

## Local affine-connection approach to the elastic constants of nematic liquid crystals

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In this paper, the affine connection approach [D. Baalss and S. Hess, *Phys. Rev. Lett.* **57**, 86 (1986)] will be defined in terms of a local transformation. Accordingly, the macroscopic anisotropy of the nematic medium will be conceived as resulting from a local transformation where, at each point of the sample, the spherical molecules of an idealized hypothetical isotropic liquid have their shape changed to the ellipsoidal form of the nematic liquid crystals molecules. When such local character is imposed to this transformation, the patterns determined by the director configuration of the nematic medium acquire an intrinsic curvature whose correct treatment requires the replacement of the techniques and methods of the usual calculus by those of the differential geometry of nonflat surfaces. Such an approach will be used in the calculus of the nematic elastic constants. As a result, the dependence of the elastic constants on the scalar order parameter, on the eccentricity of the nematic molecules, and on the interaction between them will be determined and compared with the experimental data of the 4-methoxybenzylidene-4-n-butylaniline.

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### I. INTRODUCTION

Some years ago, Hess and co-workers [1–5] had proposed that the anisotropic rheological properties of a liquid crystal could be obtained by means of an affine transformation in which the spherical potential of spherical molecules, of a hypothetical isotropic liquid, is deformed to assume the ellipsoidal shape of the liquid crystals' interacting potential. The main aim of this paper is the proposition of a geometrical method that generalizes such an approach in such a way that such deformation can be taken as position dependent.

We will start with the observation that in a usual nematic sample the director orientation is inhomogeneous and, as consequence, the molecular deformation producing the affine connection approach is position dependent and the corresponding mathematical tools must take it into consideration. Essentially, it will be shown that after such transformation the usual derivatives do not transform as usual covariant vectors and, as a consequence, they must be replaced by covariant derivatives. The mathematical tools describing such change are today usual in many branches of the physics but, to our knowledge—save for the case where the liquid crystals defects are used to simulate the behavior of a light path at the neighborhoods of cosmological singularities [6]—such an approach is not usual in the liquid crystals physics. As we will show ahead, the natural way to implement it is to consider that the use of the Hess affine connection approach maps the nematic textures on a nonflat differentiable surface.

To avoid the criticism that we are introducing an unfamiliar and unnecessary formalism, it will be used here to obtain an absolutely nontrivial result, the nematic elastic constants will be derived from a very usual and simple starting point; the free energy must be a scalar constructed with the fundamental mathematical objects of the theory [7]. The determination of the thermal behavior of elastic constants of the nematic liquid crystals (NLC) [8–10] is an old-standing

problem for which experimental [11–15], computational [16,17], and analytical methods [18–23] have been applied and, for each of these approaches, a new set of results have been found. Nevertheless, despite such developments, the understanding of the elastic constants is not yet complete [24]; only the leading terms of their dependence on the scalar order parameters is firmly established [25] and, even recently, the nature of the anchoring of the molecules of these materials at the surface of the sample has been a theme of intense research [26–29]. Due to the broadness of this subject it is impossible to quote all relevant works on the area. For example, in the last years the interest on the role of the molecular rotational entropy on the elastic constants has arisen [30–37]. Surely, many questions related with important issues remain to be investigated and will not be considered here. The main aim of this work is to emphasize that the tolls of differential geometry are relevant and may be used in the study of the nematic phenomenology. In our approach to the nematic elastic constants some fundamentals of the affine connection approach will be combined with the fundamentals of the pseudomolecular approach [38–41] to produce an expression that, blends them to obtain the elastic constants in terms of these parameters.

Finally, as an application, our results will be compared with the experimental data of the 4-methoxybenzylidene-4-n-butylaniline (MBBA). We believe that our final results are sufficiently solid to justify the introduction of such mathematical apparatus on the physics of the liquid crystals. The paper is written in a way to avoid mathematical subtleness and the physical content will be detached.

### A. Fundamentals

According to Hess [1–5], the interaction between the liquid crystals' molecules can be obtained from the interaction between the spherical molecules of a common hypothetical isotropic liquid, once their spherical potential is deformed until it assumes the ellipsoidal shape of the nematic molecules. This challenging assumption considers the geometry

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generated by the interacting potential, the essence of the anisotropic behavior found on the liquid crystals phenomenology and, if it cannot completely explain the diversity of the liquid crystals' behavior [42] it has, at least, successfully described many rheological problems [1–5]. In mathematical terms, it is assumed that the ellipsoidal interaction potential  $\Phi_E$  between nematic molecules can be transformed in a spherical interaction potential  $\Phi_S$ , once the vector  $\vec{r}$  connecting two particles is submitted to an appropriated affine transformation. That is,

$$\Phi_E(r_S) = \Phi_S(r_E), \quad (1)$$

where the indexes  $E$  and  $S$  stand for ellipsoidal and spherical symmetries, respectively. Namely, the nonspherical potential,  $\Phi_E$ , can be substituted by a spherical,  $\Phi_S$ , if the distance between two points is given by a metric in which two points on the nonspherical equipotential surface become “equidistant” from the potential center. As consequence, there would be an affine transformation leading the physics of liquids formed with spherically interacting molecules to the physics of liquids with ellipsoidal ones, and vice versa. That is, the measurements of distances in the two potentials would be connected by relations having the form

$$r_S^i = \frac{dr_S^i}{dr_E^k} r_E^k \quad \text{and} \quad \frac{d}{dr_S^j} = \frac{dr_E^i}{dr_S^j} \frac{d}{dr_E^i}, \quad (2)$$

where the first equation is the law of transformation for vectors, while the second gives the law of transformation for derivatives. Hereafter, the sum rule over repeated indexes is being assumed. Of course, these relations satisfy the inverse relations

$$\frac{dr_S^i}{dr_E^k} \frac{dr_E^k}{dr_S^j} = \delta_j^i. \quad (3)$$

An essential consequence of these hypotheses—the motive of this work—can be understood when it is assumed that the nematic sample is not homogeneously aligned, and the corresponding affine transformation becomes effectively point dependent. Under such a condition the derivatives of a vector do not behave as a tensor and a new definition of derivative must be introduced. Namely, all quantities having the form  $dv^i/dr^j$ , where  $v^i$  is the  $i$  component of any vector  $\vec{v}$ , must transform according to Eq. (2) and, consequently,

$$\frac{dv^i}{dr^j} \rightarrow \frac{dr_E^m}{dr_S^j} \frac{d}{dr_E^m} \left( \frac{dr_S^i}{dr_E^k} v_E^k \right) = \frac{dr_E^m}{dr_S^j} \frac{d^2 r_S^i}{dr_E^m dr_E^k} v_E^k + \frac{dr_E^m}{dr_S^j} \frac{dr_S^i}{dr_E^k} \frac{dv_E^k}{dr_E^m}. \quad (4)$$

When the director configuration is not homogeneous, changing from point to point, the first term of the high side of the above equation becomes non-null, revealing that  $dv^i/dr^j$  is not a tensor under the transformation given in Eq. (2). This behavior is usually found when point dependent coordinates transformations are being considered. The standard way to deal with it modifies the rule of differentiation; normal derivatives have to be changed to covariant derivatives [43] in such a way that the anomalous term of the above equation is canceled. Furthermore, even when the use

of covariant differentiation is required, it can happen that such a procedure has resulted from an “inconvenient” system of coordinates, and an appropriated change of coordinates could restore the normal derivative rule. Nevertheless, there are situations in which the use of covariant derivatives becomes unavoidable, and there is no change of coordinate able to reestablish the normal derivation rule. In this case, the surface where the physical phenomena happens has an intrinsic curvature.

