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The model of elastic multipole

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ABSTRACT

The idea of elastic multipole is based on a number of drastic simplifications. On the one hand, the theories of point-like multipoles are phenomenological as a point-like source cannot produce director distortions. On the other hand, only a spherical particle allows for analytical theory. I present a mathematically consistent analytical model of spherical elastic multipoles of a finite radius a. The core idea is to consider the general problem of a particle in an ambient distorted director field whose actual source is replaced by an equivalent source in the form of a large concentric sphere of radius $\tilde{a}$. The solution obtained up to small terms $\sim a/\tilde{a}$ gives a simple universal tool to derive all particle's interactions. For an example, the interactions of elastic dipoles, quadrupoles, and monopoles with the ambient director, as well as their pair potentials are calculated by the straightforward differentiation. The assumptions underlying the model are discussed in detail. The main ideas of elastic multipoles and their tensorial structure, which are general and do not depend on the particular particle shape, are briefly presented.

1. Introduction

The core phenomena in the physics of nematic colloids is interaction of particles in a nematic liquid crystal (NLC). Particles immersed in a NLC interact via the director field **n**. A particle produces director distortions and another one interacts with these distortions. The unique physics behind this phenomenon lies in a long range of these distortions and, as a result, in the interaction whose power-law distance dependence evokes an analogy to the electrostatic multipole interaction [1–10]. Numerous experimental [11–20], analytical [1-10,21], and numerical [22–25] studies confirmed this analogy, and nowadays colloidal particles in a NLC are widely associated with elastic multipoles. Mathematically, however, elastic multipole is a model based on a number of strong simplifications. In this paper I will be concerned with the theory of elastic multipoles.

Of course, the multipole approach both in colloidal nematostatics and electrostatics is useful only when the distances between particles are much larger than their sizes. Though experiments show that this approach gives reasonable predictions when particles' separations are as small as about their diameters, at smaller separation the situation is very different. In the electrostatics, at small separations one cannot describe a particle by its single dominating multipole. The total multipole expansion however is practically useless and, as a result, the idea of multipole is inapplicable. Nevertheless, the electrostatics remains a linear theory at any distances so that a single multipole source is replaced by a distribution of point-like charges each of which produces a Coulomb field. In nematostatics the situation at small particles' separations is much more difficult. The reason is that the elastic theory of a NLC is a nonlinear vector theory which also involves the scalar order parameter. The role of the scalar order parameter is that to save the elastic energy it diminishes in areas where the distortions of the vector field are strong thus giving rise to defects in the nematic medium. The vector order parameter in the physics of liquid crystals is called director: it has unit length and the theory is invariant with respect to its sign change (the free energy is quadratic in the director components). At a large distance, particle-induced distortions are weak, the theory can be linearized and only then, under some additional simplification, one may talk of the electrostatic analogy and elastic multipoles. But close to particle's surface the director distortions can be strong so that the theory is strongly nonlinear and may involve point-like defects and line-like defects called disclinations. Moreover, when such particles are close to each other they are often get entangled by disclination lines of a very complicated form. This kind of particles' interaction can be addressed only numerically. The recent numerical studies of the defect structures at different particle surfaces and of the interaction of particles at short distances [24,26-29] have developed in a particular area of the physics of LCs. The mathematical notions which this area operates with are very different from those of the multipole approach. In this paper we consider only particles' interaction at large separations.

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The idea that particles' interaction in a NLC is of a long range and resembles the electrostatic interaction was first brought to the broad attention by Brochard and de Gennes [30] in 1970 and later by Lopatnikov and Namiot [31]. The fast development to the modern state of the theory had begun in the late nineties after papers by Ramaswamy et al. [2] and Lubensky et al. [4].

Mathematically, the similarity between the director-mediated and electrostatic interaction lies in the massless nature of both theories and the Coulomb-like behavior of the Green functions which derives from it [7,8]. The two systems however have fundamental differences. Electrostatic potential is a scalar described by the linear Laplace equation, whereas the director **n** is a vector field described by a linear equation only in the one constant approximation and only in 2 dimensions. Because of this linearity, core of a point defect plays the role of a charge in 2 dimensions [32,33]. But in 3 dimensions the field **n** is described by highly nonlinear equations and point defects cannot be linearly connected with the distortions of **n** they induce [1,4]. As a result, the theory of a large distance interaction via the director field, the colloidal nematostatics [40], consists of two quite different problems. The first problem is to find the form of interaction between different types of colloids which supposedly are elastic multipoles. The second is to express such multipoles in terms of the director field induced by colloid's surface. The fundamental difficulty in solving these problems is that the colloidal nematostatics has no *a priori* analog of the Coulomb law. Owing to the Coulomb law, the electrostatic interaction can be presented as that of point-like charges. An electrostatic charge can be a field source in spite of its infinitesimal size because the electric potential at its location is infinitely large. In contrast, the nematic director is finite everywhere implying that the *deformation source must have a finite size*.

