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Dynamics of two colloidal particles immersed in a nematic liquid crystal

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Abstract

The dynamic equations of a colloidal particle with a homotropic anchoring are solved in the presence of another fixed particle, when hyperbolic hedgehog defects are created on one or other side of them. The velocities of the particles are obtained in terms of the parameter $q = \gamma_{\perp}/\gamma_{\parallel}$; then a polar equation of the path is calculated for $q = 3/2$. The same procedure has also been used for colloidal particles with a planar anchoring to obtain the velocity and path of a moving particle.

1. Introduction

Colloidal dispersions [1] are used extensively in our daily life, and they can be found in such substances as foods, drugs and paints. Therefore they have long been an important subject in technological and scientific research. Recently, colloidal dispersions in anisotropic host fluids such as liquid crystals [2–5] have attracted a wide interest as a different class of composite materials compared to conventional colloids with isotropic hosts. One of the interesting and important features of liquid crystal colloidal dispersions is that elastic distortions of the liquid crystal host can mediate a long-range interaction between particles immersed in it, unlike conventional colloids and emulsions [6–9]. The elastic distortions of the liquid crystal host arise from the anchoring of the mesogenic molecules on the surfaces of the dispersed particles. The resulting interaction forces mediated by the liquid crystal can be measured in experiments [6–10].

A full theoretical analysis of this problem is virtually impossible because of highly nonlinear problems in a complex geometry. A single particle breaks the continuous rotational symmetry of a liquid crystal. It behaves topologically as a core of an orientational defect, when the surface anchoring is sufficiently strong. Various types of topological defects such as a hyperbolic hedgehog, a Saturn ring, and boojums, have been recently reported in liquid crystal colloidal dispersions. Ruhwandl and Terentjev [7] found that the interaction between spherical particles with weak surface anchoring is quadrupolar, with the potential being proportional to r^{-5} , with r being the interparticle distance. Lubensky *et al* [8] showed by a phenomenological argument that particles carrying a hyperbolic hedgehog [2, 3] act as a dipole. They have formulated a theory of elastically mediated forces between particles with hyperbolic hedgehog

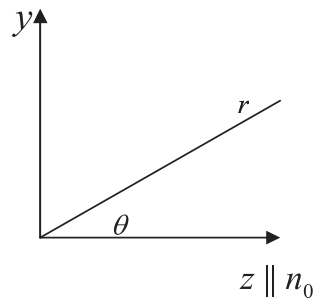


Figure 1. Polar variables r and θ with respect to n_0 .

defects [8]. The hyperbolic hedgehog defect is created to one side of the particle with a homotopic anchoring surface along the surrounding director field, in order to satisfy a total topological charge of zero. Thus induced distortion of the liquid crystalline order assumes a dipolar property. It leads to chain formation owing to the balance of the long-range dipolar attractive and the short-range defect-mediated repulsive interactions. Yada *et al* [10] reported quantitative evaluation of anisotropic interactions between solid particles dispersed in a nematic liquid crystal. They introduced two types of anisotropic spatial distribution of the trapping forces between particles with hyperbolic hedgehog defects, leading to a linear chain form. They obtained the force map and compared it with the theoretical distribution of the dipolar attractive forces between the particles.

Particles in motion give rise to a wealth of interesting physics. A theoretical treatment of particles in motion has to deal with the dynamic equations of a nematic liquid crystal, i.e. the Ericksen–Leslie equations, which couple the director field and the fluid velocity. Due to their complexity, only a few examples with an analytical solution exist [11].

However, to our knowledge, in spite of the wealth of theoretical and numerical studies on the elastic-distortion-mediated particle interactions there have been no theoretical studies to discuss the trajectory of particle motion to form a linear chain. The purpose of this paper is to present our attempt to study this subject analytically. However, we know that a full analytical analysis is virtually impossible, due to intrinsic difficulties in the treatment of the elasticity of liquid crystals, such as the nonlinear nature, the presence of topological defects, and hydrodynamic interactions.

However, we obtain the trajectory of particle motion in the presence of another particle in a nematic liquid crystal medium. The article is organized as follows. After formulation of the problem and obtaining the equations for components of the velocity of the moving particle, the trajectory of the particle is finally obtained.