The first result of this paper will be the demonstration that the affine connection approach reveals that the mathematic description of the nematic textures has necessarily associated a surface with an intrinsic curvature and, consequently, its correct description requires the use of mathematical tools consistent with it. For example, covariant derivatives must substitute the usual derivatives. As all nematic textures arise from variations of the director and, furthermore, its variations are related to the elasticity of the sample, we will apply such an approach to study the nematic elasticity. It will be shown that from very simple scalar functions, constructed with the correct covariant differentiation rule, a description of the nematic elasticity can be obtained. At the end, the results of such description will be compared with experimental data of the MBBA.

## II. CURVATURE OF NEMATIC SAMPLE

Equation (4) revealed the necessity of the use of covariant derivatives when the affine connection approach is used to describe nematic physics. In order to do that, the metric of the surface generated by the nematic textures must be determined. This is the aim of this section. To give a metric prescription we remember that the distance in a spherical geometry is given by

$$d_S^2 = \delta_{ij} r_S^i r_S^j, \quad (5)$$

while, in a nonspherical geometry, it is given by

$$d_E^2 = g_{ij} r_E^i r_E^j, \quad (6)$$

where, for the physical situation that we are studying,  $g_{ij}$  gives the metric induced by the equipotential surfaces of the nonspherical potential. The affine connection approach affirms that the physical phenomena happening in the nonspherical equipotential surface can be obtained, through an affine transformation, from one happening in a spherical equipotential surface. To obtain such law of transformation, given in Eq. (2), it will be observed that the points localized along the same ellipsoidal equipotential surface are “equidistants” from a potential center. From this point of view, the Hess hypotheses can be formulated by saying that for a ellipsoidal symmetric potential there is an associated spherically symmetric potential satisfying the rule,

$$d^2 \equiv d_S^2 = d_E^2. \quad (7)$$

Therefore the passage from the ellipsoidal potential to the spherical one, or vice versa, stated in Eq. (1), can be realized through a metric change in the surface in which the phenomenon is being studied. That is, the measurements of distances

in the two potentials must be connected by some law, determined by Eq. (2). To obtain a formal relation between the metric  $g_{ij}$  and this change of coordinate system it is enough to observe that when this equation is substituted in Eqs. (1), (5), and (6), it is obtained,

$$\delta_{ij} r_S^i r_S^j = \delta_{ij} \frac{dr_S^i}{dr_E^k} \frac{dr_S^j}{dr_E^l} r_E^k r_E^l. \quad (8)$$

That is,

$$g_{kl} = \frac{dr_S^i}{dr_E^k} \frac{dr_S^j}{dr_E^l} \delta_{ij}. \quad (9)$$

The use of superior and inferior indexes follows the usual rule of contravariant and covariant vectors and will be illustrated below, in the context of the present model. They are related with direct and inverse transformation laws; tensor components that transform according to vectors receive superior indices and are called contravariants and those that transform according with the inverse transformation receive inferior indices and are called covariants. In this way, the metric,  $g_{ij}$ , given in Eq. (6) is contravariant, and its inverse,  $g^{ij}$ , which can be obtained from the rule,

$$g_{ik} g^{kj} = \delta_i^j, \quad (10)$$

is contravariant. These rules give a metric form to the affine transformation method; once a physical quantity is known in a spherically symmetric system, Eq. (1) says that it is enough to apply on it the transformation to the ellipsoidal system to obtain the corresponding expression in the nonspherical system. Nevertheless, to obtain an explicit form to this rule it is necessary to know the metric  $g_{ij}$  that generates such a transformation. The obtainment of such a metric in terms of the nematic parameters is our next objective.

### A. Ellipsoidal order parameter

It will be assumed here that the metric  $g_{ij}$  is determined from the same matrix  $E_{ij}$  that characterizes the quadratic form of a uniaxial ellipsoid. A generalization for a biaxial NLC is straightforward and will appear elsewhere. Given a uniaxial ellipsoid there is always a local coordinate system in which it assumes the form

$$\frac{x_1^2}{a^2} + \frac{x_2^2}{b^2} + \frac{x_3^2}{b^2} = 1, \quad (11)$$

where its three main axis lengths are given, respectively, by  $\{a, b, b\}$ , each of them pointing to the directions given, respectively, by the three orthonormal vectors,  $\{\vec{e}_x, \vec{e}_y, \vec{e}_z\}$ , where

$$\vec{e}_x = (1, 0, 0), \quad \vec{e}_y = (0, 1, 0), \quad \vec{e}_z = (0, 0, 1), \quad (12)$$

$x_1, x_2$ , and  $x_3$  being the coordinates along them. In a compact form, this ellipsoid can be written as  $E_{ij}^d x^i x^j = 1$ , where

$$E_{ij}^d = \begin{pmatrix} \frac{1}{a^2} & 0 & 0 \\ 0 & \frac{1}{b^2} & 0 \\ 0 & 0 & \frac{1}{b^2} \end{pmatrix} \quad (13)$$

is the diagonalized matrix characterizing the ellipsoid, which is completely characterized by the eigenvalues,

$$\left\{ \frac{1}{a^2}, \frac{1}{b^2}, \frac{1}{b^2} \right\}, \quad (14)$$

and eigenvectors given by Eq. (12). The index  $d$  in  $E_{ij}^d$  are used to remember that the corresponding characteristic matrix  $E_{ij}^d$  is yet diagonal. The matrix  $E_{ij}$  representing an arbitrary uniaxial ellipsoid, having the same semiaxis lengths, can be obtained from the matrix  $E_{ij}^d$  through an arbitrary rotation in which its three orthonormal main axis  $\{\vec{e}_x, \vec{e}_y, \vec{e}_z\}$  are rigidly rotated to a new set of orthonormal  $\{\vec{p}, \vec{q}, \vec{r}\}$  vectors. Let us demonstrate that after such rotation  $E_{ij}$  assumes the form

$$E_{ij} = \frac{1}{a^2} p_i p_j + \frac{1}{b^2} q_i q_j + \frac{1}{b^2} r_i r_j. \quad (15)$$

To do it, it is enough to demonstrate that  $\vec{p}, \vec{q}, \vec{r}$  are the eigenvectors of  $E_{ij}$  with the set given in Eq. (14) as the eigenvalues. Using the orthonormal relations, Eq. (17), between  $\vec{p}, \vec{q}$ , and  $\vec{r}$ , it is trivial to compute eigenvectors and eigenvalues of  $E$ , and observe that

$$E_{ij} p^j = \frac{1}{a^2} p_i, \quad E_{ij} q^j = \frac{1}{b^2} q_i, \quad E_{ij} r^j = \frac{1}{b^2} r_i. \quad (16)$$

So,  $\vec{p}, \vec{q}$ , and  $\vec{r}$  are the normalized eigenvectors of  $E$  and  $\{1/a^2, 1/b^2, 1/b^2\}$  the corresponding eigenvalues. As a matrix is completely characterized by its eigenvalues and eigenvectors, the matrix given in Eq. (14) gives the rotated version of the one given in Eq. (13).

