ M_i = R_s + S_s \rho \alpha e_{i\alpha}, \]  (2.46)

Moments of the equilibrium distribution functions satisfy the following equations:

\[ \sum_i f_i^{eq} = \rho, \quad \sum_i f_i^{eq} e_{i\alpha} = \rho u_\alpha, \quad \sum_i f_i^{eq} e_{i\alpha} e_{i\beta} = -\sigma_{\alpha\beta} + \rho u_\alpha u_\beta, \]  (2.47)

\[ \sum_i G_i^{eq} = Q, \quad \sum_i G_i^{eq} e_{i\alpha} = Q u_\alpha, \quad \sum_i G_i^{eq} e_{i\alpha} e_{i\beta} = Q u_\alpha u_\beta. \]  (2.48)

Coefficients from (2.45) and (2.46), \( s = 0, 1, 2 \), are determined by evaluating the constraints on \( f_i^{eq}, G_i^{eq}, p_i, M_i \) (i.e. eqns. (2.39), (2.43), (2.47) and (2.48)) and matching terms. Coefficients \( A_s, B_s, C_s, D_s, E_s \) depend on density and the symmetric part of the stress tensor; \( J_s, K_s, L_s, N_s \) are functions of the tensor order parameter \( Q \); \( T_s \) are constants; and \( R_s, S_s \) depends on the molecular field \( \hat{H} \). The exact expressions for the coefficients can be found in [142] together with more details on the algorithm.
2.3.1.2 Recovery of macroscopic tensor order parameter equation

The continuity and Navier-Stokes equations for liquid crystals can be recovered in a similar way to isotropic fluids described above. Eq. (2.40), responsible for the evolution of the tensor order parameter, can be recovered in the following manner.

We again start with the Chapman – Enskog expansion of the distribution function [140]:

\[ G_i = G_i^{(0)} + \Delta t G_i^{(1)} + \Delta t^2 G_i^{(2)} + O(\Delta t^3). \]  

and substitute it into the expression similar to eq. (2.24):

\[ \Delta t D_i G_i + \Delta t^2 D_i^2 G_i = -\frac{1}{\tau_G} (G_i - G_i^{eq}) + M_i. \]  

Repeating the same steps as for \( f_i \), we would get the following expressions:

\[ G_i^{(0)} = G_i^{eq} + \tau_G M_i, \quad G_i^{(1)} = -\tau_G D_i G_i^{eq} + \tau_G M_i, \quad G_i^{(2)} = \tau_G^2 D_i^2 G_i^{eq} - \tau_G^2 D_i M_i. \]  

Substituting eq. (2.51) into eq. (2.50), summing over the velocity vectors, and using equations for the moments of the equilibrium distribution function (2.48), would give eq. (2.40), to the first order:

\[ \partial_t Q + \partial_\alpha (Q u_\alpha) = S(W, Q) + \Gamma H + O(\partial^2). \]  

2.3.1.3 Alternative update of distribution functions

Described above is the general approach to update the distribution functions. In our work, however, to solve equations (2.37) and (2.42), we used an algorithm suggested by Ollila et al. [143].

In order to explain the origin of equations in this algorithm, let us start with the following equation:

\[ \frac{df}{dt} = -\frac{1}{\tau}(f - \tilde{f}_i^{eq}), \]  

where \( \tilde{f}_i^{eq} = f_i^{eq} + \tau_i p_i \). Multiplying both sides of this equation by a yet unknown variable \( \mu \), we can get:

\[ \frac{\mu df}{dt} + \frac{\mu f}{\tau} = \frac{\mu \tilde{f}_i^{eq}}{\tau}. \]  

Let us find \( \mu \) that would satisfy

\[ \frac{d(\mu f)}{dt} = \frac{\mu df}{dt} + f \frac{d\mu}{dt} \]  

Comparing eq. (2.54) with eq. (2.55), it can be seen:

\[ \frac{d\mu}{dt} = \frac{\mu}{\tau} \quad \Rightarrow \quad \mu = e^{t/\tau}. \]
2.3. Lattice-Boltzmann Method for Liquid Crystals With Immersed Particle

Substitute this result into eq. (2.54) and change notation of \( t \) to \( s \):

\[
\frac{d(e^{s/\tau})}{ds} = \frac{e^{s/\tau} \tilde{f}^{eq}_i}{\tau},
\]  

(2.57)

integrate:

\[
e^{s/\tau} f|^{t+\Delta t}_{t} = \int_{t}^{t+\Delta t} e^{s/\tau} \tilde{f}^{eq}_i \frac{1}{\tau}. \tag{2.58}
\]

After simplification and factorization out the term \( e^{t/\tau} \), we would get:

\[
f_i(x + e_i \Delta t, t + \Delta t) = e^{-\Delta t/\tau_f} \left( f_i(x, t) + \int_{t}^{t+\Delta t} e^{(s-t)/\tau} \tilde{f}^{eq}_i(x + e_is, t + s) ds \right). \tag{2.59}
\]

Performing the Taylor series expansion of \( \tilde{f}^{eq}_i \) about \( s = 0 \) in the above equation at \( t + \Delta t \) would lead to:

\[
f_i(x + e_i \Delta t, t + \Delta t) = e^{-\Delta t/\tau_f} f_i(x, t) + (\Delta t - \tau_f \Upsilon_f) D_i \tilde{f}^{eq}_i(x, t) + (\tau_f^2 \Upsilon_f - \Delta t \tau_f + \Delta t^2/2) D_i^2 \tilde{f}^{eq}_i(x, t) + O(\Delta t^4) \tag{2.60}
\]

with \( \Upsilon_f = 1 - e^{-\Delta t/\tau_f} \) and

\[
\tilde{f}^{eq}_i = f^{eq}_i + \tau_f p_i,
\]

\[
D_i \tilde{f}^{eq}_i(x, t) = \frac{\tilde{f}^{eq}_i(x, t) - \tilde{f}^{eq}_i(x - e_i \Delta t, t - \Delta t)}{\Delta t},
\]

\[
D_i^2 \tilde{f}^{eq}_i(x, t) = \frac{\tilde{f}^{eq}_i(x + e_i \Delta t, t) - \tilde{f}^{eq}_i(x, t)}{\Delta t^2} - \frac{\tilde{f}^{eq}_i(x, t - \Delta t) + \tilde{f}^{eq}_i(x - e_i \Delta t, t - \Delta t)}{\Delta t^2}. \tag{2.61}
\]

The equation for updating distribution function \( G_i \) can be recovered in a similar manner and looks like

\[
G_i(x + e_i \Delta t, t + \Delta t) = e^{-\Delta t/\tau_G} G_i(x, t) + \Upsilon_G \tilde{G}^{eq}_i(x, t) + (\Delta t - \tau_G \Upsilon_G) D_i \tilde{G}^{eq}_i(x, t) + (\tau_G^2 \Upsilon_G - \Delta t \tau_G + \Delta t^2/2) D_i^2 \tilde{G}^{eq}_i(x, t) + O(\Delta t^4), \tag{2.62}
\]

where \( \Upsilon_G = 1 - e^{-\Delta t/\tau_G} \). Expressions for \( \tilde{G}^{eq}_i, D_i \tilde{G}^{eq}_i \) and \( D_i^2 \tilde{G}^{eq}_i \) are similar to (2.61).

This approach was found to be more stable compared to the standard update equations (2.37) and (2.42) for the treatment of the stiff terms that often appear due to colloidal forces [143].
2.3.2 The Object and Coupling

To accomplish the objectives of this research, discussed in sec. 1.2, we have to start with simulations of a single disc-shaped particle immersed in a nematic liquid crystal. This requires a “construction” of the disc and coupling it with the liquid crystal.

There exist a lot of studies that simulate the behavior of particles of various shapes submerged in liquid crystals – research was done on spheres, ellipsoidal particles, toruses, wires, etc. In most of these works, however, the immersed particle is not allowed to move. In this work we extend the algorithm of F. Mackay et al. [144] and provide a method that is suitable for particles of any shape, has full coupling between the liquid crystal and the immersed object, and allows the forces resulting from this coupling to move the particle. Our method also requires a discretization of the object; before, discretization was performed primarily for spheres and other geometrical shapes were represented continuously.

Sec. 2.3.2.1 covers the representation of the particle and related questions; next section, 2.3.2.2, explains how the coupling between the liquid crystal and the object is performed.

2.3.2.1 Disc Representation

When the fluid is on a discrete mesh, one can also discretize the object, as was done in this work (see fig. 2.4 and fig. 2.5). However, nodes of the object will often not coincide with the mesh sites of the liquid. That implies that the object nodes have to be distributed to the nearest mesh sites using some scheme to determine, for example, with what weights additional molecular field from conditions on the surface represented by the nodes has to be added to these sites. Conversely, the forces from the liquid crystal that would affect the object are calculated at the mesh sites and have to be drawn back together with the same scheme to be applied to the node of the object as a weighted sum. This also adds some constraints on the object representation: in order to prevent fluid from getting through the border of the object, the distance between nodes has to less than $\Delta x$, the lattice spacing; on the other hand, one should avoid creating too many nodes or it would lead to inefficient calculations. For example, all discs used here are created with 0.03 $\mu m$ distance between the nodes, while the grid spacing $\Delta x$ is 0.0625 $\mu m$.

In this work, in order to “put” the disc into the liquid crystal, we distribute nodes to nearby lattice mesh via trilinear stencil. This interpolation method is performed in the following way: each node of the object is labeled by index $\alpha$ and described by coordinates $(x_\alpha, y_\alpha, z_\alpha)$; each node is located inside a cubic cell and, thus, has 8 grid sites around it – these sites are indexed by $j \in [0..7]$ and have coordinates $(x_j, y_j, z_j)$. Next, the weights from node $\alpha$ defined via

$$\zeta_{\alpha j} = \phi_j(x_\alpha) \phi_j(y_\alpha) \phi_j(z_\alpha)$$  \hspace{1cm} (2.63)

are assigned to all eight nearest sites. Here

$$\phi_j(r_\alpha) = 1 - |\Delta r|$$  \hspace{1cm} (2.64)
2.3. Lattice-Boltzmann Method for Liquid Crystals With Immersed Particle

with $\Delta r = (\mathbf{r}_\alpha - \mathbf{r}_j)/dx$, where $\mathbf{r}_\alpha$ and $\mathbf{r}_j$ are the position of a node and lattice mesh site, respectively [145] (see fig. 2.4). As can be mentioned, $\zeta_{\alpha j}$ is the volume of a parallelogram defined by diagonal points $(x_\alpha, y_\alpha, z_\alpha)$ and $(x_j, y_j, z_j)$ (in simplified to two dimensions fig. 2.4 this volume corresponds to the shaded area). Such weights satisfy $\sum_j \zeta_{\alpha j} = 1$ for each node $\alpha$ and can be used to perform a weighted sum for getting the interpolated value at the node location (for example, this is done for the velocity value at the node location to calculate the hydrodynamic forces, as described below), or, on the opposite, the value from the node (the surface normal, for example) can be interpolated to the sites. If there are more than one node in a cubic cell, the weights from each node are summed at the sites of this cell. One may mention that values of weights $\zeta_{\alpha j}$ changes smoothly from 1 to 0 when particle, started at a node, moves to the neighboring one. When the object is distributed like this, the interaction between the object and the fluid is performed in a continuous manner.

We simulated a disc with radii $R$ and thickness $L$ (see table 3.1 for exact numbers) in two ways. In the first case (see Figure 2.5a) the object was represented by equally distributed nodes on the bases of the cylinder with the distance between bases equal to the thickness of the disc (referred to later as the “edgeless” representation). The second representation, referred to as the “edged” representation, consisted of the same nodes plus nodes on the cylindrical surface (see Figure 2.5b). There are two reasons to examine these different representations.

The first reason is that in the physical implementation (i.e. the experiment) the

Figure 2.4: Simplified to two dimensions schematic representation of the distribution of the nodes of the object to fluid mesh.
effective boundary conditions on the face of the disc should be well represented by a term such as eq. (1.13) with the preferred orientation normal to the surface. As homeotropic anchoring is typically obtained by chemical treatment of the surface, it is not clear how effective this treatment is on the edge of a very thin disc. That is, if the homeotropic anchoring was perfect on the edge one should have a defect around the disc edge even in the case when the disc’s orientation does not produce any distortion due to the conflict between the face and edge conditions for the director on the surface of the disc. This is illustrated in fig. 2.6. First, a surface normal, i.e., a unit vector perpendicular to the surface at each point, is calculated for each node of the disc (surface normals are shown by light and dark blue lines in fig. 2.6a). Next, since the nodes of the disc have to be distributed to the nearest mesh sites (see fig. 2.6b, blue and green dotted lines), the surface normal is interpolated using a trilinear stencil to the nearest mesh sites as well. However, since there is more than one node per cell, normals of all nodes in this cell are taking part in the calculation of the surface normal at a mesh site belonging to this cell. Because we use trilinear interpolations, normals of the nodes that are closer to a particular site would contribute more to the normal at the site. For example, the normal at the top site inside the green ellipse in fig. 2.6b is calculated based on normals of both the orange node on the base of the disc and the purple node on the cylindrical surface, resulting into a tilted normal vector. Finally, the orientation of liquid crystal particles at the mesh sites near the surface of the disc is calculated based on the surface normal at the sites, strength of anchoring on the surface, and surrounding director field, leading to a highly distorted area around the edge of the disc due to an abrupt change in the surface normal (fig. 2.6, c). This problem does not exist for edgeless discs, since there are no particles on the edge to contribute to the orientation of the liquid crystal director. Of course, if the surface anchoring on the edge of the disc in the experiment is very effective, it will experience a similar distortion at the edge.