2. Formulation of the problem

2.1. Hedgehog defects both on the left side of two particles

In this subsection we assume a configuration of two particles having hedgehog defects both on the left side in a uniformly aligned nematic liquid crystal. The particles are considered along a direction nearly perpendicular to the z axis (e.g. they are set by laser-trapping forces); see figure 1. If one of the particles is supposed to be trapped at the centre of the coordinate system and then the other particle is released from the trap, it starts gradually to move in an arc and to approach the fixed particle. These results have been observed in experiments by Yada *et al* [10]. In the following our aim is to calculate the mathematical equation of this arc.

Following the phenomenological theory of Lubensky *et al* [8] on the particle–particle interactions which are mediated by the nematic liquid crystal, one can write the effective free energy as

$$F = K \int d^3r \left[\frac{1}{2} (\nabla n_\mu)^2 - 4\pi P_z \partial_\mu n_\mu + 4\pi (\partial_z c_{zz}) \partial_\mu n_\mu \right] \quad (1)$$

where the dipole–bend coupling term has been neglected to leading order in deviations of the director from uniformity. The dipole moment of the particle P prefers to align with the local director n . This is nearly in the far field, which is the case under our consideration here.

The interaction energy between the particles at positions $r(0, 0)$ and $r(r, \theta)$ with respective dipole and quadrupole moments P_z, P'_z, c and c' is [8]

$$U(r) = 4\pi K [P_z P'_z V_{pp}(r) + \frac{4}{3} c c' V_{cc}(r) + \frac{2}{3} (c P'_z - c' P_z) V_{pc}(r)] \quad (2)$$

where the interaction energy functions $V_{pp}(r)$, $V_{cc}(r)$ and $V_{pc}(r)$ are

$$V_{pp}(r, \theta) = r^{-3} (1 - \cos^2 \theta) \quad (3)$$

$$V_{cc}(r, \theta) = r^{-5} (9 - 90 \cos^2 \theta + 105 \cos^4 \theta) \quad (4)$$

$$V_{pc}(r, \theta) = r^{-4} (15 \cos^2 \theta - 9). \quad (5)$$

Here we ignore the quadrupole interparticle interaction, whose contribution to the force is much smaller than that of the dipolar interaction at large distances; even when the moving particle approaches the fixed particle, $r = 2a$, this interaction is small compared to the dipolar one (see below) [8]. We consider two spherical particles of radius a , positioned at $r(0, 0)$ and $r(r, \theta)$, such that the interparticle distance is larger than the typical dimension of the particle; r and θ are the polar variables. When the particles are interacting via the dipole–dipole forces, the interaction energy is expressed in terms of the dipole moment p_z and the dipole–dipole potential $V_{pp}(r)$ from equations ((2)–(5)):

$$U(r, \theta) = 4\pi K p_z^2 V_{pp}(r, \theta) \quad (6)$$

where K is the Frank elastic constant for the nematic director field in the one-constant approximation [12], with $p_z = \alpha a$. The interparticle force can be calculated by

$$F = -\nabla U(r, \theta) \quad (7)$$

$$F = \frac{d}{r^4} \{ (1 - 3 \cos^2 \theta) \hat{e}_r - 2 \cos \theta \sin \theta \hat{e}_\theta \}$$

where \hat{e}_r and \hat{e}_θ are polar orthogonal unit vectors and $d = 12\pi K p_z^2$.

The particle positioned at $r(0, 0)$ is fixed with its centre located at the origin of the coordinate system. When the other particle is released, they are approaching each other, with the friction force balancing the dipolar force. The experimental results [10] show that the trajectory of particle motion is in the plane of the initial distance of two particles, the y -axis, and the unperturbed director n_0 , the z -axis (see figure 1). There is only one preferred direction in the problem, namely, the unperturbed director n_0 at infinity, which is along the z -axis. Therefore, the velocity $v(r)$ and the viscous force F_v should be decomposed into components parallel to z and normal to it, as follows:

$$v(r) = v_y \hat{j} + v_z \hat{k}, \quad (8)$$

$$F_v = -\gamma_{\parallel} v_z \hat{k} - \gamma_{\perp} v_y \hat{j} \quad (9)$$

where the effective coefficients of viscosity γ_{\perp} and γ_{\parallel} are independent of the variables x and y [18]. v_z, v_y, \hat{k} and \hat{j} can be written in the terms of v_r, v_θ, \hat{e}_r and \hat{e}_θ , i.e.