An important property of these eigenvectors is that they compose a complete set and, therefore, are linked by the relation [44]

$$p_i p_j + q_i q_j + r_i r_j = \delta_{ij}. \quad (17)$$

Combining this equation with Eq. (14), it is obtained

$$E_{ij} = \frac{1}{a^2} p_i p_j + \frac{1}{b^2} (\delta_{ij} - p_i p_j) = \frac{1}{1-e} \{\delta_{ij} - e p_i p_j\}, \quad (18)$$

where

$$e = 1 - b^2 \quad (19)$$

is the ellipsoid eccentricity and  $\vec{p}$  corresponds to the symmetric axis of the uniaxial ellipsoid. We have fixed the length of the uniaxial semiaxis of the ellipsoid as  $a=1$ , to be in accord with the normalization that we have adopted to the sphere with radius  $r=1$ .

So, in an arbitrarily rotated coordinate system, this ellipsoid can be written as

$$E_{ij}y^i y^j = 1. \quad (20)$$

As the condition  $e=0$  reduces the ellipsoid to a sphere of radius  $r=1$ , the anisotropy found in the rheological parameters can be interpreted as the deformation induced on the nematic medium by the nonspherical equipotential surfaces. Consequently, this anisotropy can be quantified by measuring how much this ellipsoid differs from an equivalent sphere. To obtain such a sphere we remember that, according to Eq. (13), the tensor characterizing an ellipsoid is a linear function of the inverse of the square of its axes and, furthermore, it would be reduced to a sphere if these axes become equal. Accordingly, the equivalent sphere can be defined as that one for which the radius  $r$  satisfies the relation

$$\frac{1}{r^2} = \frac{1}{3} \text{Tr}(E) = \frac{1}{1-e} \left(1 - \frac{e}{3}\right). \quad (21)$$

Namely, the square of the inverse of its radius is given by the mean of the inverse of the square of the ellipsoid semiaxis. Therefore if  $E$  is the characteristic matrix of an ellipsoid, the elements of the characteristic matrix of the equivalent sphere would be given by  $S_{ij} = \delta_{ij} \text{Tr}(E)/3$  and, consequently, the ellipsoidal deformation  $\Delta E$  could be defined by the difference between the ellipsoid and its equivalent sphere,

$$\Delta E_{ij} = E_{ij} - S_{ij} = E_{ij} - \frac{1}{3} \delta_{ij} \text{Tr}(E), \quad (22)$$

which, with the use of Eqs. (18) and (21), becomes

$$\Delta E_{ij} = \frac{e}{1-e} \left\{ \frac{1}{3} \delta_{ij} - p_i p_j \right\}. \quad (23)$$

That is, the ellipsoidal deformation  $\Delta E$  is determined by the product of two distinct terms,  $e/(1-e)$  and

$$Q_{ij}^E = \frac{1}{3} \delta_{ij} - p_i p_j. \quad (24)$$

This last term is the anisotropic component of the ellipsoidal deformation. It coincides with the quadrupolar momentum tensor [45], being formally similar to the expression of the tensorial order parameter of a nematic liquid crystal. In fact, as stated by de Gennes [7], the tensor order parameter can be measured from the difference between the anisotropic and isotropic parts of a given physical property. Its was just this that has been done with  $E_{ij}$  to arrive at Eq. (23). In that equation, the eccentricity term,  $e$ , furnishes the magnitude of the ellipsoidal elongation; different eccentricities correspond to different molecular shapes; when  $e < 0$ , we have that  $b > 1$ , corresponding to a discotic phase and when  $e > 0$ , we have that  $b < 1$ , corresponding to a calamitic phase.

Summarizing, the ellipsoidal matrix, given in Eq. (15), can be written as

$$E_{ij} = S_{ij} + \frac{e}{b^2} Q_{ij}^E = \frac{1}{1-e} \left\{ \left(1 - \frac{e}{3}\right) \delta_{ij} + e Q_{ij}^E \right\}, \quad (25)$$

where the first term corresponds to the spherical (isotropic) part of  $E_{ij}$  and the second term describes its deviation from the spherical shape. As defined by Hess, and explained above, the affine-connection approach can be realized by de-

forming a spherical interacting potential up to the point in which it assumes the ellipsoidal form of the nematic molecules. So, such deviation is described by a term that is structurally equal to the order parameter tensor. It will be from this form of  $E_{ij}$  that the metric  $g_{ij}$  will be constructed; it will consist of an isotropic part, proportional to  $\delta_{ij}$  and an anisotropic part, proportional to  $Q_{ij}$ .

## B. Thermodynamics in the metric

Above, it has been shown that the matrix  $E_{ij}$  characterizing an ellipsoid differs from a sphere by a tensorial term,  $Q_{ij}^E$ , which is formally identical to the nematic order parameter  $Q_{ij}$ . It is important to stress that—up to this point—this equality is restricted to the form of these mathematical objects, conceptually they describe different objects, this being the reason why we have introduced the superscript  $E$  on  $Q_{ij}^E$ . The aim of this section is to show that such formal equality can be improved until the point where both concepts become identical and a temperature dependent metric is obtained. This remarkable result stays in the essence of the forthcoming use of the Hess approach and its physical motivation can be easily understood: for temperatures greater than the NI phase transition point the nematic liquid is isotropic and all directions are equivalent, for temperature smaller than the NI phase transition point the liquid becomes anisotropic and, at each point, many physical properties acquire a privileged direction. So, at least from this naive point of view, it is hoped that a temperature dependent metric can be constructed. We will introduce such a study by remembering some standard considerations about the physical meaning of the microscopic order parameter and, afterwards, we will use it to construct a macroscopic order parameter. In our next developments, especially in Eq. (26), the distinction between microscopic and macroscopic order parameter is the standard one and follows the usual approach [7], they are discussed ahead for clarity of our reasoning.

