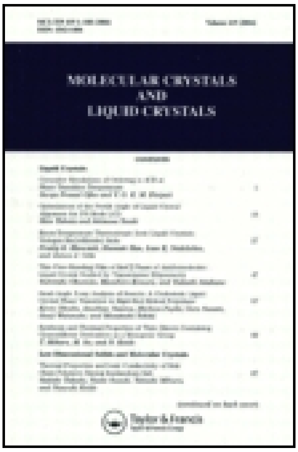

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Tatiana Kushnaryova [a] , Stanislav Kushnaryov [a] & Vitaly Pershin [a]
[a] Department of Physics, Cheliabinsk State University, Cheliabinsk, Russia
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DEFECTS OF CYLINDRICAL TYPE IN NEMATIC LIQUID CRYSTALS: DIRECTOR FIELDS OF MIRROR SYMMETRY

TATIANA KUSHNARYOVA, STANISLAV KUSHNARYOV,
VITALY PERSHIN
Department of Physics, Cheliabinsk State University,
Cheliabinsk, Russia

Abstract Within the framework of continuum theory of nematic ordering a new class of defects, which have stable director fields of cylindrical type with integer and half-integer topological invariants, has been studied.

INTRODUCTION

It is well known that the symmetry of nematic ordering allows an occurrence of line and point topological defects - disclinations and hedgehogs in nematic liquid crystals.

Classic line defects are Frank's planar disclinations[1] which in one-constant approximation of continuum theory is described by director fields $\vec{n}(\vec{r})$ of the form

$$n_x = \sin\alpha\cos\beta,\quad n_y = \sin\alpha\sin\beta, n_z = \cos\alpha \qquad (1)$$

where

$$\alpha = \pi / 2,\quad \beta = k\varphi, \qquad (2)$$

k = n/2 (n is an integer) is a disclination strength.

Equilibrium director fields of nematic distortions around point defects of axial symmetry can be approximately described by the following angular functions[2]

$$\alpha_k^*(\theta) \approx k\theta,\quad \beta_k^*(\varphi) = \varphi,\quad k = n. \qquad (3)$$

The following solutions of equilibrium equations are also possible[3,4]

$$\alpha_k^{\pm}(\theta) = 2\,\mathrm{atan}\left(C\left|\tan\frac{\theta}{2}\right|^{\pm|k|}\right),\quad C > 0, \qquad (4a)$$

$$\beta_k(\varphi) = k\varphi + C_0,\quad k = n/2 \qquad (4b)$$

where C and C_0 are arbitrary parameters.[1,4] When k = 1 Eq.(4) corresponds to well-known solution of nematic equilibrium equations for variable modifications of the radial hedgehog. For k ≠ 1 the parameter C_0 in Eq.(4b) only fixes an orientation of the defect in 3D-space, and we can take it to be equal to zero without any loss of generality.

The aim of the present work is to study topological defects in nematic liquid crystals, which have director fields described by Eqs.(4) Their structures, symmetries, energetics and topological characteristics have been considered.

STRUCTURE AND SYMMETRY

Let us consider structures of defects described by Eqs.(4). For this we take a system of differential equations for the director in cylindrical coordinates (ρ,φ,z)

$$\begin{cases} \dfrac{d(\ln\rho)}{d\varphi} = \cot\big(\beta(\varphi) - \varphi\big), \\ \dfrac{d\rho}{dz} = \tan\alpha\cos\big(\beta(\varphi) - \varphi\big), \end{cases} \tag{5}$$

The first of Eqs.(5) describes the structure within xy-plane, and the second one gives the spatial variation of the director. Substitution Eqs.(4) in Eqs.(5) gives the following expressions

$$\rho_k(\varphi, C_1) = C_1\left|\sin(k-1)\varphi\right|^{1/(k-1)}, C_1 > 0, \tag{6}$$

$$\frac{d\rho}{dz} = \frac{2Cg(\rho, z)^{\pm|k|}}{1 - C^2 g^{\pm 2|k|}(\rho, z)}\cos\big((k-1)\varphi\big), \tag{7}$$

where $g(\rho, z) = \left(\sqrt{\rho^2 + z^2} - z\right)\rho^{-1}$.