$$\hat{k} = \hat{e}_r \cos \theta - \hat{e}_\theta \sin \theta; \quad \hat{j} = \hat{e}_r \sin \theta + \hat{e}_\theta \cos \theta \quad (10)$$

$$v_z = v_r \cos \theta - v_\theta \sin \theta; \quad v_y = v_r \sin \theta + v_\theta \cos \theta. \quad (11)$$

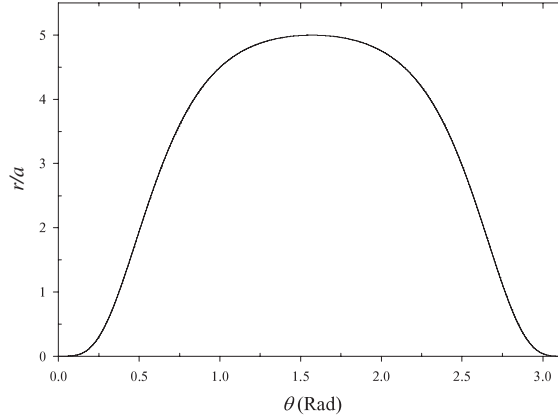


Figure 2. r/a is plotted versus θ for homotropic anchoring.

By substituting equations (10) and (11) into (9) we have

$$F_v = -\gamma_{\parallel} \{ [F(\theta)v_r + (1-q)\sin\theta\cos\theta v_{\theta}] \hat{e}_r + [Q(\theta)v_{\theta} + (1-q)\sin\theta\cos\theta v_r] \hat{e}_{\theta} \} \quad (12)$$

where $q = \gamma_{\perp}/\gamma_{\parallel}$ and

$$\begin{aligned} F(\theta) &= 1 + (q-1)\sin^2\theta \\ Q(\theta) &= q + (1-q)\sin^2\theta. \end{aligned} \quad (13)$$

The equation of motion describing the acceleration and velocity of the fluid with dispersed particles is simply Newton's law:

$$m \frac{dv}{dt} = F_d + F_v \quad (14)$$

where F_d and F_v represent the dipole–dipole interaction force and viscous force, respectively.

We limit our attention to the viscous and dipole–dipole interaction forces, which is a reasonable limitation for small particle velocity, and since in the case of small particle velocity (to be precise, small Ericksen number characterizing the ratio of the viscous and elastic forces) one may put the left-hand side of equation (14) to zero, hence we have

$$\begin{aligned} \gamma_{11} \{ v_r F(\theta) + (q-1)v_{\theta} \sin\theta \cos\theta \} &= \frac{d}{r^4} (1 - 3\cos^2\theta) \\ \gamma_{11} \{ (q-1)v_r \sin\theta \cos\theta + v_{\theta} Q(\theta) \} &= -\frac{2d}{r^4} \cos\theta \sin\theta. \end{aligned} \quad (15)$$

By solving equations (15) in terms of v_r and v_{θ} and taking the initial conditions into account, we have

$$\begin{aligned} v_r &= \frac{d}{qr^4\gamma_{\parallel}} [-2q - 1 + (7q-4)\sin^2\theta - 5(q-1)\sin^4\theta] \\ v_{\theta} &= -\frac{d}{qr^4\gamma_{\parallel}} \sin\theta \cos\theta \left(1 + \frac{5}{2}\sin^2\theta \right). \end{aligned} \quad (16)$$

By taking $r_0 = \sigma a$ and $q = 3/2$, we have

$$\frac{r}{a} = \sigma \sin^4\theta \left/ \left(1 - \frac{5}{7}\cos^2\theta \right)^{5/2} \right. . \quad (17)$$

In figure 2, r/a has been plotted versus θ for $\sigma = 5$ [10]. It is interesting to note that when the particle at r_0 , $\theta \leq \pi/2$ is released from the laser trap, the dipolar force causes the particle

to move towards smaller angles θ (i.e. the positive z -axis) whereas for $\theta_0 \geq \pi/2$ the released particle moves towards the negative z -axis (see also section 2.2). Regardless, in both cases the two particles will reach each other at angles $\theta_{c_1} = 29.23^\circ$ and $\theta_{c_2} = 150.77^\circ$.