The anisotropy of liquid crystal materials can be observed at two levels, macroscopically and microscopically. On thermodynamical measurements it appears macroscopically; but, it has a microscopic origin, the LC molecules have an intrinsic microscopic anisotropy that, when averaged, may or may not be observed on macroscopic measurements, it depends on the temperature. Let us distinguish between the microscopic and the macroscopic nature of  $Q_{ij}$  by putting a hat over its vectorial parameter  $\vec{n}$  when it denotes a microscopic unitary vector. So,  $Q_{ij}(\hat{n})$  means that  $\vec{\hat{n}}$  is a microscopic random variable—the molecular long axis—and the associated order parameter is a microscopic order parameter. Likewise, without a hat on  $\vec{n}$ ,  $Q_{ij}(n)$  means that  $\vec{n}$  is a macroscopic variable, the director, and the corresponding order parameter is a macroscopic order parameter. The connection between these two quantities is made by assuming that the microscopic random variable  $\vec{\hat{n}}$  oscillates so fast that when  $Q_{ij}(\hat{n})$  is averaged, on the time and/or on neighborhoods of a point, such average determines the macroscopic order parameter  $Q_{ij}(n)$ , where  $n$  is the usual director [7], and  $Q_{ij}$  has the same form as given in Eq. (24), with  $\hat{n}$  replaced by  $n$ , from which

the uniaxial macroscopic anisotropy can be measured. In mathematical terms [7],

$$\langle Q_{ij}(\hat{n}) \rangle = S Q_{ij}(n), \quad (26)$$

where  $\langle x \rangle$  stands for the statistical average of the random variable  $x$ . As anticipated above,  $S$  gives the intensity by which the random oscillations make the microscopic anisotropy be observed on a macroscopic scale. To get such a result it is enough to multiply the left side of the above expression by the macroscopic order parameter,  $Q^{ji}(n)$ , and take the trace of the resulting expression,

$$Q^{ji}(n) \langle Q_{ij}(\hat{n}) \rangle = S Q^{ji}(n) Q_{ij}(n), \quad (27)$$

to obtain

$$S = \frac{3}{2} \left( -\frac{1}{3} + \langle (\hat{n} \cdot \vec{n})^2 \rangle \right). \quad (28)$$

This equation is the standard expression for scalar order parameter [7].

Let us now consider that the interacting potential attached to each molecule of a nematic sample has an equipotential surface that can be represented by a matrix  $E_{ij}$ . When, in the neighborhoods of a point, a large set of such objects are taken together we can consider, in exact analogy with Eq. (26), that such a set may be, or not, aligned, generating, or not, a nematic phase. The representation of the macroscopic results of this microscopic alignment can be made through the matrix  $Q_{ij}^E$  by assuming that it satisfies the same relation of a microscopic order parameter,

$$\langle Q_{ij}^E(\hat{n}) \rangle = S Q_{ij}(n), \quad (29)$$

which means that the microscopic anisotropy of each molecule becomes coupled with the ones at its neighborhoods; the long axis of each of them oscillates along the same direction, generating a nematic phase. An important consequence of the above reasoning is that it gives macroscopic consequences to the microscopic ellipsoidal anisotropy of each nematic molecule. As  $Q_{ij}^E$  appears in the definition of  $E_{ij}$ , Eq. (25) reveals that the ellipsoidal matrix  $E_{ij}$  also has a macroscopic counterpart. That is, in giving meaning to  $\langle Q_{ij}^E \rangle$  a corresponding meaning must be also given to  $\langle E_{ij} \rangle$ . Such a matrix measures the passage from a macroscopic isotropic symmetry (determined by the term  $\delta_{ij}$ ), to a macroscopic ellipsoidal symmetry of a nematic phase. It will be assumed here that such anisotropy is realized through a macroscopic metric  $g_{ij}$ . That is,  $g_{ij} = N \langle E_{ij} \rangle$ ; or

$$\begin{aligned} g_{ij} &= N \left\{ \frac{1}{3} \text{Tr}(E) \delta_{ij} + \frac{e}{1-e} \langle Q_{ij}(\hat{n}) \rangle \right\} \\ &= \frac{N}{(1-e)} \left\{ \left( 1 - \frac{e}{3} \right) \delta_{ij} + e S Q_{ij}(n) \right\}, \end{aligned} \quad (30)$$

where  $N$  is a normalization constant introduced in order to assure the director normalization,

$$n^i n_i = g^{ij} n_j n_j = 1.$$

A straightforward calculation reveals the value of  $N$ , showing that

$$g_{ij} = \frac{1}{[3 - e(1 + 2S)]} \{ (3 - e) \delta_{ij} + 3e S Q_{ij}(n) \} \quad (31)$$

and

$$g^{ij} = \frac{1}{[3 - e(S - 1)]} \{ [3 - e(S + 1)] \delta^{ij} + 3e S Q^{ij}(n) \}. \quad (32)$$

On these equations it is assumed that the metric induced by the ellipsoidal anisotropy depends on the scalar order parameter  $S$  and, therefore, it is macroscopic and determined by the nematic temperature; at the isotropic phase ( $S=0$ ) the metric is spherical and macroscopic measurements would be isotropic. As the temperature is reduced, the nematic-isotropic phase transition creates a non-null  $S$ , which induces a macroscopic ellipsoidal anisotropy described by the order parameter  $S$  and the eccentricity  $e$ . It is important to observe that this metric has as aim the realization of the Hess hypotheses of the affine connection approach; it is a thermodynamic effect induced by the anisotropies of the nematic phase, as will be proved with the establishment of Eq. (36). It does not mean, for example, that the real metric of the space in which the phenomena happens has changed.

### C. Connections and curvature

Here, it will be shown that in the presence of nematic textures the application of the affine connection approach must be necessarily followed by the use of covariant differentiation; the Hess hypothesis leads to a nonplanar three-dimensional surface whose scalar curvature is nonzero. To arrive at these results some formulas of differential geometry will be used. Their deductions are straightforward and a ‘‘physical derivation’’ of them can be found, for example, in the classical Weinberg book [43]. To calculate the curvature associated with the metric  $g_{ij}$ , the connection,

$$\Gamma_{ij}^k = \frac{1}{2} g^{km} \left\{ \frac{\partial g_{mj}}{\partial x^i} + \frac{\partial g_{mi}}{\partial x^j} - \frac{\partial g_{ij}}{\partial x^m} \right\}, \quad (33)$$

must be evaluated. Once having  $\Gamma_{ij}^k$ , the Ricci tensor,  $R_{ij}$ ,

$$R_{ij} = R_{ikj}^k,$$

$$R_{imj}^k = \frac{\partial \Gamma_{im}^k}{\partial x^j} - \frac{\partial \Gamma_{ij}^k}{\partial x^m} + \Gamma_{im}^n \Gamma_{jn}^k - \Gamma_{ij}^n \Gamma_{mn}^k, \quad (34)$$

can be calculated. With these objects, the scalar curvature  $R$ ,

$$R = g^{ij} R_{ij}, \quad (35)$$

can be determined. All these calculations are straightforward, but lengthy. At the end, it can be shown that the connection is given by

$$\begin{aligned} \Gamma_{ij}^k &= \frac{3eS}{2[3 - e(1 + 2S)][3 - e(1 - S)]} \{ [3 - e(1 + 2S)] [n^k (\partial_i n_j \\ &\quad - \partial_j n_i) + n_j (\partial_i n^k - \partial^k n_i)] - [3 - e(1 - S)] n_i (\partial_j n^k + \partial^k n_j) \\ &\quad + 3e S n_i n^m (n^k \partial_m n_j + n_j \partial_m n^k) \}, \end{aligned}$$

and the scalar curvature is given by

$$R = \frac{9e^2S^2}{2[3-e(1-S)]^2}[\vec{n} \cdot (\nabla \times \vec{n})]^2 - \frac{3eS}{[3-e(1-S)]} \times \vec{\nabla}[\vec{n}(\vec{\nabla} \cdot \vec{n}) + \vec{n} \times (\vec{\nabla} \times \vec{n})]. \quad (36)$$

