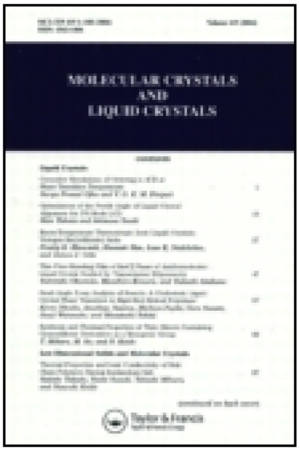

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Peculiarities of Interaction Between the Radial and Hyperbolic Point Defects in Nematics: Creation and Decay of the Cylindrical Defect P^C_{+2}

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PECULIARITIES OF INTERACTION BETWEEN THE RADIAL AND HYPERBOLIC POINT DEFECTS IN NEMATICS: CREATION AND DECAY OF THE CYLINDRICAL DEFECT P^c_{+2}

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Abstract In the framework of continuum theory of nematics we have investigated how the radial (R) and hyperbolic (H) point defects interact with each other. The force of interaction is shown not to depend on the distance, but, as well as the result of coalescence of the defects, it is only controlled by their mutual orientation. Two most important cases of mutual orientations have been considered, namely when symmetry axes of the defects are in line (the elastic field with axial symmetry) and parallel. In the first case the defects attract each other and then disappear, in the second case they repel each other. The stability of cylindrical defect P^c_{+2} with respect to decay into R- and H-defects has been analyzed. The results obtained have been generalized to pair interactions of defects with any other strengths.

INTRODUCTION

Nematic ordering allows structural defects of various dimensions and symmetry to exist.[1,2] Defect interactions cause director fields of elastic deformations $\vec{n}(\vec{r})$ to occur and the energy of nematic liquid crystal to vary. The study of defect interactions in nematics have been always restricted by the simplest cases, namely, when symmetry axis of defects are parallel (L^p_k)[1,3] or in line (P^a_k)[4]. However because of the anisotropy of a structure of director field for most of the defects their energy of interaction depends upon not only the distance between defects but their mutual orientation.

The objective of the present work is to study interaction of defects in accordance with their arrangement and orientation relative to each other. The consideration has been made in one-constant approximation of the theory of elasticity [1,3] for defects of radial (R) and hyperbolic (H) types, which are the most abundant and important.

Free R- and H-defects generate elastic fields with spherical and axial symmetry respectively. Therefore the structure of the director field and the energy of interaction of {R,H}-pair is defined by two parameters, a distance between the defects and angle γ between the symmetry axis of H-defect and the straight line passing through the both singular points. Consider two most important cases of mutual orientation of R- and H-defects: 1) $\gamma = 0$ ($\{R, H_{-1}\}$-pair, Figure 1a) and 2) $\gamma = \pi/2$ ($\{R, H_{+1}\}$-pair [1], Figure 1b).

STRUCTURE OF THE DIRECTOR FIELDS

To achieve the objective formulated let us write director components as follows

$$n_1 = \sin\alpha\cos\beta,\ n_2 = \sin\alpha\sin\beta,\ n_3 = \cos\alpha, \tag{1}$$

where α and β are the angular functions that must satisfy the equilibrium equations[1]

$$\nabla^2\alpha - \sin\alpha\cos\alpha(\nabla\beta)^2 = 0,$$
$$\nabla^2\beta + 2\cot\alpha(\nabla\alpha, \nabla\beta) = 0. \tag{2}$$

Since solving Equations (2) for the system of two defects requires complicated computations, it is usual to use analytical approximate functions $\tilde{\alpha}(\vec{r})$, $\tilde{\beta}(\vec{r})$ corresponding to a "quasi-equilibrium" director field that contains defects of given types.[4,5] The variation of parameters of these angular functions allows one to determine an evolution of a structure of the elastic field. Within the problem on two-defect interaction such parameters are a distance between defects and space angles that characterize their mutual orientation. Thus, the analysis of the situation in a system on the basis of the approximate functions makes it possible to reveal an energetically profitable arrangement and orientation of defects.