On the other hand, if the anchoring on the edge of the disc was weak, the molecules may avoid a defect along the edge and align perpendicularly to the face, even along

Figure 2.5: Schematic representation of the disc in the simulation: a) The disc is represented only by bases; b) Additional points on the cylindrical surface have been added.
Figure 2.6: The surface normal and director configuration near the edge of a disc. Nodes on the bases of the disc are represented by the orange spheres, nodes on the cylindrical surface are colored in purple. Green ellipses help to track the same group of nodes. In a): surface normal at the nodes of the edged disc (dark and light blue lines). In b): nodes of the disc have to be distributed to the nearest mesh sites (shown by blue and green dotted lines) together with the surface normal (shown by purple lines). In c): surface conditions resulted in a conflict between director field near the bases and around the edge (the snapshot is a cross-section near the center of the simulation domain viewed from above).

the edge. Our two representations model the two extremes where the edgeless case is equivalent to assuming the disc is too thin for effective chemical coating and the edged case strictly enforces the normal anchoring on the edge of the disc, which should be the case for thicker discs. For intermediate edge anchoring strengths we find that the system effectively adopts a director configuration that is similar to one of the two extreme cases we study here. For example, if the edge anchoring is sufficiently weak compared to the anchoring on the face, the system just adopts the director configuration of the edgeless disc but with some loss of order near the edge (i.e. the magnitude of $q$, the largest eigenvalue of the tensor order parameter, decreases). Conversely, if the edge anchoring is sufficiently strong, it generates a defect which is always pinned to the edge, similar the edged representation.

Since, for the edgeless case, we don’t have any particles on the cylindrical surface, in order to recover an imposed value of $Q$ from the disc onto the lattice Boltzmann mesh, the thickness of the object should be in the range $0 < L < 2dx$, where $dx$ is the size of the grid cell. Thus this type of representation can be used for thin discs and laths. The
advantage of the second case of the representation is that we can specify the conditions on the cylindrical surface, hence, there are no constraints on the thickness of the object and one can use this representation for cylindrical colloids such as wires and rods. However this requires slightly more computational time due to a larger number of points in the object representation.

### 2.3.2.2 Coupling Between Liquid Crystal and Particle

In this section we describe a new method of two-way coupling of a liquid crystal medium with a particle in it that implements no-slip condition on the surface of the object, meaning that the particle moves together with the fluid, something that has not previously been done.

Discussion of coupling between liquid crystal and immersed in it object in this work is described in the following manner: the liquid crystal is thought of consisting of a “fluid” part, that is described by Navier-Stokes eqn. (1.22) and (1.23), and “LC” part, described by eq. (1.17).

**Hydrodynamic forces**

Two-way coupling between the “fluid” and the object is performed via hydrodynamic forces, which arise when the particle moves through the liquid crystal. We simulate these by applying equal and opposite forces to mesh sites and nodes of the colloidal disc:

\[
F = \pm \lambda (v_n - u_f),
\]

where \(v_n\) is a particle node velocity and \(u_f = \sum u_j \xi_{j\alpha}\) is the velocity of the fluid trilinearly interpolated to the particle node location. In eq. (2.65) the plus sign corresponds to the force acting from the disc nodes to the sites of the fluid; the minus sign is for the force applied to the object node from the liquid crystal. Here \(\lambda\) is set to

\[
\lambda = \frac{2m_u m_v}{\tau_f (m_u + m_v)},
\]

where \(m_u\) and \(m_v\) are masses of the particle node and representative fluid mass at the node location, respectively. See Ref. [145], [144] for detailed information on how this implementation was developed and tested.

This way of implementation of hydrodynamic forces approximates no-slip boundary conditions on the surface of immersed particle (i.e. fluid velocity at the surface of the object is equal to the object’s velocity) that in this case means that the particle moves with the fluid (due to applying equal but opposite forces to both fluid sites and object nodes). Since two way interaction, i.e. object – to – “liquid” and “liquid” – to – object, is included via this force, we should not include any other information about the disc surface effects into calculation of the equilibrium distribution function \(f_i^{eq}\) to avoid double counting of this force. Hence, we perform the update of \(f_i^{eq}\) using only bulk and elastic molecular fields from eq. (1.20) (i.e. calculations of density and symmetric part of the stress tensor do not contain the molecular field from the surface conditions \(H_{SC}\), and, therefore, none of the coefficients \(A_s, B_s, C_s, D_s, E_s\) in \(f_i^{eq}\) contain \(H_{SC}\); see sec. 2.3.1.1).
2.3. Lattice-Boltzmann Method for Liquid Crystals With Immerged Particle

Effects of surface conditions

The effects of the particle presence on the "LC" part is fully defined by surface conditions and the corresponding term $H^{SC}$ from eq. (1.14). Hence, disc – to – "LC" coupling can be included into the simulation through adding $H^{SC}$ to the main bulk and elastic molecular fields in the update of equilibrium distribution function $G_i^{eq}$ (i.e. $H^{SC}$ would be included in $R_s$, $S_s$ in eq. (2.46); see sec. 2.3.1.1): the $S$ term from eq. (1.17) couples the tensor order parameter $Q$ with the flow, $H_{bulk}$ and $H_{elast}$ push system to the equilibrium, and $H^{SC}$ enforces surface conditions and, hence, account for the presence of the object. It should be mentioned that update of the equilibrium distribution function $f_i^{eq}$ uses the stress tensor containing $H^{bulk}$ and $H_{elast}$, coupling the fluid flow to order parameter and, thus, finishing the two-way coupling between the flow and order parameter.

The "LC" – to – disc coupling is more complicated. However, we may use a formula for isotropic liquids suggested by Landau and Lifshitz [146] to calculate the effect from the symmetric part of the stress tensor $\sigma^{SC}$ resulting from surface conditions:

$$F_{\alpha i} = a_{\beta} \sigma^{SC}_{\alpha \beta} \Delta S_i,$$  \hspace{1cm} (2.67)

where $\Delta S_i$ is the portion of the surface of the colloidal particle represented by node $i$, $\hat{a}$ is a surface normal and $\sigma^{SC}_{\alpha \beta}$ is based on (1.24) with $H$ replaced by $H^{SC}$. Only $\sigma^{SC}_{\alpha \beta}$ is used here because including whole $\sigma_{\alpha \beta} + \sigma^{SC}_{\alpha \beta}$ would mean double counting, since effects of $\sigma_{\alpha \beta}$ are already included via using $\sigma_{\alpha \beta}$ in $f_i^{eq}$ update (remember, $\sigma^{SC}_{\alpha \beta}$ was not included in $f_i^{eq}$). The calculations are performed, not directly at the node location, but at the outer edge of the surface, by stepping out one lattice Boltzmann distance unit, $dx$, along the surface normal as eq. (2.67) is meant to be evaluated on the outside of the surface [83]. Summation of $F_{\alpha i}$ over all nodes of the object would give

$$F_\alpha = \sum_i a_{\beta} \sigma^{SC}_{\alpha \beta} \Delta S_i.$$  \hspace{1cm} (2.68)

We call this force net surface anchoring force because it is a total force resulted from conditions on the surface of the object. The net surface anchoring force for a single disc in a uniform medium should be equal to 0 because of symmetry reasons. However, individual contributions from $F_{\alpha i}$ might lead to a torque we are interested in as it will rotate the object.

de Gennes showed [14, 147] that the torque due to a molecular field $h$ conjugate to the director field $\hat{n}$ can be calculated as:

$$\Gamma = \hat{n} \times h,$$  \hspace{1cm} (2.69)

where $\hat{n}$ is the director vector. However, since on the surface of an object with strong perpendicular anchoring the director would be the same as the surface normal, we can calculate the local torque from an immersed particle via:

$$\Gamma = \hat{a} \times h,$$  \hspace{1cm} (2.70)
where \( \hat{a} \) is unit vector of surface normal and \( h_\mu = q_{eq}(\hat{a}_\beta H^{SC}_{\mu\beta} + \hat{a}_\alpha H^{SC}_{\alpha\mu}) \). This formula can be written as [57]:

\[
\Gamma_\alpha = 2\varepsilon_{\alpha\beta\gamma} \left[ Q_{\alpha\beta} H^{SC}_{\alpha\gamma} + H^{SC}_{\beta\gamma} Q_{\beta\beta} - H^{SC}_{\beta\beta} Q_{\beta\gamma} \right]. \tag{2.71}
\]

This equation, for the uniaxial case, can be simplified using \( \tau_{\alpha\beta} = Q_{\alpha\gamma} H^{SC}_{\gamma\beta} - H^{SC}_{\alpha\gamma} Q_{\gamma\beta} \) (similar to eqn. (1.25)) to finally get the net torque \( \Gamma \) from the liquid crystal on the disc that arises due to the preferred anchoring at the surface of the disc:

\[
\Gamma_\alpha = -\sum_i 2\tau^{SC}_{\beta\gamma} \Delta V_i, \tag{2.72}
\]

where \( \alpha, \beta, \gamma \) are cyclic permutations, \( \tau^{SC}_{\beta\gamma} \) is similar to (1.25) but contains only the molecular field from surface anchoring, \( H^{SC} = \alpha_s(Q - Q^0) \), the sum is over the nodes \( i \) on the disc surface, and \( \Delta V_i \) is a local volume element. Using this formula it is now possible to calculate the local forces from \( \tau^{SC} \) in a way similar to what was done in a two dimensional simulation in [83]: for each node \( i \) one needs to apply equal but opposite forces at the neighboring nodes, that would reproduce the local torque \( \Gamma_\alpha = 2\tau^{SC}_{\beta\gamma} \Delta V_i \) at this node. However, since the sum of such forces would always give zero, and at the same time their implementation requires quite complicated calculations for the simulation in three dimensions, we include only net torque (2.71) and ignore these local forces. Therefore, eq. (2.71) finishes the coupling between the “LC” and the immersed object.

To sum up, two-way “fluid” – object coupling is performed through hydrodynamic forces (no \( H^{SC} \) in calculations of equilibrium distribution function); object – to – “LC” coupling is expressed via inclusion of \( H^{SC} \) in the driving term of \( G^{eq}_i \); “LC” – to – object coupling is due to net surface anchoring force and its resulting torque plus the torque \( \Gamma \) from \( \tau^{SC} \). See fig. 2.7 for a sketch of forces and torques used for two-way coupling between the liquid crystal and the object. When \( \varphi_{vr} = 0 \) the problem of potential double counting of some part of calculations disappears, because in this case \( \sigma \) does not contain
any molecular fields at all and $\tau = 0$, and updates of $f_i^{eq}$ and $G_i^{eq}$ are independent of each other.

It should be mentioned that this way of coupling of the liquid crystal to the object and vice versa fits to the object of any shape. This is possible because only local calculations that do not require any information about object geometry are used to couple them.

**Magnetic field**

An additional torque $T_{MF} = \mu \times B$ from the magnetic field $B$ was applied to the disc. Here $|\mu| = (0.32 \pm 0.06) \times 10^{-13} \text{A} \cdot \text{m}^2$ is the magnetic moment of the disc which is in the plane of the disc surface (see Figure 3.1). The value of magnetic moment was set to be proportional to the experimental value: both the size of the disc and its magnetic moment was taken to be about 50 times smaller than in the experiment [2]. The magnitude of the magnetic field $B$ was in the range $0.1 \text{G} - 20 \text{G}$.

### 2.4 LAMMPS

The algorithm described above was implemented within the open-source software system LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) [148]. LAMMPS allows implementation of various phenomena via a set of packages, usually named $\text{fix.package.name}$. Each such package contains the code to be completed at each time step. Such things as application of forces, controlling the temperature and updating of atom positions and velocities due to time integration are done in LAMMPS via fix commands that can be included into the input file. We, for instance, used one of the standard packages, a fix called $\text{rigid}$, to integrate the motion of the rigid object and modified it by adding the calculation of the surface normal to the code (we named the new fix $\text{fix.rigid.normal}$).

Software like LAMMPS allows a lot of flexibility for modeling fluid simulations by using different easily attachable and adjustable main and user-created packages. We took one of the user-created fixes named $\text{fix.lb_fluid}$ created by Mackay et al. that implements the lattice Boltzmann algorithm for simple isotropic fluids [144]; then we modified this fix to be suitable for liquid crystals simulations. Our fixes include calculations of all parameters necessary for the lattice Boltzmann method for liquid crystals ($f_i$, $G_i$, $f_i^{eq}$, $G_i^{eq}$, etc.), computation of all forces and torques acting on the liquid crystal from the immersed object and vise versa as described in sec. 2.3.2.2, and code for outputting parameters and the system configuration into a file for later analysis or restarts (the fix also supports the restart of simulation from the selected time step when necessary input files are provided).

We also created $\text{fix.add.torque}$ to add a torque on the object. This fix was produced in a similar way to the existing $\text{fix.add.force}$ package. In our simulations $\text{fix.add.torque}$ calculates the magnetic field torque on the object depending on the disc orientation (i.e. direction of the magnetic moment $\mu$) and the direction and magnitude of the magnetic field $B$; the same fix also performs rotation of the magnetic field.