2.2. Hedgehog defects on different sides of two particles

In this subsection we assume a configuration of two particles having hedgehog defects on different sides in a uniformly aligned nematic, i.e. $P_z = -P'_z$. The initial configuration of the problem is the same as in the problem considered in section 2.1. Since the procedures of the calculation is similar to the considered one $P_z = P'_z$, we here mention only the differences. The interaction energy and interparticle force are respectively

$$U(r, \theta) = -4\pi K p_z^2 V_{pp}(r, \theta) \quad (18)$$

$$F = -\frac{d}{r^4} \{(1 - 3 \cos^2 \theta) \hat{e}_r - 2 \cos \theta \sin \theta \hat{e}_\theta\}. \quad (19)$$

The equation of motion gives

$$\gamma_{11} \{v_r F(\theta) + (q - 1) v_\theta \sin \theta \cos \theta\} = -\frac{d}{r^4} (1 - 3 \cos^2 \theta) \quad (20)$$

$$\gamma_{11} \{(q - 1) v_r \sin \theta \cos \theta + v_\theta Q(\theta)\} = \frac{2d}{r^4} \cos \theta \sin \theta.$$

By solving the above equations with initial conditions we get

$$v_r = -\frac{d}{qr^4 \gamma_{11}} [-2q - 1 + (7q - 4) \sin^2 \theta - 5(q - 1) \sin^4 \theta] \quad (21)$$

$$v_\theta = \frac{d}{qr^4 \gamma_{11}} \sin \theta \cos \theta \left(1 + \frac{5}{2} \sin^2 \theta \right).$$

If we take $r_0 = \sigma a$, $\theta_0 \cong \pi/2$, and $q = 3/2$, we finally get the same results as equation (17), i.e.

$$\frac{r}{a} = \sigma \sin^4 \theta \left/ \left(1 - \frac{5}{7} \cos^2 \theta \right)^{5/2} \right. . \quad (22)$$

The only difference with the previous case (section 2.1) is in the direction of motion of the particle. Here if we put the moving particle initially at $r = r_0$ and $\theta = \theta_0 \leq \pi/2$ ($\geq \pi/2$), then on releasing the laser force on it, the particle will move upwards and go towards the negative (positive) direction of the z -axis.

3. Effects of the quadrupolar terms

As we mentioned previously, the long-range attraction force between droplets in a nematic solvent has been confirmed theoretically and experimentally [6, 10, 16], for dipolar interparticle interaction. For short distances this attractive dipolar force turns into a repulsive force [17]. In our problem, the main formula, equation (22), was obtained by only taking into account the dipolar forces and it is not applicable to short distances and small angles. The nearest distance in the problem is $2a$. The ratio of the magnitude of quadrupole to dipolar forces is equal to 0.03 (see below). For short distances, which is the case for planar anchoring [17], we may only consider the quadrupole forces in equations (2) and (9) and ignore the dipolar forces. If we consider the quadrupole potential [18]

$$U(r) = \frac{16\pi}{9} K c c' \frac{1}{r^5} (9 - 90 \cos^2 \theta + 105 \cos^4 \theta) \quad (23)$$

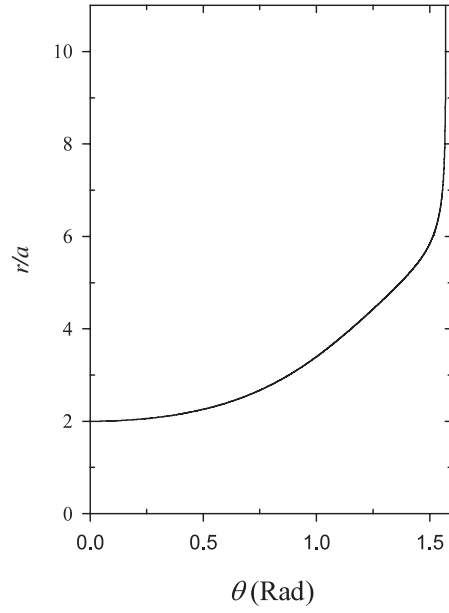


Figure 3. r/a is plotted versus θ for planar anchoring.

the quadrupole force is written as

$$F = -\nabla U$$

$$= \frac{g}{r^6} [5(3 - 30 \cos^2 \theta + 35 \cos^4 \theta) \hat{e}_r - (60 - 140 \cos^2 \theta) \cos \theta \sin \theta \hat{e}_\theta] \quad (24)$$

where c and c' are quadrupole moments, and g is defined as $g = (16\pi/3)Kcc'$.

