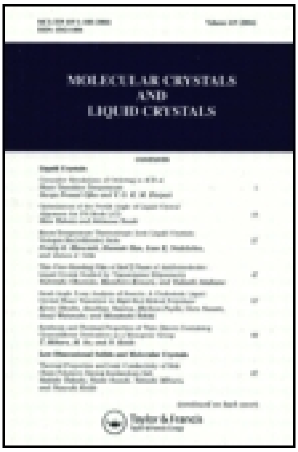

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Molecular Structure of the Hedgehog Point Defect in Nematics

F. Greco [a] & G. Marrucci [a]

[a] Dipartimento di Ingegneria Chimica, Universita' di Napoli, Piazzale Tecchio, 80125, Napoli, Italy

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Molecular Structure of the Hedgehog Point Defect in Nematics

F. GRECO and G. MARRUCCI
Dipartimento di Ingegneria Chimica, Universita' di Napoli, Piazzale Tecchio, 80125 Napoli, Italy

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In view of the limitations inherent to phenomenological approaches, the problem of the internal structure of defects in nematics is here afforded from a molecular viewpoint. By using an extension of the Maier-Saupe mean-field potential which accounts for distorted states of nematics, the general equation applicable inside a defect is obtained by self-consistency. The specific example of the hedgehog point defect is developed in detail. It is shown that the size of the defect core depends on the order parameter characterizing the undistorted nematic phase: the core size decreases when the order parameter increases.

1. INTRODUCTION

Since the early studies on nematics, various conjectures concerning the internal structure of their defects (disclinations) have been made, the most popular of them being that the defect "core" is made up of an isotropic phase. In the absence of detailed models of the defect structure, the only quantity which can be estimated, merely through a dimensional analysis, is the "energy content" of a defect. Examples of such estimates are reported in textbooks.[1]

The first calculation of the structure of a defect core is due to Fan.[2] His approach is based on a Landau-de Gennes expansion of the free-energy density of the nematic phase, inclusive of the distortion terms.[3] The expansion parameter is the order parameter tensor, which Fan takes to be uniaxial throughout the defect. As a consequence of this uniaxial assumption, the problem can be formulated in terms of a director $\mathbf{n}$ plus a scalar order parameter S. The solution obtained by Fan for a disclination line shows that, by entering the defect, S decreases continuously, and reaches zero at the defect centerline.

The assumption used by Fan was erroneous, however, because, as observed by Lubensky,[4] a distortion generally makes the order parameter tensor biaxial. Only in the linear limit, corresponding to Frank elasticity, can the distortion be considered not to affect the uniaxial character of the equilibrium nematic phase.[5] Whenever the distortion exceeds the linear limit, as is certainly the case in close proximity of defects, there is no reason to expect that the uniaxial symmetry is preserved. The same criticism applies to subsequent calculations,[6,7] also based on this arbitrary uniaxial assumption.[8]

An approach to the defect structure not based on uniaxiality is due to Sluckin and coworkers.[9,10] They also use a Landau-de Gennes formalism, but solve for the internal structure of a defect line without further assumptions. The conclusions reported in Reference 10 are: "The core is always biaxial, sometimes contains structures which resemble an isotropic-nematic interface, but never contains a core of isotropic fluid."

Independently of this biaxial *vs.* uniaxial controversy, it should be noted that all the above mentioned calculations[2,6-10] are based on phenomenological expressions for the free-energy density (such as the Landau-de Gennes expansion or similar ones). Now, because the coefficients of a phenomenological equation are material dependent, and, in the case at hand, the gradual change in the order parameter inside the defect virtually corresponds to a gradual change of the material itself, these coefficients surely vary thoughout the defect. In the absence of any information on how these coefficients change with the order parameter tensor, a phenomenological approach *cannot be used.*

It should be emphasized that this serious difficulty is intrinsic to the problem, because the order parameter, differently from temperature for example, is an internal variable. Thus, whereas the temperature dependence (to pursue our example a little further) of phenomenological coefficients can be measured, no such route is available in the case at hand, because the order parameter cannot be varied at will. This discussion will be taken up again in the last section of the paper, in the light of the results obtained. Here, the intrinsic limitations of the phenomenological approach have been mentioned merely to justify why, in the present work, the more realistic approach of molecular modeling is followed instead, in spite of its greater complexity.