A simulation runs in the following manner (see schema in fig. 2.8). Firstly, the program reads the file with coordinates of all “atoms” of all rigid bodies (i.e. the nodes
Figure 2.8: Sequence of steps in simulation of liquid crystals with LB method using LAMMPS.
representing the object surfaces). For the very first time step, fix rigid_normal just calculates the surface normal at each point of the object. Next, information about the surface normal and coordinates of the nodes is used to update the fluid and liquid crystal information, and calculate new forces and torques on the disc acting from the liquid crystal. Later, fix add_torque rotates the magnetic field and calculates the magnetic torque based on node locations. A loop of fixes, rigid_normal – liquid_crystal – add_torque repeats, and at each time step rigid_normal updates the position of all nodes based on forces and torques calculated in the liquid_crystal fix and add_torque fix. Fix liquid_crystal can also output velocity, forces, director vector fields and other parameters at desired time steps.

Another advantage of LAMMPS is that it supports the parallelization of the code. Existing packages are all parallelized using the Message Passing Interface (MPI), a standardized set of libraries for exchanging information between different computational cores. This allows a significant decrease of the computation time. The lattice Boltzmann method is very easy to parallelize, due to the fact that only local information is used for updates of all parameters, meaning only relatively small portions of data have to be exchanged between the processors. We utilized that useful property of the LB method and performed parallelization of the code with MPI in a manner consistent with LAMMPS. At the beginning of the simulation, the computation domain is equally distributed between the computation cores and during the run the cores exchange only boundary information necessary for calculations of this domain. We run simulations using the Sharncet and WestGrid computation facilities. Run time for each simulation strongly depends on the system configuration and number of cores used, but as an estimate one can expect 3 – 5 days per simulation of a medium size system (6µm × 6µm × 6µm) on 32 cores.

2.5 Chapter Summary

This chapter describes a novel algorithm for simulating objects in liquid crystals. The model includes a two-way coupling between the liquid crystal medium and the immersed particle, represented by a set of discrete nodes. The method also accounts for the backflow (i.e. the effect of the director reorientation on the fluid flow), that is very important for the accurate simulation of colloids in liquid crystals as we will show in the next chapter.

The method, implemented and parallelized in the LAMMPS environment, was used to simulate the behavior of a single thin disc inclusion in a nematic liquid crystal, and results of these simulations are described in chapter 3. Chapter 4 describes how the algorithm was updated for use in the simulation of the motion of disc pairs in a nematic and provides some results of the behavior of disc pairs.

Our code provides an opportunity to work not only with thin disc-shaped particles, but also allows discs with different aspect ratio as well, making it possible to work with not only discs but also with rod-shaped particles, laths, etc. Because the coupling between the liquid crystal and the object does not depend on the shape of the particle, the code can be used for particles of any shape, such as torus, ring, hollow cylinder, by only changing the rule for calculation of the surface normal. Our algorithm can also perform simulations for cholesteric liquid crystals as well.
3

Dynamics of a Single Disc

“I was captured for life by chemistry and by crystals.”

– Dorothy Crowfoot Hodgkin

The majority of experimental and numerical research on self-assembling inclusions has been performed on spherical particles [1,81,84,87,96], rod-shaped particles [57,100–102,149–151], or prolate spheroidal colloids [152–154], although some studies have considered more complicated shapes [155, 156]. Electrical or magnetic fields can be used to manipulate colloids, controlling their motion and organization. For example, spherical particles are often manipulated through laser traps, although the required electrical fields also affects the liquid crystal alignment [57]. On the other hand, experiments on ferromagnetic nanowires immersed in liquid crystals have used magnetic fields for particle manipulation instead. The required magnetic fields are small enough (< 20G) [101] to avoid changing the alignment of the liquid crystal particles [14]. In contrast to spherical particles, the orientation of an aspherical inclusion with respect to the liquid crystal director plays an important role, since any changes in the inclusion’s orientation affects the total elastic energy of the system. As a result, the particle experiences a torque that makes it rotate to the position of the lowest distortion energy, where elastic torque and magnetic torque are balanced. It has been shown that the torque on a rod-shaped colloid with parallel anchoring on its surface follows a linear dependence on the orientation of the particle [101] and the elastic energy changes analogous to electrostatic field energy [157], at least for small to moderate distortions. This implies that the rod will exhibit angular motion under the action of a magnetic field until it rotates by approximately $\pi$ from its original position; then the rod precesses to release the distortion in the liquid crystal. According to the latest experiments [2], a disc with perpendicular anchoring under similar conditions firstly behaves similarly and demonstrates angular motion, but the release of the liquid crystal distortion through flipping happens much earlier, closer to a rotation of $\pi/2$.

For a better understanding of this complicated motion and the associated properties of a disc-shaped inclusion and liquid crystal, we have performed 3D simulations of the behavior of an isolated ferromagnetic disc with homeotropic anchoring in a nematic liquid crystal in the presence of a rotating weak magnetic field. The aim of this work is to investigate ways of controlling the motion and the director field distortion around
the immersed particle through the disc size and properties of the magnetic field, such as its angular speed and magnitude. We also examine the role of the edge of the disc in defect generation, the flipping transition, and backflow effects (the effects of coupling between the liquid crystal director field and the velocity field) on the motion of the disc. In addition to seeing a simple flipping behavior similar to the one from the experiment, we observe and analyze more complicated situations when the disc demonstrates a mix of flipping motion and rotational motion of the face of the disc. We also observe a different way for the disc to release the distortion rather than to spin in the case of rapidly rotating magnetic fields — by creating a defect line.

3.1 Simulation Parameters

Table 3.1: The simulation parameters used for simulations of this chapter are given here.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>LC parameters</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( A_0 )</td>
<td>0.5</td>
<td>( atm )</td>
</tr>
<tr>
<td>( \gamma )</td>
<td>3.2</td>
<td>—</td>
</tr>
<tr>
<td>( K_1, K_2, K_3 )</td>
<td>9.5, 5.1, 13.8</td>
<td>( pN )</td>
</tr>
<tr>
<td>( K_1 = K_2 = K_3 = K )</td>
<td>10.7 or 15.0</td>
<td>( pN )</td>
</tr>
<tr>
<td>( \Gamma )</td>
<td>0.33775</td>
<td>( (atm \cdot \mu s)^{-1} )</td>
</tr>
<tr>
<td>( \xi )</td>
<td>0.75 or 0.52</td>
<td>—</td>
</tr>
<tr>
<td>( dx )</td>
<td>0.0625</td>
<td>( \mu m )</td>
</tr>
<tr>
<td>( \Delta t )</td>
<td>1</td>
<td>( \mu s )</td>
</tr>
<tr>
<td>( P_0 )</td>
<td>1.0</td>
<td>( atm )</td>
</tr>
<tr>
<td>( \tau_f / \Delta t )</td>
<td>0.56</td>
<td>—</td>
</tr>
<tr>
<td>( \tau_G / \Delta t )</td>
<td>0.25</td>
<td>—</td>
</tr>
<tr>
<td><strong>Disc</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>radii R</td>
<td>0.21—2.4</td>
<td>( \mu m )</td>
</tr>
<tr>
<td>thickness L</td>
<td>0.0308—0.21</td>
<td>( \mu m )</td>
</tr>
<tr>
<td>number of nodes</td>
<td>298—40162</td>
<td>—</td>
</tr>
<tr>
<td>strength of anchoring ( \alpha_s )</td>
<td>0.2—0.9</td>
<td>—</td>
</tr>
</tbody>
</table>

Parameters used in the simulations in this chapter are provided in table 3.1. All values used for simulation in this chapter were rescaled to have units of pressure (\( atm \)), time (\( \mu s \)) and length (\( \mu m \)). The simulation domain in each direction was at least 6 times bigger than the radius of the disc to reduce boundary effects. We tested a small number of simulations with a larger box and found no qualitative difference. The \( xy \)-plane had periodic boundaries in both directions. Rigid walls were located at \( z = -l/2 \) and \( z = l/2 \), where \( l \) is the height of the domain. Boundary conditions on the walls, director along the \( x \)-axis, will result in equilibrium conditions for the director of \( \hat{n} = (1, 0, 0) \) throughout the simulation domain. A disc with homeotropic anchoring on the surface
was initially placed in the middle of the domain with its normal also along the \(x\)-direction (fig. 3.1a; later figures show the top views of the shaded section). The magnetic field starts along the \(y\)-direction (\(\vartheta_{MF} = 0^\circ\), also the direction of magnetic moment of the disc) and then rotates in the \(xy\) plane by a small amount, \(0.0001^\circ \to 0.05^\circ\) every time step or \(1.7 \text{ rad/s} \to 872.5 \text{ rad/s}\), until it reaches the final position \(\vartheta_{MF}^{\text{stop}} \in [120^\circ, 180^\circ]\).

### 3.2 Slow Rotation of Magnetic Field

#### 3.2.1 Capacitance measurements

We first investigate the situation for small rotations. Without any external forces, a disc with homeotropic anchoring aligns itself in such a way that the surface normal \(\hat{a}\) is parallel to the far field director \(\hat{n}\) (fig. 3.1a). There is no distortion observed in the liquid crystal except for the distortion around the edges for the edged representation (see fig. 2.5) due to the conflict between surface conditions as was discussed in sec. 2.3.2.1. When the magnetic field \(B\) is switched on, \(B\) is parallel to \(\mu\) initially (along the positive \(y\)-axis) and and then starts turning, the nickel disc reacts to it and rotates to an angle \(\theta\) (angle between \(\hat{n}\) and \(\hat{a}\)) at which all torques are balanced, leading to a distortion of the director field (see fig. 3.1b) that costs elastic energy. This distortion appears in order to satisfy the homeotropic anchoring conditions on the surface of the disc and adds an elastic torque \(\tilde{\Gamma}\) to the system. When \(Q\) is uniaxial and defect-free, the elastic energy (1.11) can be written in the following form for the static equilibrium case [14]

\[
F_{\text{elastic}} = \frac{1}{2} [K_1 (\nabla \cdot \hat{n})^2 + K_2 (\hat{n} \cdot \nabla \times \hat{n} + K_3 (\hat{n} \times \nabla \times \hat{n})^2)].
\]  

(3.1)

For the one elastic constant approximation \((K_1 = K_2 = K_3 = K)\) and director \(\hat{n}\) of the form \(n_x = \cos \theta \sin \psi, n_y = \sin \theta \sin \psi, n_z = \cos \psi\) (3.1) can be written as

\[
F_{\text{elastic}} = \frac{1}{2} K [((\nabla \psi)^2 + \sin^2 \psi \ (\nabla \tilde{\theta})^2
+ 2 \sin \psi \hat{n} \cdot \{\nabla \tilde{\theta} \times \nabla \psi\}].
\]

(3.2)

Minimizing this with respect to the angles gives the following equations of static equilibrium [48]:

\[
\nabla^2 \psi - \sin \psi \cdot \cos \psi \cdot (\nabla \tilde{\theta})^2 = 0,
\sin \psi \nabla^2 \tilde{\theta} + 2 \cos \psi \ (\nabla \psi \cdot \nabla \tilde{\theta}) = 0.
\]

(3.3)

Assuming that for \(\theta < \frac{\pi}{2}\) the disc rotation does not produce out of plane distortions (i.e. \(n_z = 0\) and \(\psi \equiv \frac{\pi}{2}\)), eqn. (3.3) simplifies to a Laplace equation

\[
\nabla^2 \tilde{\theta} = 0.
\]

(3.4)
3.2. Slow Rotation of Magnetic Field

Figure 3.1: Schematic representation of a disc with perpendicular anchoring: a) No external forces are acting on the system; b) Disc is rotated by $\theta < \frac{\pi}{2}$; c) Director field is highly distorted when the disc is rotated by $\theta > \frac{\pi}{2}$ and is about to flip; d) configuration is stable after the transition. Pictures b-d, adapted from [2], are top views.
For \( \frac{R}{L} \to \infty \) the disc can be approximated as an oblate spheroid and under this assumption (3.4) can be solved analytically with the following coordinate change [158]:

\[
\begin{align*}
  z &= a\xi \eta, \\
  x &= a\sqrt{(\xi^2 + 1)(1 - \eta^2)} \cos \varepsilon, \\
  y &= a\sqrt{(\xi^2 + 1)(1 - \eta^2)} \sin \varepsilon,
\end{align*}
\]

where \( \xi \in [0, \infty) \), \( \eta \in [-1, 1] \), \( \varepsilon \in [0, 2\pi] \) and \( a = \frac{L}{2} \sqrt{\frac{(2R)^2}{L} - 1} \) is an inter-focal distance. Then the solution of (3.4) is

\[
\tilde{\theta} = \theta \frac{\cot^{-1}(\xi)}{\cot^{-1}(\xi_0)},
\]

where \( \xi = \xi_0 \) defines the oblate spheroid surface and \( \theta \) specifies the orientation on the surface of the disc: \( \hat{n}^0 = (\cos \theta, \sin \theta, 0) \). Integrating the elastic energy (3.2) from the static equilibrium over all space excluding the disc, we get

\[
U_{\text{elastic}} = \frac{K}{2} \int dV (\nabla \tilde{\theta})^2 = 2\pi Ka\theta^2 \left[ \tan^{-1} \frac{1}{\xi_0} \right]^{-1},
\]

corresponding to the formula for the potential of an oblate spheroidal particle immersed in the nematic liquid crystal. The analogy between the elastic free energy of the nematic liquid crystal and the electrostatic field energy of an object at a fixed potential [57,149] (\( \tilde{\theta} \) has the similar meaning to the potential) together with the experiment studies [101] suggest that the elastic energy varies with the angle of orientation \( \theta \) as

\[
U = 2\pi KC\theta^2,
\]

where in analogy to electromagnetism, \( C \) stands for the “capacitance” of the colloidal particle. Comparing equations (3.7) and (3.8) and then using (3.5), we can see that

\[
C = a \left[ \tan^{-1} \frac{1}{\xi_0} \right]^{-1} = \frac{L}{2} \sqrt{\frac{(2R)^2}{L} - 1} \left( \tan^{-1} \left( \sqrt{\frac{(2R)^2}{L} - 1} \right) \right)^{-1}.
\]