This result justifies all developments so far undertaken. It reveals that the scalar curvature associated with the textures of a nematic sample is nonzero, and given by the sum of two usual nematic textures, the bend texture term,  $[\vec{n} \cdot (\nabla \times \vec{n})]^2$ , and the saddle-splay texture term,  $\vec{\nabla}[\vec{n}(\vec{\nabla} \cdot \vec{n}) + \vec{n} \times (\vec{\nabla} \times \vec{n})]$ . As  $R$  is a scalar quantity, this quantity will be always the same in all systems of coordinates and, therefore, it cannot be eliminated. The curvature that it expresses is a basic property of the affine connection approach; it intrinsically associates the nematic textures with a nonflat surface. At the end of this work we will retake this point and discuss its physical meaning.

#### D. Naive approach to elastic energy

Above, it has been learned that when the affine connection approach is used the nematic textures must be described by a nonflat surface. Consequently, necessarily, the usual derivatives must be substituted by covariant derivatives [43],

$$\partial_i v^j \rightarrow D_i v^j \equiv \partial_i v^j + \Gamma_{ik}^j v^k. \quad (37)$$

In order to see what can be gained with such improvement, a very naive model for the elastic energy stored in the elastic textures will be now considered. The elastic constants will be computed with the use of the above derivative rule, and the results will be compared with those obtained with the use of normal derivatives. Ahead, more elaborate models will be presented.

A straightforward generalization of Hook's law to the liquid crystals medium reveals that around a given point the elastic energy must be at least proportional to the variations of the director, and the square of the scalar order parameter [46]. That is,

$$E \approx \alpha S^2 (\partial_i n^j)^2.$$

By using the usual derivatives rules it is straightforward to show that, in terms of the usual expressions for the textures of the nematic phase, this equation can be rewritten as

$$E \approx \alpha S^2 \{ (\vec{\nabla} \cdot \vec{n})^2 + (n \cdot \vec{\nabla} \times \vec{n})^2 + (n \times \vec{\nabla} \times \vec{n})^2 - \vec{\nabla}[\vec{n}(\vec{\nabla} \cdot \vec{n}) + \vec{n} \times (\vec{\nabla} \times \vec{n})] \}$$

According to this simple model, all elastic constants of the nematic liquid crystals would be identical, no difference between their values would be observed. Otherwise, when normal derivatives are substituted by covariant derivatives it is found that

$$E \approx \alpha S^2 (\partial_i n^j)^2 \rightarrow \alpha S^2 (D_i n^j)(D^i n_j) = \alpha S^2 g^{jk} g^{im} (D_i n_k)(D_m n_j).$$

After a straightforward calculation it is found that

$$E \approx \alpha S^2 \left\{ (\vec{\nabla} \cdot \vec{n})^2 + \left( 1 - \frac{3e[6-e(S+2)]}{2[3+e(S-1)]^2} \right) (n \cdot \vec{\nabla} \times \vec{n})^2 + \left( 1 - \frac{3eS}{3+e(S-1)} \right) (n \times \vec{\nabla} \times \vec{n})^2 - (\vec{\nabla}[\vec{n}(\vec{\nabla} \cdot \vec{n}) + \vec{n} \times (\vec{\nabla} \times \vec{n})]) \right\}.$$

Revealing a nontrivial expression to the elastic constants,

$$K_{11} \approx \alpha S^2,$$

$$K_{22} \approx \alpha \left( 1 - \frac{3e[6-e(S+2)]}{2[3+e(S-1)]^2} \right) S^2,$$

$$K_{33} \approx \alpha \left( 1 - \frac{3e[6-e(S+2)]}{2[3+e(S-1)]^2} - \frac{9e^2S^2}{2[3+e(S-1)]^2} \right) S^2. \quad (38)$$

The introduction of the covariant derivative has given a dependence of the nematic elastic constants on molecular eccentricity  $e$  and on the scalar order parameter  $S$ . As it will be shown below, see Eqs. (51), (52), and (55), this expression furnishes an acceptable ratio between  $K_{11}$  and  $K_{22}$ , but it strongly fails for the value of  $K_{33}$ . As an immediate inspection shows, even the simplest experimental data of calamitic compounds are always related by the rule,  $K_{22} < K_{11} < K_{33}$  [7]. Nevertheless, the above expressions obeys the relation  $K_{33} < K_{22} < K_{11}$ . Ahead, a more elaborated model will be proposed. Essentially, it will be learned from these models that the ratio  $K_{33}/K_{11}$  is also determined by the multipolar interaction between the nematic molecules, a feature which is not observed on  $K_{22}/K_{11}$ . This is the physical fact that explains the differences found on the experimental data of these ratios [24].

### III. ELASTIC ENERGY

Above, a naive model was used to evaluate the elastic energy stored on the nematic textures. Even furnishing an expression for the elastic constants as a function of the molecular eccentricity and the scalar order parameter, the expression for  $K_{33}$  disaccords with the experimental data. Here, such a model will be improved and a global agreement with the experimental data will be intended. The starting point will be the usual one; since the free energy is a scalar function, it would be constructed from scalars obtained from the simplest unitary invariants of the mathematical objects that characterize the liquid crystals theory [7]. Furthermore, in order to arrive at such expression some essential physical ingredients must be added to the ones already considered in the above naive model; beyond the geometry aspects contained in the use of covariant derivatives, the relative orientation of the interacting anisotropic molecules and the distance between them have to be explicitly considered.

Let us begin by considering the angular interaction [47], which has been extensively formulated in terms of tensorial products of the order parameter,

$$I_j^i(\hat{p}, \hat{q}) = Q^{ik}(\hat{p})Q_{kj}(\hat{q}). \quad (39)$$

This is a function of random variables,  $\hat{p}$  and  $\hat{q}$  localized, respectively, at different points  $\vec{r}_1$  and  $\vec{r}_2$ , and only the thermodynamic quantities generated by it can have macroscopic meaning. To obtain them, it will be assumed that the connected part of the two points function  $\langle Q^{ik}(\hat{p})Q_{kj}(\hat{q}) \rangle$  can be neglected and, consequently, we can approximate  $\langle I_j^i(\hat{p}, \hat{q}) \rangle$  by  $\langle I_j^i(\hat{p}, \hat{q}) \rangle = \langle Q^{ik}(\hat{p}) \rangle \langle Q_{kj}(\hat{q}) \rangle$  [48]. So, using Eq. (13), we arrive at

$$\langle I_j^i(\hat{p}, \hat{q}) \rangle = S^2 Q^{ik}(p)Q_{kj}(q) = S^2 I_j^i(p, q). \quad (40)$$