The paper is organized as follows. In Section 2, we specify the molecular model by choosing a form for the nematogenic interactions which is apt to describe distorted states. The use of an expansion procedure then produces (in Section 3), by self-consistency, the field equation for an arbitrary distorted state, the core of a defect included. Solution of this equation with prescribed boundary conditions gives the order parameter tensor as a function of the position. We have solved the problem of the hedgehog point defect in Section 4. The last section presents the results and contains a discussion of the assumptions used. The Appendix shows an alternative derivation of the field equation based on free-energy minimization.

2. THE MOLECULAR MODEL. GRADUAL VARIATION ASSUMPTION

We consider the simplest model of a nematic molecule, i.e., the rigid rod. The only degrees of freedom available to such a molecule are then its position in space, $\mathbf{R}$, and its orientation, described by the unit pseudo-vector, $\mathbf{u}$. At a fixed location $\mathbf{R}$, the orientational state is described by the distribution function $f(\mathbf{u};\mathbf{R})$ giving the probability density that a molecule centered at $\mathbf{R}$ is oriented along $\mathbf{u}$.

The molecular interactions giving rise to the nematic phase are assumed to be described by a mean-field Maier-Saupe potential.[11] However, because distorted configurations will be considered here, the potential must be written in an "extended" form,[12] such as:

$$V(\mathbf{u};\mathbf{R}) = -2\,kT\,U\{\mathbf{u}'\mathbf{u}'\}:\mathbf{uu} \tag{2.1}$$

$$\{\mathbf{uu}\} = \int d\Omega\,\mathbf{uu}\,\frac{1}{v}\int_v dv\,f(\mathbf{u};\mathbf{R}+\mathbf{r}) \tag{2.2}$$

where the symbol $\{\cdot\}$ indicates a *neighborhood* ensemble average, i.e., as shown in Equation (2.2), an average based on the distribution function in a whole neighborhood v of **R**, not merely at **R**. In Equation (2.2), a spherical neighborhood is understood, scanned by the vector **r**; this represents a simplified version of the theory considered in Reference 12, corresponding to the case where the length of the molecule is smaller than the characteristic distance of intermolecular interactions. In the homogeneous case (no distortions), $\{\mathbf{uu}\}$ reduces to the classical ensemble average, and Equation (2.1) becomes the standard Maier-Saupe potential, with kT the Boltzmann constant times the absolute temperature, and U the nondimensional "strength" of the potential.

Because we only deal with equilibrium situations, albeit distorted, the function $f(\mathbf{u};\mathbf{R})$ must be a Boltzmann distribution. In view of the mean-field potential defined above, we may then write

$$f(\mathbf{u};\mathbf{R}) = Z^{-1}(\mathbf{R})\exp(2U\{\mathbf{u}'\mathbf{u}'\}:\mathbf{uu}) \tag{2.3}$$

where $Z(\mathbf{R})$ is the local normalization factor, i.e., the "sum over states":

$$Z(\mathbf{R}) = \int d\Omega\,\exp(2U\{\mathbf{u}'\mathbf{u}'\}:\mathbf{uu}) \tag{2.4}$$

The integral over orientations in Equation (2.4), just as that in Equation (2.2), extends over the full solid angle $\Omega = 4\,\pi$.

An expansion procedure is now adopted, i.e., it is assumed that the distribution function does not vary too much over the volume v of the neighborhood of any point. It should be immediately emphasized that such a simplifying assumption does not prohibit considerable changes of the distribution function to take place within a defect core. In other words, although changes are assumed to occur "slowly," their cumulative effect can be very large. This *gradual variation assumption* (GV-assumption) will be reconsidered more thoroughly later in the paper.