Following the same procedure as in previous section, the equations of motion are obtained:

$$\gamma_{11} \{v_r F(\theta) + (q - 1)v_\theta \sin \theta \cos \theta\} = -5g (3 - 30 \cos^2 \theta + 35 \cos^4 \theta)/r^6$$

$$\gamma_{11} \{(q - 1)v_r \sin \theta \cos \theta + v_\theta Q(\theta)\} = -g (60 - 140 \cos^2 \theta) \cos \theta \sin \theta / r^6. \quad (25)$$

Solving the above equations with the initial conditions we get

$$v_r = \frac{g}{qr^6 \gamma_{11}} [(\sin^2 \theta + q \cos^2 \theta)(3 - 30 \cos^2 \theta + 35 \cos^4 \theta)$$

$$+ (q - 1)^2 \sin^2 \theta \cos^2 \theta (60 + 140 \cos^2 \theta) - 8q] \quad (26)$$

$$v_\theta = \frac{g}{qr^6 \gamma_{11}} [-15 - 45q + (-80q + 90) \cos^2 \theta + (140q - 315) \cos^4 \theta] \cos \theta \sin \theta.$$

For $r = 2a$ and $\theta = \theta_c$ the ratio of the magnitude of quadrupole to dipolar force is equal to 0.03, for $\alpha = 2.05$, $\beta = 0.2$ [17]. By taking $r_0 = 2a$ and $\theta_0 \cong 0$, the path of the particle with planar anchoring and $q = 3/2$ is

$$r/a = 2 \left[\frac{1}{29} (11 + 4 \cos^2 \theta + 14 \cos^4 \theta) \right]^{0.7}$$

$$\times \exp[1 - 1.13 \arctan(0.16 + 1.14 \cos^2 \theta)] / (\cos \theta)^{0.11}. \quad (27)$$

In figure 3, r/a has been plotted versus θ .

4. Some remarks and conclusions

We have obtained the trajectory of particle motion in the presence of another particle immersed in a nematic liquid crystal. The spherical particles, of radius a , are positioned at $r(0, 0)$ and $r(r, \theta)$. In section 2 we supposed that the long-range attraction force dominates between the particles immersed in the liquid crystal. The polar components of the velocity and the path of the particle for $q = 3/2$ have been obtained. In section 3, the path of moving particle has been obtained, for the case of quadrupole interaction between particles with planar anchoring. We are now in a position to make some remarks.

- (1) In this paper the dipole–dipole interaction has been considered in parallel and anti-parallel cases (i.e. two particles with hyperbolic hedgehog defects, accompanying defects on the same side and different sides of each particle [10]), and repulsive quadrupole interaction between two particles.
- (2) One can monitor the trajectory of the particle in the regimes in which the attractive dipolar and repulsive quadrupole forces dominate, compare it with figure 2 and 3 respectively and be sure about the value of $q = 3/2$ [11].
- (3) In a nematic liquid crystal medium, the trajectory of particle motion in the presence of another particle strongly depends on the initial conditions. In this work we only use the initial condition $r = r_0$, $\theta \approx \pi/2$, $v_0 = 0$ for homotropic anchoring and $r = 2a$, $\theta = 0$, $v_0 = 0$ for planar anchoring.
- (4) Strong homotropic anchoring results in dipolar symmetry of the director field around the particle, whereas planar anchoring conditions induce quadrupole interactions between immersed particles. Kotar *et al* [18] recently reported their experimental observation of the interaction between two particles with planar anchoring in one dimension by exerting an additional force on the moving particle. In our case there is no additional force except quadrupole and viscous forces. We then have a motion towards the top of the slab, too.
- (5) Both the interparticle force F and velocity of a moving particle in the presence of another particle follow $1/r^4$ and $1/r^6$ for long-range and short-range regimes respectively. These quantities are functions of the angle θ , too.
- (6) In the homotropic anchoring case the two particles collide with each other at angles 29.23° and 150.77° . In the results of Yada *et al* [10] the values of the angles are 10° and 130° respectively. Discrepancies presumably come from the fact that the fixed particles in our study are not fixed in their experiment.

Acknowledgments

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