This is the basic expression from which the elastic constants have been calculated [46]. To obtain scalar invariants from this tensor at least two procedures can be undertaken. It is enough to take its trace,

$$i_1(\vec{r}_1, \vec{r}_2) = \langle I_i^i(\hat{p}, \hat{n}) \rangle = S^2 I_i^i(p, n) = S^2 \left( -\frac{1}{3} + (\vec{p} \cdot \vec{q})^2 \right), \quad (41)$$

or contract it with the radius vector  $\vec{r} = \vec{r}_1 - \vec{r}_2$ , representing the distance between the nematic domains  $\vec{p}$  and  $\vec{q}$ . That is,

$$i_2(\vec{r}_1, \vec{r}_2) = \langle r^i r^j I_{ij}(\hat{m}, \hat{n}) \rangle = S^2 r^i r^j I_{ij}(m, n). \quad (42)$$

Each of these invariants will be used to obtain expressions for the elastic energy of a nematic sample. The first of them,  $i_1$ , expresses an angular interaction, the Maier-Saupe interaction [49]. That is, two directors,  $\vec{p}$  and  $\vec{q}$ , only are elastically coupled when  $S \neq 0$ , otherwise, in the isotropic phase ( $S = 0$ ), they are uncoupled. Furthermore, through the product  $r^i r^j$ ,  $i_2$  couples the anisotropic distance between the nematic molecules with this angular interaction, just the quantities that we supposed would describe the nematic elasticity. Consequently, it is from  $i_2$  that a best description of the nematic elasticity would be possible. Anyway, we will begin our study looking for the elastic constants predicted by the invariant  $i_1$ . There are two main reasons for this procedure, it will explicitly show the limits of a pure angular description of the nematic elasticity, and it will be used in the interpretation of the results that will be found ahead in the study of  $i_2$ .

So, observe that the change  $\vec{r}_2 = \vec{r}_1 + \vec{r}$  gives

$$\begin{aligned} Q_{kj}(\vec{r}_2) &= Q_{kj}(\vec{r}_1 + \vec{r}) \\ &\approx Q_{kj}(\vec{r}_1) + r^m D_m Q_{kj}(\vec{r}_1) + \frac{1}{2} r^m r^n D_m D_n Q_{kj}(\vec{r}_1). \end{aligned} \quad (43)$$

Using the mean field approximation, it is found that

$$\begin{aligned} \langle I_j^i(\vec{r}_1, \vec{r}_2) \rangle &= \langle Q^{ik}(\vec{r}_1) Q_{kj}(\vec{r}_1 + \vec{r}) \rangle \\ &\approx \langle Q^{ik}(\vec{r}_1) Q_{kj}(\vec{r}_1) \rangle + \langle Q^{ik}(\vec{r}_1) r^m D_m Q_{kj}(\vec{r}_1) \rangle \\ &\quad + \frac{1}{2} \langle Q^{ik}(\vec{r}_1) r^m r^n D_m D_n Q_{kj}(\vec{r}_1) \rangle. \end{aligned} \quad (44)$$

Now we will consider an important substitution for the product of the variables  $r^m r^n$  that will be used ahead in the com-

putation of  $i_1$  and  $i_2$ . As  $r^m r^n$  is a second rank symmetric tensor, it could be written in terms of the natural second rank symmetric tensors of the theory [25,38],  $Q^{mn}$  and  $\delta^{mn}$ ,

$$r^m r^n = A Q^{mn} + B \delta^{mn}, \quad (45)$$

where  $A(r)$  and  $B(r)$  are constants to be determined, whose physical meaning will be important to interpret our elastic theory. As the trace of  $Q^{mn}$  is null,  $\text{Tr}(Q^{mn}) = 0$ , we immediately have

$$B(\vec{r}) = \frac{r^2}{3},$$

which shows that  $B(\vec{r})$  measures the isotropic component of  $r^m r^n$ , as is already evident in Eq. (45). Nevertheless, the meaning of  $A(r)$  is not so evident. Using the facts that  $Q^{mn} Q_{nm} = 2/3$  and  $Q^{mn} \delta_{nm} = 0$ , we straightforwardly obtain

$$A(\vec{r}) = \frac{2}{3} r^m r^n Q_{mn},$$

which shows that  $A(r)$  is proportional to the quadrupolar energy term, at the point  $\vec{r}$  [50].

Using these definitions on  $\langle I_j^i(\vec{r}_1, \vec{r}_2) \rangle$  we get

$$\begin{aligned} \langle I_j^i(\vec{r}_1, \vec{r}_2) \rangle &= \langle Q^{ik} Q_{kj} \rangle + \langle Q^{ik}(\vec{r}_1) r^m D_m Q_{kj}(\vec{r}_1) \rangle \\ &\quad + \frac{1}{2} \langle Q^{ik}(\vec{r}_1) [A(\vec{r}) Q^{mn} + B(\vec{r}) \delta^{mn}] D_m D_n Q_{kj}(\vec{r}_1) \rangle. \end{aligned} \quad (46)$$

On the above equation we have made the change  $\delta^{ij} \rightarrow g^{ij}$ , defined in Eq. (9).

Now, all the formalism developed so far will be gathered to compute the nematic elastic constants. It will be assumed that the term  $i_1$  contributes to the free energy through a term with the form

$$F_1 = F_0 + \int d^3 r_1 d^3 r_2 a_1(\vec{r}_2 - \vec{r}_1) \langle I_j^i(\vec{r}_1, \vec{r}_2) \rangle, \quad (47)$$

where  $a_1(\vec{r}_1 - \vec{r}_2)$  expresses the coefficients of the energy in terms of  $\langle I_j^i(\vec{r}_1, \vec{r}_2) \rangle$ . Making the change of the parameters of integration defined above, we get

$$\begin{aligned} F_1 &= F_0 + \frac{1}{2} \int d^3 r_1 d^3 r a_1(\vec{r}) \\ &\quad \times \{ \langle Q^{ik}(\vec{r}_1) (A Q^{mn} + B \delta^{mn}) D_m D_n Q_{kj}(\vec{r}_1) \rangle \} \\ &= F_0 + \frac{1}{2} \int d^3 r_1 \\ &\quad \times \{ \langle Q^{ik}(\vec{r}_1) (C_A Q^{mn} + C_B \delta^{mn}) D_m D_n Q_{kj}(\vec{r}_1) \rangle \}, \end{aligned} \quad (48)$$

where we have disregarded the linear term in  $r^m D_m$ , a cholesteric term [25,38], and

$$C_A = \int d^3 r a_1(\vec{r}) A(\vec{r}) = \frac{2}{3} \int d^3 r a_1(\vec{r}) r^m r^n Q_{mn},$$

$$C_B = \int d^3 r a_1(\vec{r}) B(\vec{r}) = \frac{1}{3} \int d^3 r r^2 a_1(\vec{r}). \quad (49)$$