The distribution function is expanded in space in the following way:

$$f(\mathbf{u};\mathbf{R}+\mathbf{r}) = f(\mathbf{u};\mathbf{R}) + \nabla f\cdot\mathbf{r} + \frac{1}{2}\nabla\nabla f:\mathbf{rr} + \ldots \tag{2.5}$$

where it is understood that the spatial gradients are calculated at **R**, for any fixed **u**. This expansion will be substituted in the integral of Equation (2.2) where, because of symmetry, the first order term integrates to zero. For this reason, the expansion is carried out up to second order.

Substitution gives:

$$\{\mathbf{uu}\} = \mathbf{S} + \frac{1}{2}\ell^2\Delta\mathbf{S} \tag{2.6}$$

$$\mathbf{S} = \langle\mathbf{uu}\rangle \tag{2.7}$$

where $\langle\cdot\rangle$ indicates the ensemble average at $\mathbf{R}$.

The first term in Equation (2.6) results from the zeroth order term of the expansion in Equation (2.5). The term containing the Laplacian of $\mathbf{S}$, arising from the second order term of the expansion, is obtained by considering that, in the innermost integral of Equation (2.2), the second gradient $\nabla\nabla f$ is a constant. The innermost integral then becomes

$$\frac{1}{v}\int_v dv\,\mathbf{rr} = \ell^2\,\mathbf{1} \tag{2.8}$$

where $\mathbf{1}$ is the unit tensor, and ℓ is a characteristic interaction distance.

3. THE GENERAL PROBLEM OF DISTORTIONS. THE FIELD EQUATION FOR S

The general problem to be solved when distortions are present is a formidable one, because it consists in finding the orientational distribution function $f(\mathbf{u};\mathbf{R})$ at all points. Our choice of a spherical shape for the interaction domain v and, more importantly, the GV-assumption greatly simplify the problem, however. Indeed, as shown by Equation (2.6), our task is now reduced to the determination of $\mathbf{S}(\mathbf{R})$.

The tensor field $\mathbf{S}(\mathbf{R})$ is determined by a self-consistent equation, conceptually analogous to that used by Maier and Saupe for the undistorted case. In fact, by using Equations (2.3), (2.4), and (2.6), the definition of $\mathbf{S}$ (see Equation 2.7) becomes:

$$\mathbf{S} = \frac{\displaystyle\int d\Omega\;\mathbf{uu}\,\exp[2U(\mathbf{S} + \frac{1}{2}\ell^2\Delta\mathbf{S}):\mathbf{uu}]}{\displaystyle\int d\Omega\,\exp[2U(\mathbf{S} + \frac{1}{2}\ell^2\Delta\mathbf{S}):\mathbf{uu}]} \tag{3.1}$$

With a similar approximation as used previously to obtain Equation (2.6), i.e., in the spirit of the GV-assumption, we can expand the term $\exp(U\ell^2\Delta\mathbf{S}:\mathbf{uu})$ in Equation (3.1). Then, by neglecting second order terms in the resulting fraction, Equation (3.1) is finally rewritten as:

$$\mathbf{S} = \mathbf{P} + U\ell^2(\mathbf{Q} - \mathbf{PP}):\Delta\mathbf{S} \tag{3.2}$$

In Equation (3.2), **P** and **Q** are symmetric tensors of second and fourth rank, respectively, defined as

$$\mathbf{P}(\mathbf{S}) = \frac{1}{g}\int d\Omega\ \mathbf{uu}\exp(2U\,\mathbf{S}:\mathbf{uu}) \tag{3.3}$$

$$\mathbf{Q}(\mathbf{S}) = \frac{1}{g}\int d\Omega\ \mathbf{uuuu}\exp(2U\,\mathbf{S}:\mathbf{uu}) \tag{3.4}$$

where g is the scalar

$$g(\mathbf{S}) = \int d\Omega\exp(2U\,\mathbf{S}:\mathbf{uu}) \tag{3.5}$$

For a given U-value, **P** and **Q** are **S**-dependent. Thus, Equation (3.2) defines **S** implicitly. By solving this implicit differential equation, the tensor field **S**(**R**) is obtained; of course, specific boundary conditions must be assigned as well. For the special case where the boundary conditions dictate a spatial homogeneity, Equation (3.2) reduces to $\mathbf{S} = \mathbf{P}(\mathbf{S})$, which is the classical self-consistent equation of Maier and Saupe (written here in tensor form).