If we place R- and H-defects at points $(0,0,\pm a)$ as shown in Figure 1a the approximate solutions of Equations (2) will be the following[4]

$$\begin{cases} \tilde{\alpha}_{R,H_{-1}}(\vec{r}) = \pi - \cos^{-1}\dfrac{z+a}{\sqrt{x^2+y^2+(z+a)^2}} + \cos^{-1}\dfrac{z-a}{\sqrt{x^2+y^2+(z-a)^2}}, \\ \tilde{\beta}_{R,H_{-1}}(\vec{r}) = \tan^{-1}\dfrac{y}{x}. \end{cases} \tag{3}$$

If symmetry axes of the defects are parallel (Figure 1b) and intersect x-axis at the points $(\pm a,0,0)$ the angular functions will take the other form[5]

$$\begin{cases} \tilde{\alpha}_{R,H_{+1}}(\vec{r}) = 2\tan^{-1}\left[\tan\dfrac{\alpha_-}{2}\cdot\tan\dfrac{\alpha_+}{2}\right]^{\pm 1}, \\ \tilde{\beta}_{R,H_{+1}}(\vec{r}) = \beta_- + \beta_+ + \pi \end{cases} \tag{4}$$

where $\alpha_\pm = \cos^{-1}\dfrac{z}{\sqrt{(x\pm a)^2+y^2+z^2}}$ and $\beta_\pm = \tan^{-1}\dfrac{y}{x\pm a}$.

[1] Here the subscript labels the structure of hyperbolic defect in the plane of interaction: "-1" corresponds to the hyperbolic structure (Figure 1a) and "+1" - to the radial one (Figure 1b).

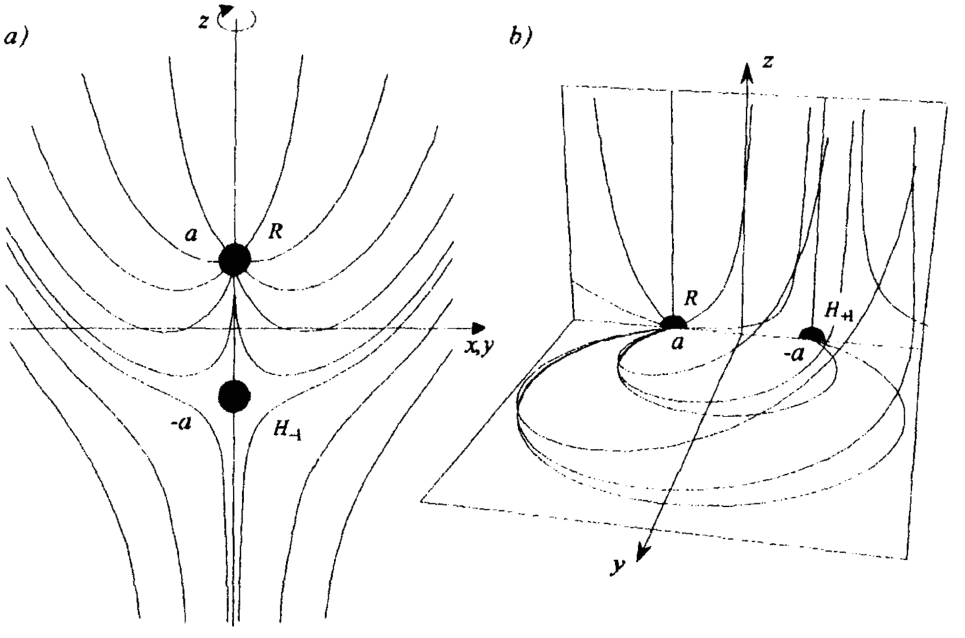

FIGURE 1. The structure of director fields a) $\{R, H_{-1}\}$-pair; b) $\{R, H_{+1}\}$-pair.

ELASTIC ENERGY OF DEFORMATIONS

To determine the relation between the energy of elastic deformations and distance between defects in the both cases under investigation let us substitute angular functions (3) and (4) into the formula for the free energy[1]

$$E_\gamma(a) = \frac{K}{2}\int_V \left\{(\nabla\alpha)^2 + \sin^2\alpha(\nabla\beta)^2 + 2\sin\alpha\left(\vec{n}[\nabla\alpha, \nabla\beta]\right)\right\} dV. \quad (5)$$