Using the definition of covariant derivative given above, and after a straightforward—but not short—calculation we arrive at

$$F_1 = F_0 + \frac{1}{2} \int d^3r_1 \{ K_{11} (\vec{\nabla} \cdot \vec{n})^2 + K_{22} (n \cdot \vec{\nabla} \times \vec{n})^2 + K_{33} (n \times \vec{\nabla} \times \vec{n})^2 + K_z T f \} \quad (50)$$

where

$$K_{11}^{(1)} = - \frac{2C_B S^2 [(3-e)^2 + 2e^2 S^2]}{3[3-e(1+2S)][3-e(1-S)]^2} (3(3+\rho S) - e\{3-S[3-\rho(1+2S)]\}),$$

$$K_{22}^{(1)} = \left( 1 - \frac{3eS [6-e(S+2)]}{2 [3+e(S-1)]^2} \right) K_{11}^{(1)},$$

$$K_{33}^{(1)} = - \frac{2C_B S^2 (3-2\rho S) [(3-e)^2 + 2e^2 S^2]}{3[3-e(1-S)]^2}, \quad (51)$$

and  $\rho = C_A/C_B$  is proportional to quadrupolar momentum, defined in Eq. (49). A noticeable aspect of these relations is that the ratio

$$r_{21} = \frac{K_{22}^{(1)}}{K_{11}^{(1)}} = 1 - \frac{3eS [6-e(S+2)]}{2 [3+e(S-1)]^2} \quad (52)$$

is exactly equal to the one already found in Eq. (42) and does not depend on  $\rho$ , the quadrupolar momentum of the nematic molecule, it is completely determined by the eccentricity  $e$  and scalar order parameter  $S$ . Below, in Eq. (55), this same kind of relation will be found again in the description of the elasticity given by  $i_2$ . Otherwise, contrasting with this property, the relation  $r_{31} = K_{33}/K_{11}$  also depends on the parameter  $\rho$ , that is,

$$r_{31} = \frac{(3-2\rho S)[3-e(1+2S)]}{3(3+\rho S) - e\{3-S[3-\rho(1+2S)]\}}. \quad (53)$$

Therefore a plot of the experimental data of  $r_{21}$  as a function of  $S$  can be used to determine the values of  $e$ . Afterwards, once having the value of  $e$ , a plot of the ratio  $r_{31}$  as a function of  $S$  can be used to determine the ratio  $\rho$ . As the elastic constants depend on  $e$ ,  $\rho$ ,  $C_B$ , and  $S$ , a further single determination of  $C_B$  would be enough to simultaneously determine the values of  $K_{11}$ ,  $K_{22}$ , and  $K_{33}$  as a function of  $S$ . We have employed this procedure to the determination of the elastic constants, and the results are plotted in Fig. 1. The values for  $S$  have been taken from the universal order parameter profile [51–53], and the experimental data of the elasticity of the MBBA have been taken from [12]. A simple examination of this figure shows that notwithstanding the agreement of the curves of  $K_{11}$  and  $K_{22}$  with the experimental data is good, the same does not happen with  $K_{33}$ . Indeed, there is not any agreement between the two curves and, it can be affirmed without doubt, that the use of  $i_1$  to the calculus of  $K_{33}$  is poor. Nevertheless, we have presented such results here because even being negative for the calculus of  $K_{33}$ , it strongly exhibits the reasons for the differences for the ratios

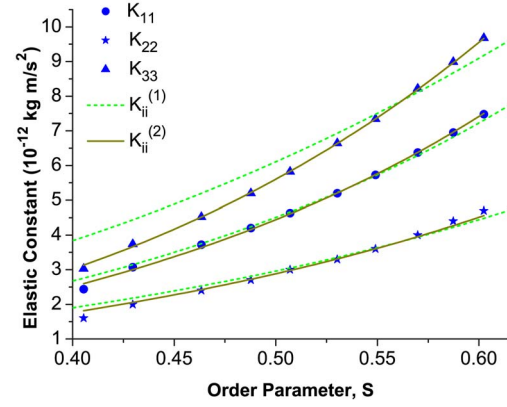


FIG. 1. (Color online) Elastic constants of the 4-methoxybenzylidene-4-n-butyliline (MBBA). The dots correspond to the experimental data, as measured by Jeu *et al.* [12]. The dashed line corresponds to the fitting obtained with the use of Eq. (51). As explained along the work, the fitting was performed in such a way that the ratio  $r_{21}$ , Eq.(52), was used to obtain the value of the eccentricity,  $e=0.78$ , the ratio  $r_{31}$  was used to obtain the value of  $\rho=-2.51$ , which is proportional to quadrupolar momentum, Eq. (49). The overall constant assumed the value  $c_1=-8.28$ . The fact that, differently from  $r_{21}$ ,  $r_{31}$  depends on the quadrupolar moment suggests that to obtain a better fitting to  $K_{33}$ , the invariant from which the elastic constants are calculated must contain the quadrupolar momentum from the beginning. The invariant  $i_2$  is in accord with this requirement; the continuous line over the experimental data corresponds to the fitting obtained with it. The adjustment was obtained by a procedure similar to the one described above, where the parameter  $e=0.78$  was obtained from the ratio  $r_{21}$ , and  $\rho_1=-1.44$  and  $\rho_2=8.27$  have been determined from the data of  $r_{31}$ . The overall constant assumed the value  $c_1=-4.94$ .

$r_{21}$  and  $r_{31}$  already reported in the literature [24]. It becomes clear when the procedure used to arrive at the results of Fig. 1 is remembered. According to the relations found above, through the eccentricity parameter  $e$  and scalar order parameter  $S$ , the ratio  $r_{21}$  is completely determined by the geometry of the correlated volume. Otherwise, the ratio  $r_{31}$  also depend on the quadrupolar momentum of the nematic molecule, and it would also strongly depend on the coupling between the relative distance of the interacting molecules and its relative orientations. So, this fact would be contained in our starting relation for the calculations of  $K_{33}$ . As we see in Eq. (42) this is exactly the physical fact stressed by  $i_2$ , consequently, it is a better starting point for the calculus of the elastic energy than  $i_1$ .

Let us now consider the elasticity predicted by  $i_2$ ,

$$F_2 = F_0 + \int d^3r_1 d^3r_2 a_2(\vec{r}_2 - \vec{r}_1) \langle r^i r^j I_{ij}(\hat{m}, \hat{n}) \rangle$$

$$= F_0 + \frac{1}{2} \int d^3r_1 d^3r_2 a_2(\vec{r}) \{ (A Q^{ij} + B g^{ij}) Q_j^k(\vec{r}_1) \times (A Q^{mn} + B g^{mn}) D_m D_n Q_{ki}(\vec{r}_1) \}, \quad (54)$$

where Eq. (45) has been used. Following the same procedure



used above we arrive at an equation similar to Eq. (45), but with the elastic constants given by

$$K_{11}^{(2)} = \frac{-c_1 S^2}{27[3 - e(1 - S)]^3 [3 - e(1 + 2S)]} \Omega_1,$$

$$K_{22}^{(2)} = \left(1 - \frac{3eS [6 - e(S + 2)]}{2 [3 + e(S - 1)]^2}\right) K_{11}^{(2)},$$