As shown in the Appendix, the same field equation for **S**, Equation (3.2), can also be obtained by minimizing free energy. The calculations are more lengthy, however, and less direct.

4. THE HEDGEHOG DEFECT

Despite its apparent simplicity, Equation (3.2) is very difficult to solve in most cases, and generally predicts a biaxial tensor field **S**(**R**). Uniaxial fields are also possible, of course, under appropriate conditions; this is true in particular when Equation (3.2) reduces to the field equation of the Frank elasticity limit, e.g., far away from defects. In fact, in the Frank elasticity limit, not only is the local uniaxial symmetry preserved, but also the scalar order parameter is a constant throughout, keeping the same value of the spatially undistorted situation.

The hedgehog example considered in this paper is also a case where, for plain reasons of symmetry, the tensor **S** must remain uniaxial everywhere, i.e., up to the center of the defect. Contrary to the Frank elasticity case, however, the scalar order parameter departs considerably from its undistorted value, reaching zero at the defect center (see Equation 4.13 below).

It should be stressed that the hedgehog defect is *the single defect* where tensor **S** remains uniaxial; for all other defects, the possible symmetries are anyhow insufficient to preserve uniaxiality of **S** at all points of the defect "core." Although we will not explicitly consider biaxial examples in this paper, we again remark that the uniaxial character of the following calculations is dictated by the spherical symmetry of the hedgehog point defect, and is not an arbitrary, unrealistic assumption as in the cases considered in References 2 and 6–8.

For the hedgehog defect, **S** takes the uniaxial form

$$\mathbf{S} = S(\mathbf{nn} - \frac{1}{3}\mathbf{1}) + \frac{1}{3}\mathbf{1} \tag{4.1}$$

where $\mathbf{n}(\mathbf{R})$ is the unit vector in the radial direction, $S(R)$ is the scalar order parameter, and it is understood that R is the radial coordinate, i.e., the distance from the defect center. (Note that Equation (4.1) fulfills the condition $tr\mathbf{S} = 1$, dictated by the definition of **S** in Equation (2.7).)

Because of the spherical symmetry, the only unknown in the "structure" of the hedgehog defect is $S(R)$, i.e., the general problem of finding the tensor field $\mathbf{S}(\mathbf{R})$ is here reduced to that of determining a single scalar function of a single scalar variable. Thus, the hedgehog defect constitutes the simplest case of a "large" distortion, i.e., of a distortion falling outside the range of validity of the Frank elasticity.

We now proceed to derive the scalar equation for $S(R)$ from the tensorial equation previously obtained, Equation (3.2). To this end we first note that, because of the local uniaxial symmetry, all tensors appearing in Equation (3.2) can be expressed in terms of the unit vector **n** (specifying the local symmetry axis) and of their appropriate scalar invariants. Therefore, scalar multiplication of Equation (3.2) by **nn** will leave a relationship among the scalar invariants only.

Because $tr\mathbf{P} = 1$ (compare Equation 3.3), the uniaxial form of **P** is

$$\mathbf{P} = P\left(\mathbf{nn} - \frac{1}{3}\mathbf{1}\right) + \frac{1}{3}\mathbf{1} \tag{4.2}$$

Equation (4.1) and Equation (4.2) imply, respectively,

$$\mathbf{S}:\mathbf{nn} = \frac{2}{3}S + \frac{1}{3} \tag{4.3}$$

$$\mathbf{P}:\mathbf{nn} = \frac{2}{3}P + \frac{1}{3} \tag{4.4}$$

so that Equation (3.2) gives:

$$\frac{2}{3}S = \frac{2}{3}P + U\ell^2[\mathbf{Q}:\mathbf{nn} - \left(\frac{2}{3}P + \frac{1}{3}\right)\mathbf{P}]:\Delta\mathbf{S} \tag{4.5}$$