A spherical volume of radius R is considered as a domain of integration. On going to spherical coordinates (r,θ,φ) and making the change of variables $\xi = r/a$ we obtain after the corresponding transformations

$$E_0(a) = 5\pi Ka\cdot I\left(\frac{a}{R}\right) = 5\pi Ka\int_0^{\frac{R}{a}} \frac{\xi}{\xi^2+1}\ln\left|\frac{1+\xi}{1-\xi}\right| d\xi \quad (6)$$

and $$E_{\frac{\pi}{2}}(a) = 4Ka\int_0^{\frac{R}{a}}\int_0^{\frac{\pi}{2}}\int_0^{\pi} \sin^2\alpha_{R,H_{+1}}\left\{\sum_{i=1}^{4} J_i(\xi,\vartheta,\varphi)\right\}\xi^2\sin\vartheta\, d\xi\, d\vartheta\, d\varphi, \quad (7)$$

where $$J_1 = \frac{3\xi^2\sin^2\vartheta+1}{B^+B^-} + \frac{1}{A^+A^-}\left[1 + \frac{\xi^2\cos^2\vartheta\left(\xi^2\sin^2\vartheta - 1\right)}{B^+B^-}\right], \quad (8)$$

$$J_2 = C^- \cos\beta_{R,H_{+1}} \cos\varphi, \quad J_3 = C^+ \sin\beta_{R,H_{+1}} \sin\varphi, \tag{9}$$

$$J_4 = \xi \cos\alpha_{R,H_{+1}} \cos\vartheta \left[\frac{1}{A^- B^-} + \frac{1}{A^+ B^+} + \frac{\xi^2 \sin^2\vartheta - 1}{B^+ B^-} \left(\frac{1}{A^-} + \frac{1}{A^+} \right) \right], \tag{10}$$

$$A^{\pm} = \left(\xi^2 + 1 \pm 2\xi \sin\vartheta \cos\varphi\right)^{1/2}, \quad B^{\pm} = \xi^2 \sin^2\vartheta + 1 \pm 2\xi \sin\vartheta \cos\varphi,$$

$$C^{\pm} = \frac{2\xi \sin\alpha_{R,H_{+1}} \sin\vartheta}{B^+ B^-} \left(\frac{1}{A^-} + \frac{1}{A^+} \right) \left(\xi^2 \sin^2\vartheta \pm 1\right). \tag{11}$$

From the condition $\beta_{R,H_{+1}}(\pi - \varphi) = 2\pi - \beta_{R,H_{+1}}(\varphi)$ it follows that

$$J_i(\pi - \varphi) = \begin{cases} -J_i(\varphi), & i = 2,3, \\ J_i(\varphi), & i = 1,4 \end{cases}.$$

Hence $\int_0^{\pi} J_i d\varphi = \begin{cases} 0, & i = 2,3, \\ 2\int_0^{\pi/2} J_i d\varphi, & i = 1,4. \end{cases}$, and Equation (7) reduces to the simpler form

$$E_{\frac{\pi}{2}}(a) = 8Ka \int_0^{\frac{R}{a}} \int_0^{\frac{\pi}{2}} \int_0^{\frac{\pi}{2}} \sin^2\alpha_{R,H_{+1}} \{J_1 + J_4\} \xi^2 \sin\vartheta \, d\xi \, d\vartheta \, d\varphi \tag{12}$$

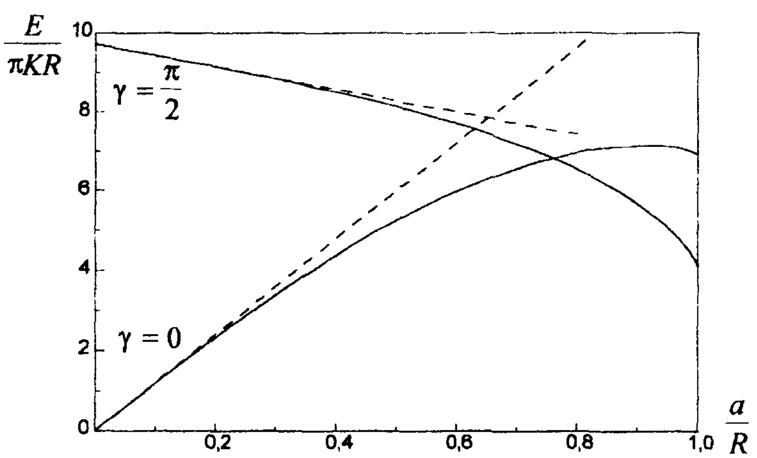

FIGURE 2. The energy-distance functions for $\{R, H_{-1}\}$ ($\gamma = 0$) and $\{R, H_{+1}\}$ ($\gamma = \pi/2$).