An alternative calculation of the capacitance of a finite-length conducting cylindrical tube, which can only be worked out approximately, was derived by Butler and Jackson [159,160] for \( \frac{R}{L} \gg 1 \):

\[
C = 4\pi^2 \frac{R}{\log \frac{32R}{L}}.
\]

Equation (3.8) implies a linear dependence between the elastic torque \( \tilde{\Gamma} = \frac{\partial U}{\partial \theta} \) and the orientation of the disc defined by \( \theta \) when there is no out-of-plane distortion. We test this relationship using simulations with the edgeless disk and one elastic constant,
3.2. Slow Rotation of Magnetic Field

Figure 3.2: Capacitance as a function of thickness and radii of the disc. Open markers (triangles and squares) are results from our simulations whereas the line is the analytical prediction of eqn. (3.9) for an oblate spheroid. For a given $2R/L$, the open triangles correspond to a faster rotation than the open squares, which are faster than the open squares with the x. Inset: The dependence of the elastic torque on the angle $\theta$ of rotation of the disc. It is linear when the rotation angle $\theta$ is small, disc is small, and the magnetic field is turning slowly (hollow diamonds); if the magnetic field rotates too fast (hollow circles) the linear dependence is violated and that leads to deviations in capacitance (dotted lines shows linear fits).
$K = 15.0 \text{ pN}$ (for all simulations in this section backflow effects are not included as we are examining the static limit; net forces due the surface anchoring (2.68) are off since the symmetry implies no net displacement of the center of mass). A couple of examples of the resulting torque versus $\theta$ is shown in the inset of Figure 3.2. It can be seen from the inset of Figure 3.2 that our simulation produces a smooth linear relationship between $\tilde{\Gamma}$ and $\theta$ when the magnetic field turns slowly enough (i.e. for $2R/L = 4, 8.7 \text{ rad/s}$), i.e. the static limit of elastic energy appears to be achieved. Measuring the slope of the torque $\tilde{\Gamma}$, one can measure the value of the capacitance of the disc using the equations

$$\tilde{\Gamma} = \frac{\partial U}{\partial \theta} = 4\pi KC\theta \Rightarrow \frac{\partial \tilde{\Gamma}}{\partial \theta} = 4\pi KC. \quad (3.11)$$

However, when the magnetic field turns rapidly, this linear dependence is violated (Figure 3.2, $2R/L = 56, 87 \text{ rad/s}$ in the inset) and this formula gives poorer results. The angular velocity of the magnetic field where deviations from the static results occur depends on the size of the disc, strength of anchoring on the surface, and magnitude of the magnetic field. The smaller the disc is, the faster the magnetic field can rotate without violating the linear dependence of elastic torque on $\theta$. For example, for a disc with $R = 0.27 \mu m, L = 0.075 \mu m$ and magnetic field $|B| = 6 \text{ G}$ that rotates at $0.005^\circ/\mu s$, a linear dependence is found, but the same magnetic field acting on a disc with $R = 2.07 \mu m$ and $L = 0.075 \mu m$ results in a non-linear dependence. The non-linearities are a result of the fact that the simulations include the dynamics, resulting in hydrodynamic effects that are dependent on the size of the disc and its rotational velocity. Figure 3.2 shows the results of simulations (symbols) with discs of different radii $R$ and thickness $L$ ($R$ varied from $0.2 \mu m$ to $2.4 \mu m$ while $L$ varied from $0.075 \mu m$ to $0.21 \mu m$). In all cases, a linear fit of the values of $\tilde{\Gamma}$ versus $\theta$ obtained in the simulation was used to obtain the capacitance, using the known elastic constant (i.e. this is an “average” slope when $\tilde{\Gamma}$ versus $\theta$ is non-linear). The solid line gives the formula for the capacitance of the oblate spheroid (3.9). It can be seen from Figure 3.2 that the simulations for small discs ($2R/L < 30$) give good agreement with the theoretical predictions. Discs of bigger radius require the magnetic fields to turn more slowly to satisfy the linear dependence of torque with respect to $\theta$ and determine a capacitance in agreement with theoretical predictions, which essentially assumes a static director field (compare squares with triangles). Figure 3.2 for the most slowly rotating discs does give a linear dependence of $2C/L$ on $2R/L$, although the effective capacitance is slightly larger for the edgeless disc than for the oblate spheroid. We have taken into account the effects of discretization in Fig. 3.2 as the discretization “spreads” the disc nodes making it effectively slightly larger [161] by about $\Delta x/3$.

If the capacitance of the disc is known, along with the direction and magnitude of the magnetic field, one could measure the rotation of the disc to find the elastic constant $K$, similar to what has been suggested for rods [57].
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Figure 3.3: The simulation of the motion of the edgeless disc under the action of turning magnetic field. Panels I, II correspond to the case of no backflow, II gives detailed views of the disc motion during the flip. The snapshots are a cross-section near the center of the simulation domain viewed from above with the disc in the center (disc is represented by spheres located at the positions of the nodes; the spheres are made about 2 times larger than the real node size for better visibility). Dark blue areas would indicate the position of a disclination line defect, light-blue contour around the disc is a high level of distortion (“softening”), and gray cloud exhibits a light disturbance. The green arrow indicates the direction of the magnetic field. The director appears shorter near the disc in f, g because it is pointing out of the plane. The insets in Panel I show director “streamlines” in the vicinity of the disc. These “streamlines” are everywhere parallel to the local director field and demonstrate the director behavior around the disc during the flip. As can be seen, the motion undoes the bend in the streamlines without breaking or kinking them (i.e. no defect is created).
Figure 3.4: The simulation of the motion of the edgeless disc under the action of turning magnetic field. Panels III, IV show the results of the simulation where the backflow effects are on, III shows motion of the disc during the flip. The snapshots are a cross-section near the center of the simulation domain viewed from above with the disc in the center (disc is represented by spheres located at the positions of the nodes; the spheres are made about 2 times larger than the real node size for better visibility). Dark blue areas would indicate the position of a disclination line defect, light-blue contour around the disc is a high level of distortion ("softening"), and gray cloud exhibits a light disturbance. The green arrow indicates the direction of the magnetic field. The director appears shorter near the disc in f, g because it is pointing out of the plane.
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3.2.2 Flip

The equivalence of both directions of the nematic director $\hat{n}$, $+\hat{n}$ and $-\hat{n}$, implies the torque on a colloidal particle in equilibrium should be symmetric about $\theta = \frac{\pi}{2}$. However, the experiments on rods immersed in nematic liquid crystals [101] show that the torque continues to increase linearly as $\theta$ increases past $\pi/2$ caused by the metastability of the distorted state (similar to fig. 3.1, c) and followed by a spin of a wire along its long axis by $180^\circ$ at $\theta \approx \pi$. In contrast, the disc with homeotropic anchoring under the same conditions behaves differently [2] (see fig. 3.1c,d). When $\frac{\pi}{2} < \theta < \pi$ the configuration becomes unstable, the surface normal $\hat{a}$ goes out from the plane of the picture and tilts so that the disc goes through a flipping motion much earlier than a rod.

To study this behavior of the disc we have looked at the changes in the director field, measured the critical angle $\theta$ at which the flip starts, analyzed the speed of the flip and rotation in the plane of the disc, and checked how the behavior of the disc changes depending on the magnitude and angular velocity of the rotating magnetic field. We were especially interested in possible defects in the liquid crystal that can be seen on the 3D plot by making a density plot of the largest eigenvalue $q$ of the tensor order parameter $Q$.

The results of our simulations are presented in figures 3.3, 3.4, and figures 3.9, 3.10. These figures show the cross-section of the middle part of the simulation domain, viewed from above, with a disc in the center. Figures 3.3, 3.4 demonstrate the disc with the edgeless representation (fig. 2.5a), and fig. 3.9, 3.10 has the disc of the edged type (fig. 2.5b).

3.2.2.1 Slowly rotating edgeless discs

We now examine the complete rotation of the magnetic field where non-linear effects, such as the disc flipping are evident. Here we will focus on 2 specific realizations. Both of them are working with a "small" edgeless discs with $R = 0.3 \mu m$ and $L = 0.15 \mu m$ consisting of 634 nodes under the action of the same magnetic field of magnitude $0.5G$ and rotational frequency $0.005^\circ/1\mu s$ (or $87\ rad/s$) that rotates by $180^\circ$ from its original position along the $y$-axis. However, the simulation shown in fig. 3.3I, II does not include backflow effects, while the simulation with results shown in fig. 3.4III, IV has backflow. We look at these two cases because, first of all, it is useful for future simulations to know if the backflow is needed as it is a significant computational cost, and also comparison of two cases are of interest from physical point of view, to know the origin of some of the observed effects. Both simulations use the one elastic constant approximation with $K = 10.72\ pN$. The linear size of the simulation boxes is 6 times larger than the disc radius in all directions.

No backflow. Initially the surface normal of the disc is parallel to the director field and no distortion in the liquid crystal is observed (fig. 3.3Ia). Then the magnetic field is switched on, initially aligned with the magnetic moment of the disc $\mu$, and starts to turn, followed by the disc rotating, geared towards minimizing the distortion torque as was discussed in the previous section 3.2.1. During this motion the director field around the disc is distorted but no defects are observed (fig. 3.3Ib and Ic). The disc slows down after getting through $\theta \sim \frac{\pi}{2}$. As $\theta$ increases further, the distortion area enlarges, and,
at a critical angle $\theta_{\text{crit}}$, the disc starts to flip (fig. 3.3Id and 1e). The “softening” cloud (very slight decrease in the largest eigenvalue, but not enough to create a defect) around the disc during the flip firstly grows and then collapses back on the surface of the disc (pictures e-g in fig. 3.3I). The final position of the disc corresponds to a less distorted director field and, thus, to a smaller free energy of the system.

To better understand the flipping motion of the disc, we study the time dependence of angles associated with the disc. We first examine the angle $\beta_{yz}$, that is the angle between the $z$-axis and the projection of the surface normal $\hat{a}$ on the YZ plane, i.e. the plane perpendicular to the far-field director $\hat{n}$, as was done in the experimental study [2] (see fig. 3.5a). Results for $\beta_{yz}$ for different discs and various magnetic fields are presented in fig. 3.6. It can be seen that our results here are similar to experiments [2]: sigmoidal shape dependence of $\beta_{yz}$ as a function of time. However, using this angle alone works well only for a description of simple flipping motion with big $\theta_{\text{crit}}$ and with only insignificant rotational motion of the disc face. For example, in fig. 3.6, the dashed orange line with filled symbols corresponds to a simulation in which the second half of the flip happens in the XZ plane and results in a different form of the curve; however, using other angles like $\beta$ (to be introduced below), shown in the inset, demonstrates that this simulation does not actually differ from the others. We found two other angles, $\beta_{xy}$ and $\beta$, more informative for the purpose of our analysis. The first of them, $\beta_{xy}$, is the angle between

![Diagram](https://via.placeholder.com/150)

**Figure 3.5:** Schematic explanation of the angles used for motion analysis throughout the article: a) angles related to projecting surface normal $\hat{a}$ on YZ plane, b) angles related to the projection of $\hat{n}$ on XY plane.
3.2. Slow Rotation of Magnetic Field

Figure 3.6: The dependence of angle $\beta_{yz}$ on time for different edgeless discs and magnetic fields; inset: angle $\beta$ for the same simulations. Origin of time is set to the location of the extrema of $\beta$. Until the surface normal goes out of plane $\beta_{xy}$ tracks $\pi - \theta$, before increasing again towards $\pi$ during the flip. Results for this increase are shown on fig. 3.7b. For the second angle determined by $\beta = \arccos(\hat{a} \cdot \hat{k})$, where $\hat{k}$ is a unit vector along the $z$-axis, results are presented on fig. 3.7c. One should remember that discs in all simulations do not start to flip at the same time but rather unless otherwise noted, the time scale was shifted to 0 at the minimum (or maximum) value of $\beta$ (discs can flip both clockwise or counter clockwise) during the flip. The angle at which the disc flips, $\theta_{\text{crit}}$ is plotted in fig. 3.7a. $\theta_{\text{crit}}$ depends on the size of the disc, angular speed and magnitude of magnetic field $|\mathbf{B}|$, and its maximum rotation angle $\theta_{\text{stop}}^{MF}$. As can be seen, increasing $|\mathbf{B}|$, with other factors constant, generally increases the critical angle (the disc flips later). A weaker trend is seen with increasing angular frequency decreasing $\theta_{\text{crit}}$.