The mathematical treatment of point sources is much easier and more familiar from the electrostatics, and the theory of interaction in nematic emulsions has been first developed phenomenologically for point-like colloids [1,2,4-6]. The phenomenological free energy (FE), resulting in a $1/r^5$ interaction of point-like sources and interpreted as the elastic quadrupole (Q)-quadrupole interaction, was proposed in [2]. Then in [4] this approach was further developed as to incorporate both point-like elastic $1/r^5$ and $1/r^3$ interactions, and the last was interpreted as the elastic dipole (d)-dipole interaction. This approach did not allow for finding the multipole moments as this task requires a finite size source. Lev and Tomchuk [5] and Lev et al. [6] combined a point-like source with a virtual (and arbitrary) enclosing surface whose symmetry was associated with that of the source multipole. This allowed the authors to demonstrate a possible tensorial structure of elastic multipoles, but the field of a surface cannot be adequately represented by any point-like source, and this useful approach was heuristic.

The model of elastic multipoles of a finite size, which allowed for establishing their tensorial structure, symmetry, and strength, has been developed in a series of papers by Pergamenshchik and Uzunova [7-10,40]. This theory based on the Green function technics establishes the elastic analog of charge density and Coulomb interaction. Recently, the author considered the interaction of elastic d and Q with the field of nematic distortions [34]. The result suggests a simple and universal description of both multipole-director and multipole-multipole interaction. Here I present the model of elastic multipoles based on this unified approach. The assumptions of the model are stated and discussed in Section 2A. The model is not phenomenological, but explicitly considers a spherical particle as the only possibility to get mathematically consistent analytical results. The main ideas of elastic multipoles and their tensorial structure are briefly presented in Sections 2B. and 2C. In Section 3, the general problem of the FE of a spherical particle in an ambient field is considered. The core result is the Green function which gives the general expression for the director field and its derivatives in the proximity of the particle surface, Section 3B. In Section 4, it is demonstrated that this result provides a simple universal tool which allows one to easily calculate all possible multipole's interactions. For an example, the interactions of elastic dipoles, quadrupoles, and monopoles with the ambient director, as well as their pair potentials are calculated by the straightforward differentiation. In concluding Section 5, the structure of the model and the main result are briefly summarized.

2. The multipole approach in the physics of nematic colloids

2.1. Main assumptions of the elastic multipole model

The main ideas and assumptions of the multipole approach to nematic colloids have been presented in a number of papers [4-8,40]. Nevertheless, it is instructive to begin our consideration with their explicit statement. The familiar multipole expansion in a power series of the inverse distance $1/r$ is the solution of linear Laplace's equation. This expansion is uniquely determined by the potential distribution over particle's surface. The electrostatic potential is governed by Laplace's equation at any distance from the source. However, a particle is well represented by its main multipole only at distances r much larger than the particle size. At small distances when particle size $\sim r$ this approach is meaningless as here the higher order multipoles cannot be neglected and particle can be described only by the total untruncated multipole expansion: at small separations the fields produced by particles and their interaction can generally be found only numerically. Implementing of the multipole approach to particles in a NLC is based on the same idea, but requires more elaboration.

First, Laplace's equation, generating the $1/r$ expansion, appears only in the one-constant approximation which therefore is ubiquitous in the physics of nematic colloids. Second, deformations of the homogeneous director are weak and governed by Laplace's equation only far from a general particle, whereas close to particle's surface the deformations can be strong and satisfy highly nonlinear equations even in the one-constant approximation. Thus, the elastic multipole approach can be useful at large r as usual, but now the inner boundary S of the linear "Laplace's zone" is the outer boundary of the nonlinear near zone rather than particle's surface, Fig. 1. Then the boundary S between the near and far zones must be taken as the effective surface of a colloidal particle, its radius must be taken as the effective particle's radius a, and one arrives at the following picture.

A particle induces distortions of a uniform director in an unrestricted medium. These are *bare distortions* as other particles and

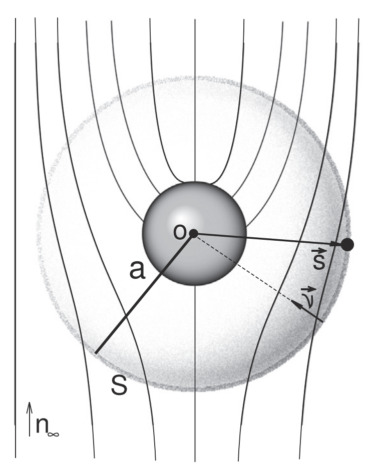

Fig. 1. The particlelike distortion domain around a real particle (darkened). At the enclosing spherical surface S of radius a, the director component normal to the unperturbed uniform director $\mathbf{n}_\infty$ is small, whereas at the particle's real surface it can be large. The area between the real surface and S is a nonlinear zone; the area outside S is a linear zone.