$$K_{33}^{(2)} = \frac{-c_1 S^2}{27[3 - e(1 - S)]^3} \Omega_3, \quad (55)$$

where

$$\begin{aligned} \Omega_1 = & 9[3 - e(1 - S)]^2 [63 - 3e(14 + S) + e^2(7 + S + 10S^2)] \\ & - 3S\{40e^4 S^4 + (3 - e)[(3 - e)^3 + 52(3 - e)^2 eS + 33(3 - e)e^2 S^2 + 22e^3 S^3]\} \rho_1 - 2S^2[4(3 - e)^3 + 18(3 - e)^2 eS \\ & - 3(3 - e)e^2 S^2 + 10e^3 S^3](3 - e(1 + 2S)) \rho_2 \end{aligned}$$

$$\begin{aligned} \Omega_3 = & (9[3 + e(-1 + S)]\{63 - 6e(7 + 2S) + e^2[7 + 4S(1 + 4S)]\} - 3S[-19(-3 + e)^3 + 48(-3 + e)^2 eS - 12(-3 + e)e^2 S^2 + 64e^3 S^3]) \rho_1 + 2S^2[-5(-3 + e)^3 + 42(-3 + e)^2 eS + 12(-3 + e)e^2 S^2 + 32e^3 S^3] \rho_2) \end{aligned} \quad (56)$$

and

$$c_1 = \int d^3 r a_2(\vec{r}) [B(\vec{r})]^2 = \frac{1}{9} \int d^3 r r^4 a_2(\vec{r}),$$

$$\rho_1 = \frac{\int d^3 r a_2(\vec{r}) B(\vec{r}) A(\vec{r})}{\int d^3 r a_2(\vec{r}) [B(\vec{r})]^2} = 2 \frac{\int d^3 r a_2(\vec{r}) r^2 r^m r^n Q_{mn}}{\int d^3 r r^4 a_2(\vec{r})},$$

$$\rho_2 = \frac{\int d^3 r a_2(\vec{r}) [A(\vec{r})]^2}{\int d^3 r a_2(\vec{r}) [B(\vec{r})]^2} = 4 \frac{\int d^3 r a_2(\vec{r}) r^m r^n r^p r^q Q_{mn} Q_{op}}{\int d^3 r r^4 a_2(\vec{r})}. \quad (57)$$

Again, from the ratio between the elastic constants, will see that the ratio  $r_{21}$  remained equal to the one found before. Nevertheless, now  $r_{31}$  depends on two parameters,  $\rho_1$  and  $\rho_2$ . As an easy inspection can show,  $\rho_1$  measures the quadrupolar momentum, being, therefore, similar to the parameter  $\rho$  found in Eq. (51). There is in fact only a new parameter  $\rho_2$ , which is quadratic in the quadrupolar momentum. Using the exact same procedure described above; use of  $r_{21}$  to determine  $e$  and  $r_{31}$  to determine  $\rho_1$  and  $\rho_2$ , we have found the value for MBBA, the fitting curve is also exhibited in Fig. 1. The quality of the global agreement that has been found indicates that our model gives a very good estimative for the elastic constants. General comments on this model will be made in the next section.

#### IV. FINAL REMARKS AND CONCLUSION

In this work we have shown that a nematic liquid crystals' sample, with a nonhomogeneous director profile, can be described as a nonflat differentiable manifold with a non-null scalar curvature determined by two kinds of usual nematic textures; the bend and the saddle-splay terms, both related with the nematic elasticity. So, it would be important to discuss the physical meaning of the non-null value found for the scalar curvature  $R$ . We have proved that according to the affine-connection approach the textures of a nonhomogeneous nematic sample are described by a three-dimensional non-null curved surface, which is, by construction, the surface determined by the nonhomogeneous director profile along the sample. A non-null  $R$  implies that there is not a system of coordinates where  $R$  can be made null; or, using a "physical analogy," such a surface cannot be continuously deformed to another surface with a homogeneously aligned director profile [43]. This is the reason why the twist and splay elastic deformations are not present in  $R$ . As it is well-known, the twist texture can be visualized as a sequence of planes in which, in each of them, the director is homogeneously aligned. As for a twisted texture a simple rotation could restore the homogeneous global alignment and it would have a null curvature. Likewise, save for a point—the singular point—the splay texture is flat; it has a null curvature. In fact, it would have the same topology of a cone, which also has a null curvature and a singular point at its pole. An interesting aspect of this result is that it exposes a curious contrast between the elasticity and curvature of a nematic sample; there are elastic deformations that do not contribute to the curvature as well as there are curvature terms that do not present a contribution to the elasticity. Namely, while the splay and twist terms contribute to the elasticity, they do not present any direct contribution to the scalar curvature and, otherwise, while the saddle-splay term only contributes to the elastic energy at the surface of the sample, its contribution to the curvature is spread along the entire nematic sample.

As a consequence of these results, the differentiation rules have been modified with the introduction of a metric that realizes the affine connection hypothesis: the potential generated by an ellipsoidal nematic molecule can be obtained through the distortion of the potential of a spherical molecule, which is deformed until it assumes the form of the corresponding ellipsoid. As the deformation of a sphere to an ellipsoid is described by an object that has the same form of the order parameter, it can be taken as a microscopic order parameter and, in the passage from the microscopic order parameter to a macroscopic order parameter the induced metric becomes temperature dependent. It is important to detach that the present theory applies to any LC whose molecules interact via a potential with ellipsoidal symmetry, even if the molecules themselves are not ellipsoidally shaped.

As an exercise of the application of this formalism we have applied it to the description of the bulk elasticity terms of a nematic sample, and compared to the results with the experimental data of the MBBA. With this procedure we have described the profile of the experimental data with very secure accuracy and estimated the values of some parameters

of our model, mainly the eccentricity  $e$  of the nematic molecules. We have also obtained an estimate for the quadrupolar moments of the interaction.

As important as the quality of the profiles that we have obtained, other important aspects of the nematic elasticity have been revealed. First, our approach suggests an explanation to the recently reported systematic differences found in the values of the ratios  $r_{21}=K_{22}/K_{11}$  and  $r_{31}=K_{33}/K_{11}$  [24]. While  $r_{21}$  is completely determined by the molecular eccentricity  $e$  and the scalar order parameter  $S$ , the ratio  $r_{31}$  also depends on the quadrupolar moments of the molecules. Furthermore, there are some suggestions in the liquid crystals' literature [46] that, in the absence of a nematic-solid or a nematic-smectic transition, the elastic constants would diverge as  $S \rightarrow 1$ . Our result is consistent with this speculation, but only with the additional condition that  $e \rightarrow 1$ , an infinitely thin nematic molecule.

Our result also suggests that a further study of the nematic elasticity must be undertaken in such a way that the above parameters,  $e$ ,  $\rho_1$ , and  $\rho_2$  may be compared for some liquid crystal compounds. This work is under execution and the results will appear elsewhere.

Finally, we would like to point out that the use of the above formulas is not restricted to the calculus of the elastic constant. In fact, the affine connection approach has been originally introduced to the calculus of the nematic viscosity, and the approach introduced here can be used for the calculus of any aspect of the nematic fluid dynamics.

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