The expression in square brackets in Equation (4.5) is a second rank tensor with a zero trace. The latter property derives from the identity $tr(\mathbf{Q}:\mathbf{nn}) = \mathbf{P}:\mathbf{nn}$, which follows from the definitions of **P** and **Q**, Equations (3.3) and (3.4), respectively. Therefore, by using once more the uniaxial symmetry, we can write:

$$\mathbf{Q}:\mathbf{nn} - \left(\frac{2}{3}P + \frac{1}{3}\right)\mathbf{P} = M\left(\mathbf{nn} - \frac{1}{3}\mathbf{1}\right) \tag{4.6}$$

Equation (4.6) is substituted into Equation (4.5). However, because $\mathbf{1}:\Delta\mathbf{S} = 0$ (Laplacian and trace are linear operators which commute), Equation (4.5) is rewritten as

$$S = P + \frac{3}{2} U\ell^2 M\, \mathbf{nn}:\Delta\mathbf{S} \tag{4.7}$$

Now, double differentiation of Equation (4.1), followed by scalar multiplication by **nn**, gives

$$\mathbf{nn}:\Delta\mathbf{S} = \frac{2}{3}\Delta S + 2S\,\mathbf{n}\cdot\Delta\mathbf{n} = \frac{2}{3}\Delta S - 4S/R^2 \tag{4.8}$$

where the latter equality makes use of the spherical symmetry of the **n**-field. Finally, by writing ΔS explicitly in the same symmetry, the hedgehog defect equation is obtained as:

$$S = P(S) + UM(S)\left(\frac{d^2S}{dR^2} + \frac{2}{R}\frac{dS}{dR} - \frac{6}{R^2}S\right) \tag{4.9}$$

where R has been made nondimensional with respect to ℓ, and the scalar functions $P(S)$ and $M(S)$ are given by

$$P(S) = (3I_2 - I_0)/2I_0 \tag{4.10}$$

$$M(S) = 3(I_4 I_0 - I_2^2)/2I_0^2 \tag{4.11}$$

with

$$I_n = \int_0^1 dx x^n \exp(2USx^2), \qquad n = 0, 2, 4 \tag{4.12}$$

Equation (4.10) is derived from Equation (4.4) (together with the definition of tensor **P**, Equation 3.3). Similarly, Equation (4.11) is obtained by scalarly multiplying Equation (4.6) times **nn**, and by using the definition of tensor **Q**. It may be worth noting that the product $\mathbf{n}\cdot\mathbf{u}$ which repeatedly appears in these operations is the cosine of the angle that the rodlike molecule makes with the symmetry axis; the integrations over the solid angle in Equations (3.3) and (3.4) are therefore reduced to the integrals over $x = \mathbf{n}\cdot\mathbf{u}$, as defined by Equation (4.12).

The boundary conditions of Equation (4.9) are:

$$\text{at } R = 0 \quad \begin{cases} S = 0 & (4.13) \\ dS/dR = 0 & (4.14) \end{cases}$$

The condition in Equation (4.13) makes the singularity of the **n**-field at $R = 0$ "compatible" with the continuity of the **S**-field (compare Equation 4.1). In fact, the tensor **S** must obviously *exist* everywhere, just because the orientational distribution of the molecules is defined at all points, center of the defect included. Notice that $S = 0$ implies $\mathbf{S} = (1/3)\,\mathbf{1}$, i.e., the ellipsoid representing the uniaxial symmetry gradually approaches a sphere as R approaches zero.

The condition in Equation (4.14) is dictated by the spherical symmetry, which imposes $\nabla\mathbf{S} = 0$ at $R = 0$.

5. RESULTS AND DISCUSSION

As mentioned before, Equation (4.9) is implicit, i.e., it contains the unknown function $S(R)$ also "inside the coefficients" P and M. Numerical solution of this equation is simple, however, if the functions $P(S)$ and $M(S)$ are pre-tabulated; in this way, the current values of P and M needed at each step of the integration of Equation (4.9) can be obtained by interpolation.