In the experiment the magnetic field set-up and abrupt motion implies a symmetric
Figure 3.7: a) Dependence of the angle at which the disc flips $\theta_{\text{crit}}$ versus $|B|$ for different systems. b) The dependence of angle $\beta_{xy}$ on time for different edgeless discs and magnetic fields. Time is shifted to have 0 at the minimum of $\beta$. Legend for (b)-(c) plots is shown in c.)
Figure 3.7 (Continued): c) The dependence of angle $\beta$ on time for the same simulations as in b). d) The time dependence of angle $\varphi^{\text{rot}}$ for the same simulations as in b) and c). Time is shifted to have 0 at the minimum of $\beta$. Legend for (b)-(c) plots is shown in c).
position of the disc just before and right after the flip, i.e. \( \beta_{yz} \) and \( \beta_{xy} \) changes by \( \pi \), while in our case the positions of the disc before and after the flip are not symmetric due to the difference in the motion of the magnetic field. However, a symmetric flip can be obtained by making the disc go through the flipping motion when \( \mathbf{B} \) is parallel to \( \mathbf{\mu} \) by tuning the magnetic field: by increasing the magnitude of the magnetic field, the disc rotates by \( \pi \) compared to lines with smaller squares that represent the results for weaker magnetic fields (e.g. fig. 3.7b, squares). The case of a symmetric position of the disc right before and after the flip would correspond to \( \min(\beta) \rightarrow 0 \) in fig. 3.7c. Looking at these plots and comparing the lines with open squares (they correspond to the same simulations except for the magnitude of magnetic fields), we can conclude that by tuning only the magnitude of magnetic field it is possible to control the moment of the flip and the final position of the disc. Also, as seen in fig. 3.7b, since the inclination of the lines is bigger for stronger magnetic fields, the speed of flipping is higher when the magnitude of the magnetic field is bigger, which means that the flipping is faster for larger \( \theta_{\text{crit}} \) (disc’s rotational angle at which flip starts, Fig. 3.7a). One may also note from fig. 3.7c that plots are not perfectly symmetric with respect to \( t = 0 \). That means that the first half of the flip goes faster, while after getting to the minimum value of \( \beta \), flipping slows down. This is probably due to the fact that even though there is no backflow, there are hydrodynamic forces and the disc has to push the fluid out of the way during the motion and this is harder in the initial stages of the flip when the fluid is not already moving in the right direction.

Fig. 3.7d demonstrates the rotational properties for the same simulations as in fig. 3.7b and c via plotting the time dependence of an angle \( \varphi^{\text{rot}} = \arccos(\hat{\mathbf{k}} \cdot \mathbf{\mu}) \), where \( \hat{\mathbf{k}} \) is a unit vector along \( z \)-axis (see fig. 3.5). Here by rotational properties we mean the properties of the rotational motion of the disc face, that can be easily seen by tracking the specially marked green particle in fig. 3.3II and measured by angle \( \varphi^{\text{rot}} \). The plot in fig. 3.7d demonstrates that stronger magnetic fields acting on the discs provoke more rotation and that discs can rotate both ways (compare, for example, the line with hollow circles with filled circles line and lines with empty squares). From this picture we can also conclude that for the edgeless discs \( \varphi^{\text{rot}} \) tends to go to \( \pi/2 \) at the end of simulation, meaning that there is no tilt in the disc position in the end.

**With backflow.** All the results demonstrated above do not include backflow effects, which means the orientation of the liquid crystal particles does not affect the velocity field. However, as demonstrated in [69] and [72], backflow may play a significant role in the motion of liquid crystals. By visual comparison of fig. 3.3I and fig. 3.4IV, it is easy to see that there are differences in results for simulations without backflow effects and with them, although the qualitative flipping behavior is present in both simulations. First, the distortion cloud around the disc during the flip for the case with backflow is smaller (lighter coloring in the density plot of the largest eigenvalue of the tensor order parameter \( Q \) corresponds to less disorder) because backflow effects allow the disc to move fluid to relax the distortion. This appears to result in more rotation in the plane of the face of the disc as discussed below (rotation is easy to see from figures II and III in figures 3.3 and 3.4). Second, \( \theta_{\text{crit}} \), describing the position of the disc right before the moment when
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Figure 3.8: Comparison of $\beta_{xy}$ for simulations with/without backflow. Dashed lines correspond to no backflow, continuous - with backflow. The simulations are performed on the edgeless disc of $R = 1.02 \mu m$, $L = 0.0616 \mu m$ consisting of 7250 nodes under action of magnetic field of magnitude $4G$ rotated by $180^\circ$. The inset shows the rotational motion measured by $\varphi^{rot}$ for the same simulations.

the flip begins, is different: compare fig. 3.3Id with fig. 3.4IVd and snapshots of disc positions in fig. 3.3II and fig. 3.4III. By looking at this figure and tracking the motion of the specially marked green particle, one notices that both discs shown in rows II and III demonstrate not only flipping but also a distinguishable rotational motion of the disc face. To measure quantitatively this face rotational behavior, we again plot the time dependence of $\varphi^{rot} = \arccos \left( \frac{\hat{k} \cdot \mu}{|\mu|} \right)$, where $\hat{k}$ is again a unit vector along the $z$-axis (see fig. 3.5). The inset of fig. 3.8 compares the levels of rotation for similar simulations with and without backflow. It can be seen that backflow forces stimulate more rotational motion of the disc face. On the graph of $\beta_{xy}$ with respect to time in fig. 3.8, we can compare the dashed line (without backflow) to the solid line (with backflow effects): there is a significant difference in results that emphasizes the necessity of backflow for accurate predictions of the disc’s motion. Though results without backflow provide qualitatively similar flipping behavior, to predict the moment of the beginning of the flip and position of the disc after it, backflow effects are vital.
Figure 3.9: The simulation of the motion of the edged disc under the action of turning magnetic field. Pictures I, II correspond to the case of no backflow. II gives detailed views of the disc motion during the flip. The snapshots are a cross-section near the center of the simulation domain viewed from above with the disc in the center (disc is represented by spheres located at the positions of the nodes; the spheres are made about 2 times larger than the real node size for better visibility). Dark blue areas indicate the position of a disclination line defect (discontinuities in this line are a result of a graphic projection: the line is a physically continuous loop around the edge of the disc), light-blue contour around the disc is a high level of distortion ("softening"), and gray cloud exhibits a light disturbance. The green arrow indicates the direction of the magnetic field. The director appears shorter near the disc in e-g because it is pointing out of the plane.
Figure 3.10: The simulation of the motion of the edged disc under the action of turning magnetic field. Pictures III, IV demonstrate the results of the simulation where the backflow effects are on. III shows motion of the disc during the flip. The snapshots are a cross-section near the center of the simulation domain viewed from above with the disc in the center (disc is represented by spheres located at the positions of the nodes; the spheres are made about 2 times larger than the real node size for better visibility). Dark blue areas indicate the position of a disclination line defect (discontinuities in this line are a result of a graphic projection: the line is a physically continuous loop around the edge of the disc), light-blue contour around the disc is a high level of distortion ("softening"), and gray cloud exhibits a light disturbance. The green arrow indicates the direction of the magnetic field. The director appears shorter near the disc in e-g because it is pointing out of the plane.
3.2.2.2 Slowly rotating \textit{edged} discs

In this section we look in detail at 2 simulations. The first one corresponding to fig. 3.9I \\
& II has an edged disc of $R = 0.3 \mu m$ and $L = 0.09 \mu m$ that consists of 634 nodes; the disc is under the action of a rotating magnetic field of magnitude $0.25G$ that rotates at $0.001^\circ/1 \mu s$ (or $17.325 \text{ rad/s}$) and stops at $160^\circ$ with respect to $+y$-axis. This simulation does not include backflow effects and uses the one elastic constant approximation with $K = 10.72 pN$. The discs’ center-of-mass does not move appreciably during the simulation implying that the net force remains negligibly small. The linear size of the simulation boxes is 6 times larger than the disc radius in all directions. The second simulation, results of which are shown in fig. 3.10III & IV works with the same disc and same magnetic field, but has backflow acting on the system. Both discs demonstrate flipping behavior similar to the edgeless discs described in the previous section: at the beginning of the simulation the surface normal $\hat{\mathbf{a}}$ is parallel to the far-field director $\hat{\mathbf{n}}$; when the magnetic field is switched on, the disc follows its rotation (fig. 3.9Ib-d and fig. 3.10IVb-d) and then flips to reduce the free energy of the system (fig. 3.9Ie-i and fig. 3.10IVe-i).

These simulations indicate that there are no line defects observed in the liquid crystal except for on the edge of the disc (due to the conflict between the surface conditions on the bases and on the cylindrical surface, not present on the edgeless representation). Further, the presence of the defect line around the edged disc results in less distortion away from the disc, compared to the edgeless representation (see, for example, fig. 3.3Ie versus fig. 3.9Ie). As the disc flips, there is a spherical region around the disc where the director tilts out of plane to accommodate the normal anchoring on the face of the disc. For the edged representation, with the defect line, this spherical region has almost exactly the same radius as the disc itself (fig. 3.9If), whereas for the edgeless representation this region is quite a bit larger than the disc (seen in fig. 3.3Ig). This has to do with the way the distortion is handled by the edgeless disc. In the absence of a disclination line, there is a flattened S-shaped (or O-shaped) distortion with the middle of the S tangential to the disc edge (c.f. fig. 3.3Ic-f fig. 3.4IVc-f). This is in contrast to the edged configuration where the presence of the disclination localizes the distortion right at the disc edge. These observations appear, at first glance, to potentially be at odds with the experiments [2] where a defect line seems to appear. We do not believe this to be the case, however, and will discuss this in more detail in Section 3.2.2.5.

The time dependence of the angles $\beta_{xy}$ and $\beta$ for simulations performed without backflow dynamics, shown in fig. 3.11a demonstrates, similar to the edgeless discs, that the speed of the flip is higher for a bigger magnetic field. However, for strong magnetic fields that were rotated by $180^\circ$ (lines with two largest circle markers shown in red and purple), hydrodynamic effects that are not observed in simulations for edgeless discs can be seen: the disc overshoots after it reaches its maximum $\beta_{xy}$, similar to the effect of optical bounce described in [162]. However, fig. 3.11a shows this is not the case for (i) fields rotated by a smaller angle, i.e. by $120^\circ$ or $160^\circ$: see line without markers; (ii) and weaker magnetic fields, whatever the final position of the magnetic field is (compare the two lines with the smallest circle markers). Results for $\beta = \arccos(\hat{\mathbf{a}}.\hat{\mathbf{k}})$ in fig. 3.11b demonstrate that discs may flip both clockwise and counter clockwise. This implies that edged discs are very sensitive to even small changes in distortion. Also, edged discs tend
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Figure 3.11: The dependence of the angles (a) $\beta_{xy}$, (b) $\beta$, and (c) $\varphi^{\text{rot}}$ on time for different magnetic fields acting on the edged disc of $R = 1.02 \mu m$, $L = 0.0616 \mu m$ consisting of 8534 nodes. Time is shifted to have 0 at the minimum of $\beta$ in all cases and the legend for all plots is shown in b).
Figure 3.11 (Continued): The dependence of the angles \( \beta_{xy} \), \( \beta \), and \( \varphi^{\text{rot}} \) on time for different magnetic fields acting on the edged disc of \( R = 1.02 \mu m \), \( L = 0.0616 \mu m \) consisting of 8534 nodes. Time is shifted to have 0 at the minimum of \( \beta \) in all cases and the legend for all plots is shown in b).
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to stay a bit tilted in their final position when $\theta_{MF}^{\text{stop}} = 180^\circ$ ($\beta$ is not tending to reach $\pi/2$, while edgeless discs are approaching $\pi/2$, as seen in Fig 3.7d).

Though inclusion of the backflow effects in the simulation does not change the qualitative flipping behavior, similar to edgeless discs, it changes the position of the disc before the beginning of the flip (fig. 3.10IVd and fig. 3.9Id). Figures 3.9II, 3.10III give more snapshots of the flip, where II has no backflow and III has backflow. From this figure it is easy to see that the two discs start the flip at different positions, then during the flip one of them rotates clockwise and the other one - counter clockwise; then they finish at the same position (forced by magnetic field) but the disc that was also under action of backflow is a mirror image of the disc on fig. 3.9 vs fig. 3.10 (darker and lighter sides of the disc got switched). The quantitative analysis of rotational motion for both simulations, i.e. the time dependence of $\phi^{\text{rot}}$, is similar to that shown in the inset of fig. 3.8: backflow leads to more rotation. The same dependence for other discs under action of various magnetic fields is demonstrated on fig. 3.11c.

These results show that the edged disc’s flipping motion, position before and after the flip, and velocity of the flip can be controlled by only tuning the magnitude of magnetic field and its angular velocity. As for backflow effects, they are more important for edged discs than for edgeless discs. They change the disc’s position before and after the flip, and the flipping motion itself by adding more rotation. Thus, for accurate predictions of the motion of the disc, backflow effects have to be taken into account for both edged and edgeless discs.

Figure 3.12: Comparison of $\beta_{xy}$ for simulations on edgeless vs edged discs. The discs have $R = 1.02 \mu m$, $L = 0.0616 \mu m$. 
3.2.2.3 Edgeless vs. edged representation

We also looked at how switching from an edgeless representation to the edged one changes the dynamics of the disc. In fig. 3.12 results for two discs are shown. Red dotted lines correspond to the discs of the same size ($R = 1.02 \mu m$, $L = 0.0616 \mu m$) under the action of the same magnetic field (0.8G rotates $0.02^\circ/1\mu s$, i.e. 346.5 rad/s), but the one with filled triangles has a disc with additional particles on the cylindrical surface (edged representation, number of nodes in the object is 8534) compared to dotted line without any markers (edgeless disc consisting of 7250 nodes). As expected, the final position and the flip velocity has changed by shifting from the edgeless disc to the edged one, meaning that the anchoring on the edge of the disc affect the dynamics even for thin discs.