On integrating Equations (6) and (12) by means of computing and taking into account Equations (8)–(11) we obtain the energy-distance dependence $E(a)$ illustrated in Figure 2. To exclude the influence of the boundary of the domain of integration, consider next only the values $a/R \in [0; 0.001]$. In this interval the energy-distance functions are linear and can be approximately described by the following relations

$$E_0(a) \approx 5\pi K a \cdot I(0) = \left(\frac{5\pi^2}{4} a\right)\pi K, \quad (13)$$

$$E_{\frac{\pi}{2}}(a) = \left(9.7168R - \sqrt{8}a\right)\pi K. \quad (14)$$

DISCUSSION

From Figure 2 we notice that the energy of two-defect interaction for $\{R, H_{-1}\}$ and $\{R, H_{+1}\}$ are well described by functions (13) and (14) up to values of the order $a/R \approx 0.4$ and $a/R \approx 0.2$ respectively. The analysis of the dependencies shown in Figure 2 allows us to conclude that defects $\{R, H_{-1}\}$ attract each other and then annihilate creating an undistorted structure with zero elastic energy. Approaching defects $\{R, H_{+1}\}$ must occur with an increase of the elastic energy and leads to a creation of cylindrical defect P^c_{+2} of energy $E_{\frac{\pi}{2}}(0) \approx 9.7168\pi KR$ (Figure 3).[6] Besides, the graphical dependencies $E_0(a)$ and $E_{\frac{\pi}{2}}(a)$ intersect each other at the point $a^* \approx 0.6R$. Therefore in the process of a decay of P^c_{+2}-defect into the $\{R, H_{+1}\}$-pair reorientation of the hyperbolic defect $H_{+1} \to H_{-1}$ can occur at a certain distance of the order a^*, and then the $\{R, H_{-1}\}$-pair generated approaches and annihilates into a uniform director field. As this takes place at a point a^* the repulsion with the force $F_{\frac{\pi}{2}} = \sqrt{8}\pi K$ replaces by the attraction with the force $F_0 = -\frac{5\pi^3}{4}K$. This energetically profitable process can be depicted as the following scheme

$$P^c_{+2} \xrightarrow{a=0} \{R, H_{+1}\} \xrightarrow{a=a^*} \{R, H_{-1}\} \xrightarrow{a=0} E.$$

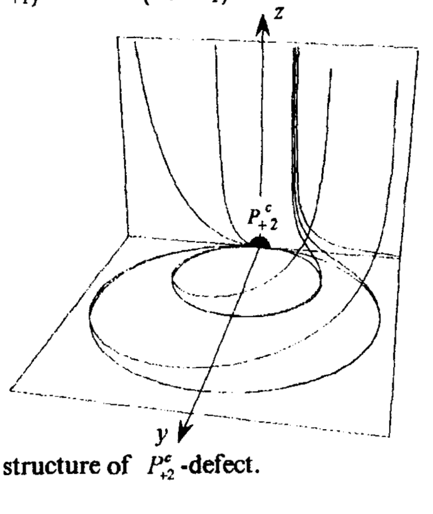

FIGURE 3. The structure of P^c_{+2}-defect.

Thus, according to their mutual orientation the R- and H-defects can attract or repel each other, the force of interaction in both cases not depending upon a distance between defects. Such a behaviour of H-defect can be associated with its special structure. In the symmetry plane of the director field of H-defect that is perpendicular to the defect symmetry axis director lines are radial. Hence, in this section the singular point is characterized by the positive topological invariant $k_{\perp} = +1$.[2] But in the director field of H-defect there also exist lines of hyperbolic type, which are peculiar to a singularity with the negative invariant $k_{\parallel} = -1$.[2] For the $\{R, H_{-1}\}$-pair the singularities with invariants opposite in sign in the plane of interaction arise; and they attract each other ($k_{\parallel} + k_R = 0$, Figure 1a). For the $\{R, H_{+1}\}$-pair the singularities in the plane of interaction have invariants of the same sign and they repel each other ($k_{\perp} + k_R = +2$, Figures 1b,3).

Existence of director lines both of radial and hyperbolic types is a peculiar property of all point defects with negative strength, so their interaction can also be an attraction or repulsion in accordance with their initial orientations with respect to the other defects of the system. Defects with positive strengths have only radial lines so they always repel each other, and their different mutual orientation influences only the magnitude of the force of repulsion.

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