For any given U-value, these functions are then pre-calculated through Equations (4.10–12) in the interval $0 < S < S_0$, where $S_0(U)$ is the value of the order parameter in the undistorted situation, i.e., far away from the defect center. By way of example, Figure 1 reports $P(S)$ and $U \times M(S)$ for $U = 3.70$, corresponding to $S_0 = 0.6$. Similar curves are obtained for different U-values.

Because Equation (4.9) contains R in the denominator, the limiting behavior as R approaches zero needs to be discussed. In that limit, Equation (4.9) becomes:

$$\frac{d^2S}{dR^2} + \frac{2}{R}\frac{dS}{dR} - \frac{6}{R^2}S = 0 \tag{5.1}$$

Indeed, in Equation (4.9) $S = P = 0$ at $R = 0$, whereas, from Equation (4.11), $M(0) = 2/15$. The general solution of Equation (5.1) is

$$S = K\,R^2 \tag{5.2}$$

with K a constant. Equation (5.2) automatically satisfies the boundary conditions of our problem, Equations (4.13–14).

Therefore, the numerical procedure adopted to solve Equation (4.9) is as follows. First, a trial value of K is assigned, so that the starting values of the function $S(R)$ in a neighborhood of $R = 0$ are known *via* Equation (5.2). Then, as R grows, a Runge-Kutta integration of the complete equation, Equation (4.9), is performed. A single value of K will exist which causes the function $S(R)$ to approach the value of S_0 as R grows indefinitely. Such a K-value is found by an appropriate trial-and-error convergent scheme.

Figure 2 reports the results of these calculations for several values of U. In particular, we have chosen those U-values which give S_0 equal to 0.5–0.8. As is immediately apparent in Figure 2, the asymptotic approach to S_0 occurs the more

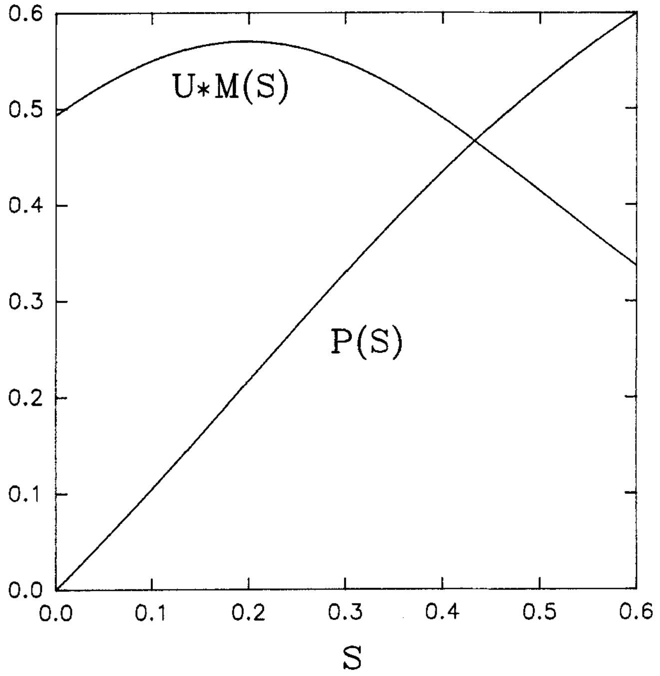

FIGURE 1 The functions of the order parameter appearing in Equation (4.9), for the case $U = 3.70$ (corresponding to $S_0 = 0.6$). The curve representing the function $P(S)$ runs very close to the diagonal, thus indicating the validity of the GV-assumption.

steeply the larger is S_0 itself. In other words, the defect core "shrinks" with increase in the order parameter of the undistorted state.

Curves very similar to those reported in Figure 2 were recently obtained by Palffy-Muhoray and Saupe.[13] The theory advanced by these authors is very different, however, from that developed here and in the previous paper,[12] although both theories are based on self-consistency. Indeed, the mean-field potential proposed in Reference 13 still contains the local "macroscopic" director, and it accounts for spatial distortions through the use of a phenomenological ansatz. Our approach is more strictly molecular: the mean-field potential, instead of invoking a director, remains based on the molecular orientational distribution throughout a suitable neighborhood.[12] In comparing the two approaches, significant differences are then generally expected. By way of example, the three elastic constants predicted in Reference 12 show a quite different S-dependence with respect to the ansatz proposed in Reference 13.