3.2.2.4 Simulations with different elastic constants

We now relax the one-elastic constant approximation and do a simulation with $K_1 = 9.5 \ pN$, $K_2 = 5.1 \ pN$, and $K_3 = 13.8 \ pN$. Comparison of simulations performed with one elastic constant approximation to simulations where $K_1 \neq K_2 \neq K_3$ on different edgeless and edged discs affected by various magnetic fields shows that the behavior of the disc is similar, except that the distortion spreads much further from the disc (easily seen on the edges of the domain on fig. 3.13, b vs e). This is probably due to the fact that for the unequal elastic constants case we examined, $K_2$ was smaller ($K_2 = 5.1 \ pN$ versus 10.72 $pN$ in the one-elastic constant case) even though the average elastic constant was similar. The system takes advantage of the weakest elastic constant and concentrates any distortion that can be accommodated by twist (corresponding to $K_2$) rather than splay or bend. Similar effects were found for rods in [57]. An additional effect of this weaker distortion mode is that the disc rotates slightly further before the distortion energy has built up enough to induce a flip (a disc from the one elastic constant approximation rotates by about $105^\circ$ compared to $107^\circ$ for the different elastic constants case). This also takes more time because the disc also rotates more slowly as $\theta$ increases (almost two times more: 175415 $\mu s$ for different $K$s vs 83036 $\mu s$ for the one elastic constant case). After the flip both simulations behave similarly and the final positions of the discs are very close (fig. 3.13, c and f show the end of simulation when the flip is almost done). Considering that switching to the one elastic constant approximation does not qualitatively change the main features of the dynamics but saves computational time, the simulations in the following chapter are performed within this approximation.

3.2.2.5 Light transmission

To analyze the optical effects of the disc’s flipping motion and to provide detailed interpretation of experimental results, the intensity of light going through the liquid crystal sample with a disc in it was studied. Our approach, details of which can be found below, has the advantage of choosing any view point (compared to the experimental set-up) and provides an opportunity to study how the light transmission changes from plane to plane and is affected by distortion and defects. Simulations in this section do not include backflow effects.
3.2. Slow Rotation of Magnetic Field

Figure 3.13: Three frames from simulations with the one elastic constant approximation with $K_1 = K_2 = K_3 = K = 10.72 \, pN$ (left column) and a simulation performed with $K_1 = 9.5 \, pN$, $K_2 = 5.1 \, pN$, $K_3 = 13.8 \, pN$ (right column), where the green arrow represents the direction of the magnetic field and the color scale of the largest eigenvalue is the same as on fig. 3.9. Time since beginning of simulation is at the bottom of each frame on the left, on the right the angle of disc rotation is shown. Both discs are edged and consist of 8534 nodes, have radius $R = 1.02 \, \mu m$ and thickness $L = 0.0616 \, \mu m$ and rotated under the action of a magnetic field $2 \, G$ with the same rotational velocity $0.04^\circ/1 \, \mu s$. 

- Same elastic constants
  - Frame a: 6209 $\mu s$, 43.1656
  - Frame b: 83036 $\mu s$, 105.356
  - Frame c: 368440 $\mu s$, 143.7067

- Different elastic constants
  - Frame d: 6318 $\mu s$, 43.1642
  - Frame e: 175415 $\mu s$, 107.368
  - Frame f: 830631 $\mu s$, 143.7604
Figure 3.14: The calculation scheme of the intensity of light, going through the liquid crystal with disc represented by the red dots immersed in it.

To study light transmission, each simulation layer of the liquid crystal along the $z$ direction was considered to be a polarizer with the input amplitude of light $\bar{A}_s^{in} = \bar{i}_i|A_s^{in}| + \bar{j}_j A_s^{in}$ defined at each point $(i,j)$ of the site mesh on the layer $s$ consisted of a component $||A^s$ in the $x$ direction and $\perp A^s$ in the $y$ direction and output amplitude $\bar{A}_s^{out} = \bar{i}_i|A_s^{out}| + \bar{j}_j A_s^{out}$ calculated via

$$\bar{A}_s^{out} = (\bar{A}_s^{in} - 1)^{(\bar{i}_i \cdot \bar{n}_s)}(\bar{j}_j \cdot \bar{n}_s)(1 - q) \cos^2 \theta.$$  

(3.12)

$\bar{A}_s^{out}$ is at the same time the input amplitude for the next layer (see fig. 3.14). Here $\hat{b}$ is a projection of the director $\hat{n}^s$ at the site mesh $(i,j)$ on the $xy$-plane, $\theta$ is the angle between the $z$-axis and director, $0 < q < 1$ is the corresponding eigenvalue of the tensor order parameter $Q$, $J$ is the orthogonal matrix.

Formula (3.12) has the following explanation. The first term calculates what part of the input light determined by $\bar{A}_s^{in}$ would propagate along the director of the layer $s$. We
3.2. Slow Rotation of Magnetic Field

Figure 3.15: Normalized intensity of light through the liquid crystal with the disc colloid in the middle (nodes of the disc are shown in orange) in crossed polarizers. On pictures (a) the results for an edged disc are presented ($R = 1.02 \mu m$ and $L = 0.0616 \mu m$ under action of magnetic field of magnitude $3G$ had a rotation frequency of $87 \ rad/s$). Pictures in (b) correspond to an edgeless disc of the same size and same conditions. The set of pictures (c) corresponds to a simulation with an edgeless disc of $R = 0.3 \mu m$ and $L = 0.15 \mu m$ and magnetic field $3G$ with rotation frequency of $87 \ rad/s$. Enlarged numbers on the gray scale are the values of plotted contours on both sets.

To treat each layer $s$ as a polarizer with a direction of polarization along the director $\hat{n}^s$. If the liquid crystal is perfectly aligned (that is equivalent to $q = 1$), no light perpendicular to the direction of polarization (i.e. $(\vec{A}_{in}^s \cdot (\vec{J}^s))(\vec{J}^s)$) would get through. However, liquid crystals are not perfect polarizers ($q < 1$) meaning that some leakage is always presented; this leakage is described in eq. (3.12) by the term $(1 - q)$. The last multiplier, $\cos^2 \theta$, is necessary to account for out-of-plane director orientations: when the director is pointing along the vertical axis, $Oz$, all the light would to get through (corresponds to $\theta = 0$ and $\cos^2 \theta = 1$); when the director is in the $xy$ plane, $\cos^2 \theta = 0$ and we just have the first term corresponding to polarization. Thus, $\cos^2 \theta$ varies between this two extreme cases, 0 and 1, and measures how much light would get through the areas where director has out-of-plane tilts that appears during the flip of the disc.

On the $0^{th}$ layer $\vec{A}_{out}^0 = \vec{i} \parallel A_{out}^0$ due to the presence of the light polarizer (or $\vec{A}_{out}^0 = \vec{i} \perp A_{out}^0$, depending on the type of polarizer). And, similarly, on the last ($N+1$)th layer where another polarizer is located, depending on if it is crossed with the first one or not, the output amplitude is $\vec{A}_{out}^{N+1} = \vec{i} \parallel A_{out}^N$ or $\vec{A}_{out}^{N+1} = \vec{i} \perp A_{out}^N$. If the disc is found to be on the way of the light beam, the transmitted light is extinguished and $\vec{A}_{out} \equiv 0$ at this $(i,j)$. Finally, the intensity of the light that got through the liquid crystal sample is...
calculated as the square of the amplitude from the last layer.

Results of these calculations are presented in fig. 3.15. Black means that no light is getting through, while white corresponds to transmittivity close to 100%. The distortion changes the amount of light that goes through the area resulting in light gray areas. These results can be compared to experimental pictures produced by Rovner et al. [2]. It can be seen that results of the simulations with the edgeless discs presented on fig. 3.15b, c provide a picture similar to the experimental ones and give details of the level of distortion in the area close to the disc surface. One notices the area corresponding to the value of normalized intensity \(0.95 - 1\) that appears right after the flip starts. The disc performs the flipping motion inside this area, which firstly grows and then shrinks back to the surface of the disc during the flip and disappears when the flip is completed. However, the pictures for the edged discs (fig. 3.15a) are different: the shell does not appear and the distortion stays closer to the surface of the particle. The defects on the edge of the disc “consume” part of the distortion and, thus, do not let it spread. Therefore, we can conclude, that the chemical treatment of the disc particle in the experiments of Rovner and co-workers [2] didn’t set strong or medium-strong perpendicular surface anchoring on the edge of the disc but rather set it either weak or left unchanged. Also their “defect” is probably an effect of the director changing from in-plane to out-of-plane as seen in fig. 3.3I. This will look similar to a defect line under the microscope, as we see here.

### 3.3 Rapidly Rotating Magnetic Field

All results discussed so far are for situations when the magnetic field was rotating fairly slowly. In this case both edged and edgeless discs rotate following the magnetic field and at an angle \(\theta_{\text{crit}}\) flip around the axis perpendicular to the axis of rotation. However, different behavior was observed for rapidly rotating magnetic fields for discs of both types of representation, edgeless and edged. Here “slowly” and “rapidly” angular velocities are relative and somewhat different for each disc depending on the type of representation, disc size and magnitude of magnetic field.

At high rotational velocities when the angle of the disc’s rotation \(\theta\) become greater then \(\pi/2\) and distortion around the disc grows, two symmetrical defects are formed on both sides of the disc (see fig. 3.16Ic and IIc). As can be seen from pictures Ic1-Ic2 and IIc1-IIc2 (the side views of the snapshots Ic and IIc), the defect for an edgeless disc is D-shaped, while the defect around the edged disc is C-shaped. The formation of the defects is probably due to the inability of the liquid crystal medium away from the edge to react rapidly to the changes in the orientation of the disc. After these defects are formed, they affect the liquid crystal director farther from the edge of the disc and reorient particles in that area leading to the disappearing of the S-shaped distortion (fig. 3.16Id and IIc) and relaxation of the distortion without flipping of the disc. After that, the disc aligns itself with the magnetic field (fig. 3.16Ie and IIe). Simulations from fig. 3.16 were performed with backflow, however this behavior was tested in simulations without backflow effects and similar results were obtained.
Figure 3.16: Snapshots of the top view of the simulations of edgeless (a) and edged (b) discs under action of a rapidly rotating magnetic field. The disc is shown in dark-to-light orange colors (disc is represented by spheres located at the positions of the nodes; the spheres are made about 2 times larger than the real node size for better visibility), and a green arrow represents the direction of magnetic field. Level of distortion is represented as color density plot of the largest eigenvalue of tensor order parameter $q$. Here dark blue areas indicate the position of a disclination line defect (discontinuities in this line are a result of the graphic projection: the line is a physically continuous loop around the edge of the disc), light blue contour around the defects is a high level of distortion ("softening"), and gray cloud exhibits a light disturbance. Additional pictures c1-c2 on I and II corresponds to the side views of snapshots number Ic and IIc and include sharper contours to better illustrate the shape of the defect lines.
3.4 Chapter Summary

To conclude, in this chapter we numerically studied the behavior of a disc-shape ferromagnetic colloidal particle in the nematic phase of a liquid crystal and demonstrated good agreement with experiments.

In this work we demonstrate how to measure the capacitance of an immersed disc particle with knowledge of the values of elastic constants of the liquid crystal. Or, vice versa, one could define the elastic properties of the liquid crystal if the capacitance of the immersed disc colloid is known.

At small deviations from the initial configuration, due to a slowly rotating magnetic field, the distortion of the director field can be predicted with help of equation (3.8). At large deviations it is hard to analytically predict the motion of the disc. In this work we have shown that the behavior under this situation can be controlled by the angular speed of the magnetic field and its magnitude. During our investigation, we showed that:

(i) the critical flipping angle depends on the angular velocity of the magnetic field and its magnitude,

(ii) for slowly rotating magnetic fields no defects are formed during the whole rotational and flipping motion (except for the areas at the edges of the disc due to the conflict in surface conditions),

(iii) the distortion during the flip stays mainly inside a softening cloud,

(iv) the size of the cloud strongly depends on the twist elastic constant of the liquid crystal and whether or not the anchoring is effective on the edge of the disc,

(v) the light transmission is strongly affected by the director pointing out of plane during the flip and this can give the (false) impression of a disclination line where the director is perpendicular to the plane of observation,

(vi) the flip may be avoided by increasing the rotational velocity of the magnetic field,

(vii) backflow effects are vital for calculations, while net forces may be neglected as the centre-of-mass does not move appreciably.

To sum up, this suggests a potential new approach for controlling colloidal interactions in liquid crystals and optical properties of colloidal disc sets.

We also want to emphasize that our results suggest the edgeless disc representation fits the experiments better than the edged representation for chemical treatments similar to the one performed by Rovner et al. [2]. After performing analysis of light transmission we can conclude that the line around the disc seen in the experiment that was interpreted as a defect is actually the edge of the area where the director is pointing out of plane.
4

Pairs of Discs in Nematic Liquid Crystal

“To know when to go away and when to come closer is the key to any lasting relationship.”

– Doménico Cieri Estrada

In Chapter 3 we studied the behavior of a disc in a nematic liquid crystal using the numerical algorithm described in Chapter 2. Calculations of the disc’s capacitance via simulations compared with analytical predictions, together with optical image analysis have demonstrated that the numerical algorithm we developed can be used to describe the dynamics of a disc in a nematic liquid crystal. The next step of this research is to move from a single particle to groups of discs. However, before simulations with multiple objects can be run, we need to update the algorithm: the algorithm described in chapter 2 and used in chapter 3 has no forces that would prevent two closely located discs from merging into one to minimize the distortion. After we include the force that would prevent particles from overlapping, we can start running simulations with multiple objects of any form (only an adjustment of a surface normal calculations would be required).

The previous chapter has also shown, that the edgeless disc representation provides better agreement with experiments compared to the edged representation, because it is very hard to perform a chemical/mechanical treatment to guarantee perpendicular anchoring on the edge surface. Due to that reason, all the simulations of this chapter are performed on thin edgeless discs.

The purpose of this chapter is to study potential interactions between the discs that present a special interest since they may lead to new methods of particles self-organization. The force between discs could change from repulsion to attraction depending on the distance between the objects and current configuration of the system (orientation of the liquid crystal molecules, local velocities, strength of the magnetic field, etc.).

This chapter is constructed in the following way: in the first section we introduce the repulsion forces into the model; the next section describes the setup of the simulations; results of simulations and some preliminary analysis are described in the subsequent sec. 4.3; chapter is finished with a conclusions section that summarize the results and
discuss potential future work.

4.1 Potentials for Objects Repulsion

The algorithm now can be expanded to be used for any number of disc-shaped objects, by only adding a short but finite range force between each pair of nodes representing the objects that would prevent objects from overlapping. This can be done, for example, by adding a hard shifted and truncated (as shown in fig. 4.1) Lennard-Jones potential from the standard LAMMPS package (pair_style lj/cut command):

\[
V(r) = 4\epsilon_{\text{well}} \left[ \left( \frac{\sigma_0}{r} \right)^{12} - \left( \frac{\sigma_0}{r} \right)^6 \right], \quad r < r_c
\]

where \( r \) is the distance between centers of mass of the particles, \( r_c \) is the cut-off radius (at distances larger than \( r_c \) the energy is set to 0), \( \sigma_0 \) is the zero-crossing distance for the potential (in our case it is the distance between the nodes of different discs, at which the repulsion appears; was set to be equal to \( 2dx \)), and \( \epsilon_{\text{well}} \) is called the depth of the potential well. The graph of this potential is shown in fig. 4.1 by the red dashed line.

![Figure 4.1: Potentials](image)

Figure 4.1: Potentials: the standard Lennard-Jones potential eq. (4.1) is represented by the red dashed line; the potential shown by the green continuous line is the Lennard-Jones potential shifted up by the depth of the potential well and truncated at \( r_c = r_m \) to remove attraction; the potential shown by the dotted blue is the soft potential described by eq. (4.2).
When \( r_c = r_m = \sigma_0 \sqrt{2} \) the potential is cutoff at the minimum and \( V(r_c) = -\epsilon_{\text{well}} \). Thus, setting the cut-off radius equal to \( r_m \) would remove the attraction part of the potential, and a shift up by \( \epsilon_{\text{well}} \) would set the value at \( r_m \) equal to 0, allowing repulsion forces to start from 0 at the cut-off point and gradually grow with a decrease of distance between particles, preventing them from overlapping. This potential is shown in fig. 4.1 as a continuous green line. However, the increase in potential energy is very steep and this may lead to stability issues (when the time step is relatively big, particles may move significantly closer in one time step, and the Lennard-Jones potential would increase sharply and move particles far away from each other, blowing up the simulation).

LAMMPS has multiple other potentials, including some that were created specifically to prevent particles from overlapping. In our research, the potential called \( \text{soft} \) was used:

\[
V_s(r) = A_{sp} \left( 1 + \cos \frac{\pi r}{r_c} \right),
\]

(4.2)

where \( r \) is the distance between particles, \( r_c \) is a cut-off radius (we set it to the same value as for Lennard-Jones potential), and \( A \) is an energy constant. This potential is also shown in fig. 4.1 as a dotted line. While the Lennard-Jones potential blows up at very small distances, the maximum value of the soft potential, eq. (4.2), is bounded and controlled via the energy constant \( A \). We used both of these potentials in the simulations demonstrated in this Chapter. With this potential added, the numerical method from Chapter 2 now can be used to simulate the behavior of groups of disc-shaped particles immersed in a liquid crystal.

4.2 Simulation setup and parameters

The setup of the simulations in this chapter is very similar to that used for the single disc simulations: the simulation box is periodic in both \( x \) and \( y \) directions, while two rigid walls with fixed surface conditions are located at \( z = -l/2 \) and \( z = l/2 \), where \( l \) is the height of the domain (\( l \) is always bigger then \( 4R \), where \( R \) is the disc radius, to allow the director to adjust to the distortion that appears around the disc during the simulation). Boundary conditions on the walls, director along the \( x \)-axis, result in equilibrium conditions for the director of \( \hat{n} = (1,0,0) \) throughout the simulation domain. The size of the domain in the \( x \) and \( y \) direction varies depending on the desired concentration of the discs, i.e. on the distance between disc pairs (picture the domain effectively repeating itself due to the periodicity).

Both discs, as before, have perpendicular anchoring on the surface.

As before, a weak magnetic field (\(< 20G\)) starts along the \(+y\)-direction (\( \vartheta_{\text{MF}} = 0^\circ \), which is the direction of magnetic moment of the disc) and then rotates in the \( xy \)-plane by a small amount, 0.0001°–0.005° every time step or 1.745 rad/s – 87 rad/s, until it reaches its final position along \(-y\)-axis, i.e. \( \vartheta_{\text{MF}}^{\text{stop}} = 180^\circ \).

All simulations of this chapter are performed on an edgeless disc of \( R = 0.72 \mu m \), \( L = 0.075 \mu m \) with magnetic moment \( |\mu| = (0.32 \pm 0.06) \times 10^{-13} A \cdot m^2 \) (\( |\mu| \) the same as the one from Chapter 2). Other parameters used in the simulations in this chapter are provided in table 4.1.
Table 4.1: Parameters used in simulations of disc pairs.

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<th>Value</th>
<th>Units</th>
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<td>$A_0$</td>
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<td>atm</td>
</tr>
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<td>3.2</td>
<td>—</td>
</tr>
<tr>
<td>$K_1 = K_2 = K_3 = K$</td>
<td>10.72</td>
<td>pN</td>
</tr>
<tr>
<td>$\Gamma$</td>
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<td>$(atm \cdot \mu s)^{-1}$</td>
</tr>
<tr>
<td>$\xi$</td>
<td>0.75 or 0.52</td>
<td>—</td>
</tr>
<tr>
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<td>$\mu m$</td>
</tr>
<tr>
<td>$\Delta t$</td>
<td>1</td>
<td>$\mu s$</td>
</tr>
<tr>
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<td>atm</td>
</tr>
<tr>
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<td>—</td>
</tr>
<tr>
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<td>$\mu m$</td>
</tr>
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</tr>
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<td>$\varepsilon_{well}$</td>
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<td>$pJ$</td>
</tr>
<tr>
<td>$A_{sp}$</td>
<td>0.5 and 0.0000005</td>
<td>$pJ$</td>
</tr>
</tbody>
</table>

### 4.3 Discs Interaction

The simplest case of a system with two discs would be the one when two discs are immersed in a liquid crystal but they are too far apart to affect each other. In this case when a weak slowly rotating magnetic field switches on, the two discs would rotate and flip independently from each other to repeat the motion described in sec. 3.2.2. Since such simulations require a big simulation domain and, thus, significant computation time, and at the same time does not contain any new information on disc behavior, this case was skipped.

The next possible configuration is when two discs are very close to each other initially. When a magnetic field starts to rotate, it should be followed by the discs. Soon after that the discs would just come in touch with each other, one on top of another (that would be effectively like a disc with double thickness), to decrease the distortion area and lower the free energy of the system. After that, they would carry on the motion acting as one disc and flip together. This case is of no interest as well, since this motion has already been studied in the previous chapter.

From these two cases it is already clear, that the interaction between discs depends on the initial distance between them and, thus, the interesting situations are where discs are neither too close or too far apart from one another. Two such configurations that produced an interesting behavior are described below.
Figure 4.2: Motion of discs pairs. Discs are represented in orange, their magnetic moments are shown as semitransparent red and purple lines. Green arrow corresponds to the direction of a magnetic field. The center part on each picture is an actual simulation domain, while pictures on the left and right are the same domain repeated periodically. Color scale on the right shows the correspondence between the largest eigenvalue and colors from dark blue to light gray.
Figure 4.3: Motion of the centers of mass of the discs. In a): changes of the distance between the centers of mass of the discs from the middle domain in figures 4.2 with time. In b): changes in \( x \) (continuous lines), \( y \) (dashed lines), \( z \) (dotted lines) coordinates of the centers of mass of the discs with time. Here disc 1 corresponds to the left disc in the center domain in figure 4.2, disc 2 corresponds to the right one.
4.3 Discs Interaction

4.3.1 Semi-stable tilted configuration

The simulation described in this section uses a relatively small domain (a bit less than 4R, where R is the radius of the discs, i.e. two discs can barely fit into the domain if they both lay horizontally in one line). Small domains also decrease the computational time. In addition, with such a domain size we can see a periodic image that corresponds to a highly packed structure of disc particles. The next section, 4.3.2, demonstrates results for bigger domains, where the disc pair is affected by the neighboring pairs due to periodic boundary conditions, but does not have to touch other disc pairs unless the discs get moved close to the edge of the domain.

Two discs of the same size \((R = 0.72\mu m, L = 0.075\mu m)\) and with the same magnetic moment \((|\mu| = (0.32 \pm 0.06) \times 10^{-13} A \cdot m^2)\) are started at a distance of 1.227\(\mu m\) or 1.72\(R\) between their centers of mass and are shown in fig. 4.2a. A magnetic field with magnitude 0.5G acts on the system and rotates with angular velocity 87 rad/s starting from the direction of the \(+y\) axis and stopping after rotating by 180°. The domain size for this simulation was 3.0\(\mu m\) \(\times\) 3.0\(\mu m\) \(\times\) 3.0\(\mu m\). All snapshots in fig. 4.2 are a cross-section near the center of the simulation domain viewed from above. On each snapshot the center region (with director field shown in black) is the actual simulation domain, while the two domains on the left and right (where the director field is shown in gray) are the periodically repeated images. Discs are represented by surface nodes, indicated by spheres located at the positions of the nodes; the spheres are made about 2 times larger than the real node size for better visibility. Red and purple semitransparent lines starting from the centers of the discs represent the direction of the magnetic moment of each disc. The green arrow, as before, corresponds to the direction of the magnetic field. The color scale on the right reflects the coloring for the largest eigenvalue: starting from the dark blue colors that would indicate the position of a disclination line defect to light gray color to exhibit a light disturbance in the order parameter field.

 Initially, the discs start to rotate, following the magnetic field (fig. 4.2, b and c), similar to what was observed for one disc in sec. 3.2. Rotation of the discs leads to a distortion that reaches the boundary of the domain; this, together with periodic boundary conditions, implies that this distortion affects the neighboring discs. The rotation motion of the discs is accompanied by a translation motion (compare fig. 4.2, c and d; also see fig. 4.3a). As can be seen from fig. 4.3b, the motion of both discs is symmetric and happens mainly along the \(x\)-axis (continuous red lines corresponds to an \(x\)-coordinate change) with only slight repulsion and followed by attractive motion along the \(y\)-axis (purple and blue dashed lines). At the same time the \(z\)-coordinate of the centers of mass of the discs stays unchanged and no rotation in the plane of the face of the discs is observed at any time of the simulation. It also can be mentioned that no defects were formed during the simulation.

Rotation and translation of discs continues, until the discs rotate by 82°, when they finally lock up and lean on each other’s side (corresponds to fig. 4.2e). Similar to observations of a single disc, the magnetic field torque is stronger at this point than the liquid crystal torque from the distortion in the liquid crystal, and each disc wants to carry on the clockwise rotation, but neighbor discs leaning on both sides of it prevent this from happening and rather lead to the balance between all forces in the system. From fig. 4.2e
one may also note that in this configuration the director field is symmetric as well as the position of all discs (i.e. each disc touch the neighbor at about the same point). Therefore, the translation motion seems to leave the discs in a configuration, in which each disc is interacting equally with both the second disc in the domain and the neighbor disc from the periodic image.

Continuation of the simulation shows no changes in configuration (both orientation and location of the discs stay the same, that corresponds to the horizontal part of the curve from the fig. 4.3a), meaning that this state is a semi-stable state, and a kick is required to move out from this configuration.