On the basis of the results obtained, it becomes possible to look into the GV-assumption more quantitatively. The ultimate consequence of this assumption is Equation (3.2), in which the "correction" due to distortions is the term containing the Laplacian. This correction is readily estimated from the difference $\mathbf{P} - \mathbf{S}$, i.e., for the hedgehog defect, by looking at the deviation of the $P(S)$ curve from the "diagonal" in Figure 1. For the case $S_0 = 0.6$, Figure 1 shows that these deviations are extremely small thoughout the entire S-range. The same comparison for other

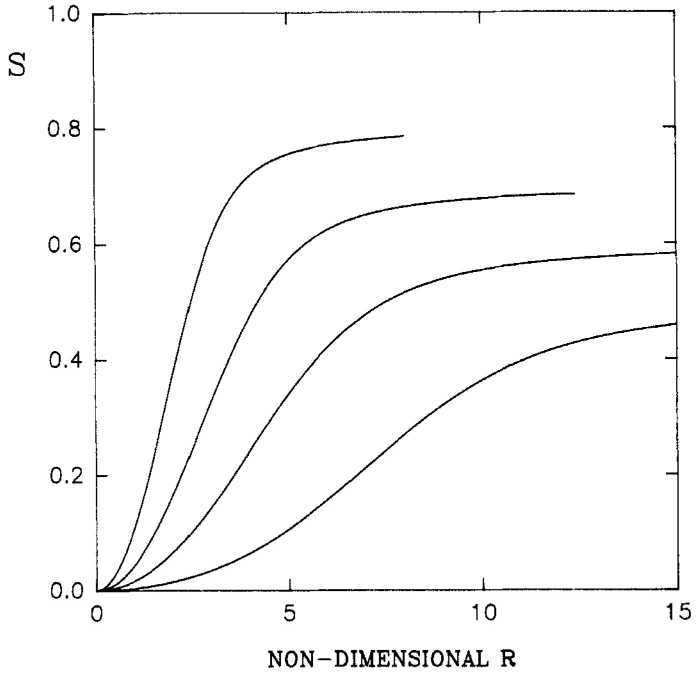

FIGURE 2 Behavior of the order parameter inside the hedgehog defect. The abscissa is the ratio between the distance from the defect center and the interaction length ℓ. Each curve asymptotically approaches its own bulk value of the order parameter.

cases indicates that the deviations increase with increasing S_0-values. Now, because the use of the GV-assumption implies that, in Equation (3.2), the order of magnitude of the error (i.e., of the neglected terms in the expansions) is given by the *square* of the Laplacian term, the conclusion may be drawn that the GV-assumption is legitimate, at least as long as S_0 is not too large.

This conclusion on the GV-assumption is confirmed by looking at the "size" of the defect core, as it can be inferred from Figure 2. At low values of S_0, the asymptote is reached after more than 10 nondimensional units, i.e., at a distance from the defect center larger than 10 times the molecular interaction length ℓ. It is thus confirmed that the transition from $S = 0$ to $S = S_0$ occurs *gradually*, without too large a change over one "molecular" distance ℓ. The core size dramatically reduces to a few nondimensional units (and the GV-assumption begins to break down) when S_0 is raised to 0.8 or more. For S_0 approaching unity, the defect core becomes of molecular dimensions in a strict sense.

Although already discussed in the Introduction, another point worth mentioning again concerns the intrinsic limitations of the phenomenological approach. We now know that, even within the context of our simple molecular model, the equation which describes the defect structure, Equation (3.2), is highly nonlinear in the order parameter. The validity of the GV-assumption (when it holds) only guarantees that the equation is linear in the Laplacian of the order parameter; the "coefficients" in the equation remain S-dependent nevertheless, and in a very complex way. From the phenomenological viewpoint, the linearity in the Laplacian can surely be anticipated, but there is no hope of envisaging what the **S**-dependence of the coefficients might be.