Stability of this configuration can also be explained in terms of the capacitance, introduced in sec. 3.2.1. When discs are locked in this configuration, they effectively can be roughly approximated by an infinite (due to periodic boundary conditions) prolate spheroidal particle. In order to find the formula for the capacitance of the prolate spheroid, we repeat the same steps we did in sec. 3.2.1 to get the capacitance of the oblate spheroid, and again get the Laplace equation

\[ \nabla^2 \tilde{\theta} = 0, \quad (4.3) \]

under the same notation as was used in sec. 3.2.1. In this case we use a coordinate change corresponding to the prolate spheroid to solve it [158]:

\[
\begin{align*}
    z &= \frac{1}{2}a\xi \eta, \\
    x &= \frac{1}{2}a\sqrt{(\xi^2 - 1)(1 - \eta^2)} \cos \varepsilon, \\
    y &= \frac{1}{2}a\sqrt{(\xi^2 - 1)(1 - \eta^2)} \sin \varepsilon,
\end{align*}
\]

(4.4)

where \( \xi \in [0, \infty), \eta \in [-1, 1], \varepsilon \in [0, 2\pi], \) and \( a = L \sqrt{1 - \left(\frac{2R}{L}\right)^2} \) is an inter-focal distance. According to [158] the solution to this equation is

\[
\tilde{\theta} = \theta \frac{\ln \frac{\xi + 1}{\xi - 1}}{\ln \frac{\xi_0 + 1}{\xi_0 - 1}},
\]

(4.5)

where \( \xi = \xi_0 \) determines the surface of the oblate spheroid and \( \theta \) specifies the orientation of the liquid crystal molecules on the surface of the particle. The integral of the elastic energy over all space excluding the discs would give

\[
U = \frac{K}{2} \int dV (\nabla \tilde{\theta})^2 = 2\pi Ka\theta^2 \left[ \ln \frac{\xi_0 + 1}{\xi_0 - 1} \right]^{-1}.
\]

(4.6)

Applying eq. (4.6), using similar reasoning as to eq. (3.7), substituting the expression for the inter-focal distance, and switching back to \( x, y, z \) coordinate system would lead to the following formula for the capacitance of the prolate spheroid:
4.3. Discs Interaction

\[
C = a \left[ \ln \left( \frac{\xi_0 + 1}{\xi_0 - 1} \right) \right]^{-1} = L \sqrt{1 - \left( \frac{2R}{L} \right)^2} \left[ \ln \left( \frac{1 + \sqrt{1 - \left( \frac{2R}{L} \right)^2}}{1 - \sqrt{1 - \left( \frac{2R}{L} \right)^2}} \right) \right]^{-1},
\]  

(4.7)

where \( R \) is the radius of the spheroid and \( L \) is its length.

We now can define the energy of this configuration using eq. (3.8), i.e.

\[
U = 2\pi KC\theta^2 = 2\pi K\theta^2 L \sqrt{1 - \left( \frac{2R}{L} \right)^2} \left[ \ln \left( \frac{1 + \sqrt{1 - \left( \frac{2R}{L} \right)^2}}{1 - \sqrt{1 - \left( \frac{2R}{L} \right)^2}} \right) \right]^{-1}.
\]  

(4.8)

This expression means, that the value of energy associated with this tilted configuration is proportional to \( L \). However, since the chain of laying discs is infinite, the length of the spheroid that approximates them, has an infinite length too, i.e. \( L \to \infty \), and, thus, \( U \to \infty \).

This dependence implies, that we need an infinite amount of energy to change or move this configuration. In order to relax the distortion, discs would have to either flip together, all at the same time, or the whole line of discs has to rotate together by about 90° in order to satisfy both the perpendicular surface conditions and orientation of the particles on the top and bottom walls. The first scenario would not happen because the angle of rotation of the discs is too far from the critical flipping angle (\( \theta < 90^\circ \)). The second scenario requires an infinite amount of energy to rotate the infinite number of discs and, hence, is also impossible. Thus, the discs will stay in this tilted locked configuration until the chain is broken in some way by an external interference.

4.3.2 Two discs flip

Another interesting configuration was observed with the following set up. Two discs of the same size, radius \( R = 0.72\mu m \) and thickness \( L = 0.075\mu m \), and same magnetic moment \( |\mu| = (0.32 \pm 0.06) \times 10^{-13} \text{A} \cdot \text{m}^2 \), were located at a distance \( 1.227\mu m = 1.72R \) between their centers of mass as in the previous section, but the simulation domain for this run was taken to be \( 4.5\mu m \times 4.5\mu m \times 4.5\mu m \) (see fig. 4.4a). A bigger domain means that disc pairs on the left and right are now further away, thus allowing the discs to move without touching the neighboring disc pairs. Fig. 4.4 demonstrates the motion of two discs showing a cross-section near the center of the simulation domain viewed from above with the discs (in orange) in the center; the discs are represented by spheres located at the positions of the nodes; magnetic moments of the discs are shown as semitransparent red and purple lines; the green arrow shows the direction of the magnetic field. The color scale for the largest eigenvalue is the same as the one from fig. 4.2.

As before, the discs starts to follow the rotation of a weak magnetic field \( (|\mathbf{B}| = 0.75G \) turning until rotated by 180° with angular velocity of 125.94 rad/s), as can be seen in fig. 4.5b – d. During this motion, the discs initially try to move apart from each other, but after they rotate by more then 90° from their original orientation, it becomes less
Figure 4.4: Motion of the discs pair. Discs are represented in orange, their magnetic moments are shown as semitransparent red and purple lines. Green arrow corresponds to the direction of a magnetic field. Color scale is the same as in fig. 4.2.
Figure 4.5: Motion of the centers of mass of the discs started at distance $1.72R$. In a): changes of the distance between the centers of mass of the discs with time. In b): changes in $x$ (continuous lines), $y$ (dashed lines), $z$ (dotted lines) coordinates of the centers of mass of the discs with time. Here disc 1 corresponds to the left disc in figures 4.4, disc 2 corresponds to the right one.
Figure 4.6: Motion of the centers of mass of the discs started at distance $3.4R$. In a): changes of the distance between the centers of mass of the discs with time. In b): changes in $x$ (continuous lines), $y$ (dashed lines), $z$ (dotted lines) coordinates of the centers of mass of the discs with time.
4.3. Discs Interaction

expensive energy-wise for them to come closer together (fig. 4.4, e - f and fig. 4.5, a and b). However, after one disc slides on top of the other (minimum of the distance between centers of mass of the discs in fig. 4.5a, close to $100000 \mu s$ after beginning of the simulation), the translational motion does not stop but rather continues (fig. 4.4g and increase of the distance between centers of mass in fig. 4.5a). Now the motion is not only happening in the $x$ direction, but also significant sliding can be seen in the $y$ direction. Also the discs start to move vertically (dotted green lines in fig. 4.5b), enlarging the distance between them. A distortion cloud appears around the discs due to a high distortion in the director field. After that both discs start the flipping motion accompanied by the rotation of the discs in the plane of their faces to lower the free energy of the system (to see that one may track the motion of the magnetic moments of the discs in fig. 4.4, h - k). The distortion cloud shrinks back to the surface of the disc, that is similar to what was observed in simulations of the motion of a single disc described in sec. 3.2.2. During the flip the translation motion continues and takes the discs further apart to finally fix them in a configuration shown on fig. 4.4l) with no distortion in the system and all the motion stopped. As can be seen, the two discs have switched their places (the one that was initially on the left now is on the right side of the domain, easily distinguishable via the color of the magnetic moment), thus the $x$ coordinate of the centers of mass of the discs changed its sign (fig. 4.5b). Also the discs’ centers of mass have shifted slightly in the $z$ direction and moved significantly along the

Figure 4.7: Stable periodic structure of discs resulted from a flipping motion (top view). Discs are represented as a set of nodes colored in orange.
Chapter 4. Pairs of Discs in Nematic Liquid Crystal

$y$ axis (see fig. 4.5b). Since the system is periodic in $x$ and $y$ directions, we can repeat the picture along this axes to get a periodic configuration shown on fig. 4.7 (keep in mind that this figure gives the top view of the configuration, but discs are also shifted along the $z$ direction as well). This implies, that one can create a stable periodic structure of a desired configuration via tuning the initial density of the discs and magnitude and rotational velocity of the magnetic field.

We also performed another simulation with the same configuration except for the initial distance between the centers of mass of the discs – in this case it was set to be equal to $2.379 \, \mu m = 3.3R$. Since the discs behave similarly and demonstrate the same flipping behavior as the previous simulation, we only provide plots of the distance between the centers of mass of the discs and coordinate change with time (in fig. 4.6). The only difference from the previous simulation (corresponds to fig. 4.5) and this one was that in this simulation discs initially started to move closer, while in the previous configuration with smaller initial distance they firstly move apart and only after about 70000 $\mu s$ started to approach each other.

In relation to the change of coordinates, we can see a similar shape of the curves as on fig. 4.5: there is a significant change in $x$ and $y$ coordinates; discs moved slightly along the $z$ direction; discs switched their places. However, comparison of fig. 4.5b and fig. 4.6b shows that although the initial position of the discs was different, their final coordinates are very similar. This behavior leads to an idea, that one may balance the distance between each two paired discs by a single rotation of the magnetic field, and then subsequent additional rotations of the magnetic field might equalize the distance between other pairs and finally produce a stable crystal structure. Nevertheless, additional simulations are required before reaching any conclusions on this matter.

4.4 Chapter Summary

Preliminary analysis of disc pair motion shows that the level of interaction between discs immersed in a nematic liquid crystal strongly depends on the distance between objects. One can receive a stable chain configuration of discs similar to the one described in sec. 4.3.1 and potentially tune the tilt angle in the configuration via the magnitude the angular velocity of magnetic field.

We also observed another stable structure, described in sec. 4.3.2 and shown in fig. 4.7. Structures similar to this one can be of a significant importance for applications that require periodic structures, such as creation of porous medium and membranes. Based on the results for a single disc, we may expect that the final distance between paired discs and the distance to nearest disc pairs can be tuned via the initial position of discs and position at which disc starts the flipping motion, that can be controlled via magnitude and rotational velocity of the magnetic field. Yet further analysis of the behavior of disc pairs is necessary to predict the motion accurately and come to conclusions on the behavior controls.
Conclusions

In this thesis we have numerically studied first the behavior of a stand-alone disc-shaped particle under the action of slowly rotating magnetic field; then, based on successive results for a stand-alone disc, we examined groups of disc particles under differing conditions.

After an introductory chapter about the main properties of liquid crystals, in Chapter 2 we described a novel method for simulating the dynamics of disc particles. The main advantage of our method is the two-way coupling between the object and liquid crystal and ability of the particle to move under action of forces that arise due to this coupling. Another significant strength of the method is that although the method was originally developed for disc particles, it can be used for colloids of any shape, since the method does not use any specific information about the particle geometry other than the surface location and the local surface normal.

In Chapter 3 we used the algorithm from Chapter 2 to simulate the behavior of a single disc immersed in a nematic liquid crystal under the action of a weak rotating magnetic field. Comparison of the results of simulations with the experiments demonstrated not only a good agreement with expected rotational and flipping behavior but also unveiled additional insights that provided an explanation and reason for the peculiar motion observed in the experiments. In this chapter we also suggested a simple yet effective method to calculate the intensity of light through the liquid crystal slab with a particle inside it. This algorithm accounts for complicated configurations where significant distortion and defects might be present; the algorithm also allows detailed study of how the light intensity changes from layer to layer. As a result of analysis of our simulations with a single disc, we came to the conclusion that the motion of the disc particle can be controlled via properties of the magnetic field – its magnitude, angular velocity and final orientation. This allows tuning of the start of the flipping motion (and, thus, orientation of the disc when the flipping begins), speed of flipping, amount of rotation of the disc in the plane of its face during the flip, and provides the ability to control the final orientation of the disc.

In the next chapter we extended the algorithm by adding a repulsive potential. This update prevents objects from overlapping and allows the method from Chapter 2 to be used for simulations of multiple particles submerged in a liquid crystal. The updated algorithm was used to simulate the motion of disc pairs of different densities in a nematic
liquid crystal under the action of a weak rotating magnetic field. Though more simulations are required before reaching final conclusions, we can give the following preliminary analysis of their motion.

I. Different particle densities lead to different stable configurations.

High density configurations end up in a stable state in which all discs lean on the side of the neighbor disc and form a chain.

Relatively low densities of disc pairs lead to a similar flip behavior that was observed for a single disc: both discs rotate after the magnetic field and, after the system reaches the critical state of highest energy, discs start to flip simultaneously to release the distortion; the final configuration does not have any distortion in the orientation of liquid crystal molecules. However, now the rotational motion of discs is accompanied by a translational motion. This leads to a switch between discs (i.e. the disc that was on the left ends on the right side) and change in the position of discs compared to the initial configuration.

These results implies, that one can control the translational motion of the discs and, thus, their final configuration (their orientation and the distance between them) via the initial density of discs in the system.

II. For the low density disc pairs the relatively small change in initial distance between particles leads to the same final position of the discs (unless particles are taken too far away from each other to interact).

This means that when discs in the liquid crystal are unequally distributed, half a circle rotation of the magnetic field can even the distance between them.

III. Based on the results for a single disc, one may expect that the final position of two discs depends on the position and orientation of the discs right before the start of the flip and, thus, could be controlled via tuning the magnitude, angular velocity and final orientation of the magnetic field.

Thus changes in the characteristics of the magnetic field and its motion can alter the final position of the discs and distance between them.

There is also a possibility that subsequent rotations of the magnetic field (and, consequently, of the discs) may lead to equally spaced discs, i.e. a stable crystal structure. The ability to produce stable crystal structures with tunable lattice distances from hardly ordered disc particles in nematic liquid crystals looks very promising and would be of a great interest for development of optical devices and porous materials. This is the most interesting direction for further research.

There is a number of other ways this work might be continued. One may try to tune the motion of the discs using different ferromagnetic materials, that would result in a different magnetic moment and, thus, different rotational velocity of two discs. Another possibility is to combine objects of different shapes, such as pair a torus with a spherical particle to produce a stable configuration. Current code is also suitable for simulations
of cholesteric liquid crystals; results of simulations of discs in cholesterics may lead to
the another parameter of control over the disc motion – the cholesteric pitch.

Another thing would be for experimentalists to try stronger fields and fast rotations
to see if they can reproduce the defect-mediated relaxation seen in chapter 3. It would
also be interesting to investigate the behavior of disc pairs in a nematic liquid crystal as
well and compare the results from the experiments with our numerical predictions.

To sum up, results of this work discover a promising area for computational soft matter
research and lead to new ways of self-organization of disc-shaped colloidal particles and
may result in discovery of the novel methods of manipulation of colloidal particles with
future research in the area.
Bibliography


Appendix A

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