The actual form of these dependences on the order parameter is dictated by the specific molecular model. In this respect, it has to be emphasized that the model adopted in this paper, Equations (2.1–2), is certainly the simplest possible one. Since the length of the rodlike molecule has been entirely neglected, the model actually corresponds to a *pointlike* quadrupole interaction. In terms of Frank elasticity, this same model[12] gives rise to the so-called one-constant approximation.

When the molecular length is no longer negligible with respect to the interaction length, the quadrupole interaction leads to three different elastic constants.[12] Correspondingly, the defect equation also becomes more complex. It can readily be demonstrated that, together with the Laplacian of **S**, the "mixed" second order derivatives of **S** would also appear in the equation. Although the details of the hedgehog defect structure would then certainly change, the main features are expected to remain the same as those reported in Figure 2.

In conclusion, the results of this work have effectively shown the internal structure of the hedgehog defect in nematics. The same self-consistent equation derived here can also be used to investigate defects, like the disclination lines, the internal structure of which is expected to be biaxial.

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APPENDIX. DERIVATION OF EQUATION (3.2) THROUGH ENERGY MINIMIZATION

The free-energy density $A(\mathbf{R})$ is given by

$$A(\mathbf{R}) = \nu\,[kT\,\langle \ln f(\mathbf{u};\mathbf{R})\rangle + \frac{1}{2}\langle V(\mathbf{u};\mathbf{R})\rangle] \tag{A.1}$$

where ν is number of molecules per unit volume, and the $\frac{1}{2}$ factor arises from the mean-field nature of the potential. By using Equations (2.1) and (2.3), Equation (A.1) becomes:

$$A(\mathbf{R}) = -\nu[kT\ln Z(\mathbf{R}) + \frac{1}{2}\langle V(\mathbf{u};\mathbf{R})\rangle] \tag{A.2}$$

Use of the GV-assumption allows one to write the logarithmic term in Equation (A.2) as

$$\ln Z = \ln g + U\ell^2\,\mathbf{P}:\Delta\mathbf{S} \tag{A.3}$$

where g and $\mathbf{P}$ are defined in Equations (3.5) and (3.3), respectively. Similarly, the ensemble average of the potential becomes:

$$\langle V \rangle = -kTU(2\mathbf{S}:\mathbf{S} + \ell^2\mathbf{S}:\Delta\mathbf{S}) \tag{A.4}$$

The free-energy density is then given by:

$$A(\mathbf{R}) = \nu kT\left[-\ln g + U\mathbf{S}:\mathbf{S} + U\ell^2\left(\frac{1}{2}\mathbf{S} - \mathbf{P}\right):\Delta\mathbf{S}\right] \tag{A.5}$$

where the $\mathbf{R}$-dependence of g, $\mathbf{S}$, $\mathbf{P}$, and $\Delta\mathbf{S}$ is understood. In order to obtain the field equation for $\mathbf{S}$, a minimization of the volume integral of $A(\mathbf{R})$ must be made, i.e.:

$$\delta \int A(\mathbf{R})dv = 0 \tag{A.6}$$

By regarding the expression of the free-energy density in Equation (A.5) as a function of $\mathbf{S}$ and $\Delta\mathbf{S}$, the variational problem of Equation (A.6) is solved by the Lagrange equation:

$$\frac{\partial A}{\partial \mathbf{S}} + \Delta\left(\frac{\partial A}{\partial \Delta\mathbf{S}}\right) = 0 \tag{A.7}$$

Performing the indicated derivatives, Equation (A.7) becomes:

$$\mathbf{S} = \mathbf{P} + U\ell^2(\mathbf{Q} - \mathbf{PP}):\Delta\mathbf{S} + \frac{1}{2}\ell^2\Delta(\mathbf{P} - \mathbf{S}) \tag{A.8}$$

Equation (A.8) differs from Equation (3.2) of the text only because an additional term is present. This term is irrelevant, however, because it can be recognized as a "surface" term. Indeed, for an arbitrary $\mathbf{S}$-field, the volume integral of $\Delta(\mathbf{P} - \mathbf{S})$ can be written as a surface integral; a possibility which is denied to all other terms in Equation (A.8).

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