One can see from Eq.(6) that in the xy-plane there is a point singularity, which has exactly the same director field around it as a Frank disclination of the strength k; the director lines in this plane are symmetric about rotations through the π/|k-1|-angles for k=(2n+1)/2 and 2π/|k-1|-angles for k=n respectively. What this means is spatial director lines lie in the cylindrical surfaces (6). Because of

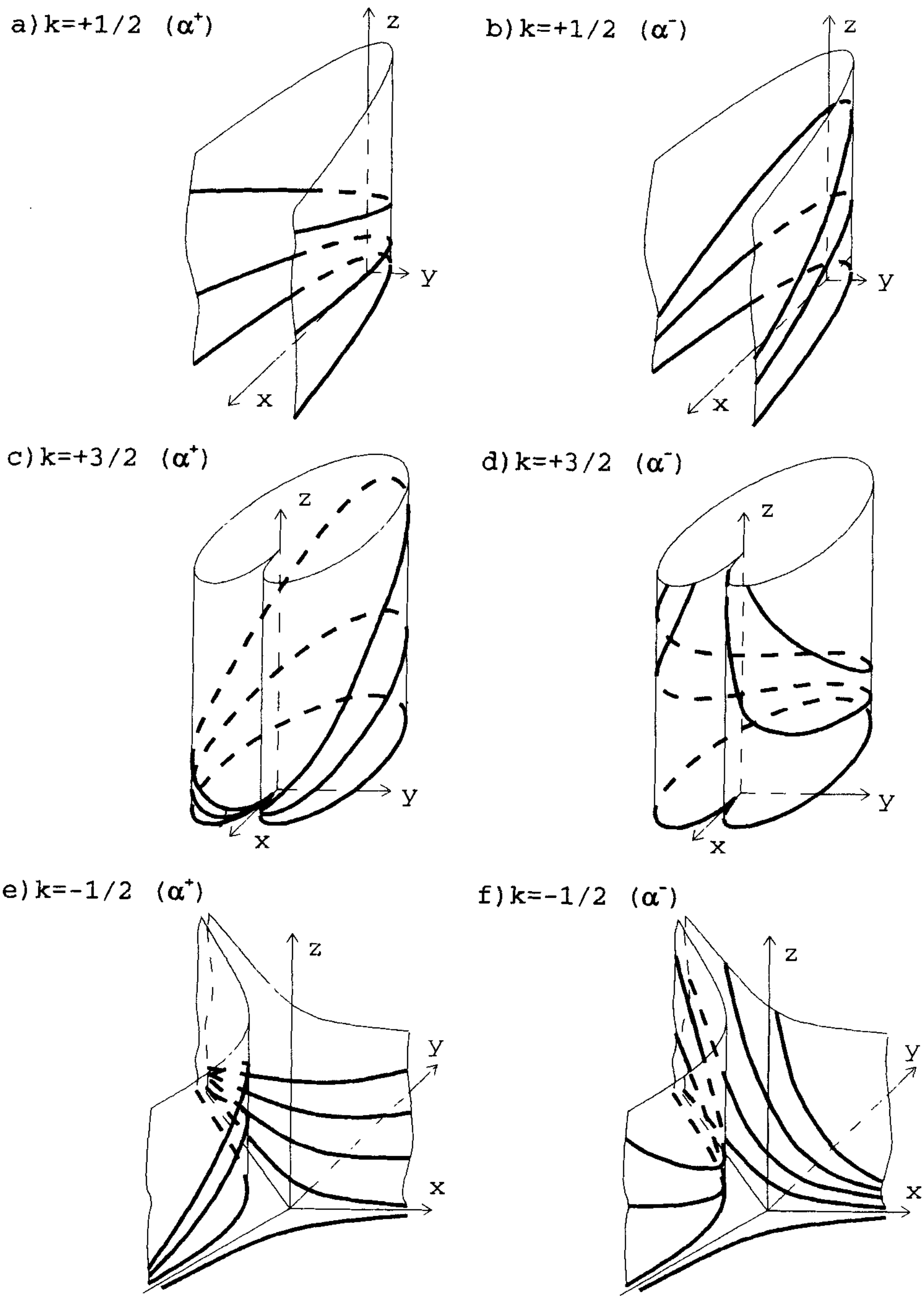

FIGURE 1 Half-integral defects of cylindrical type.

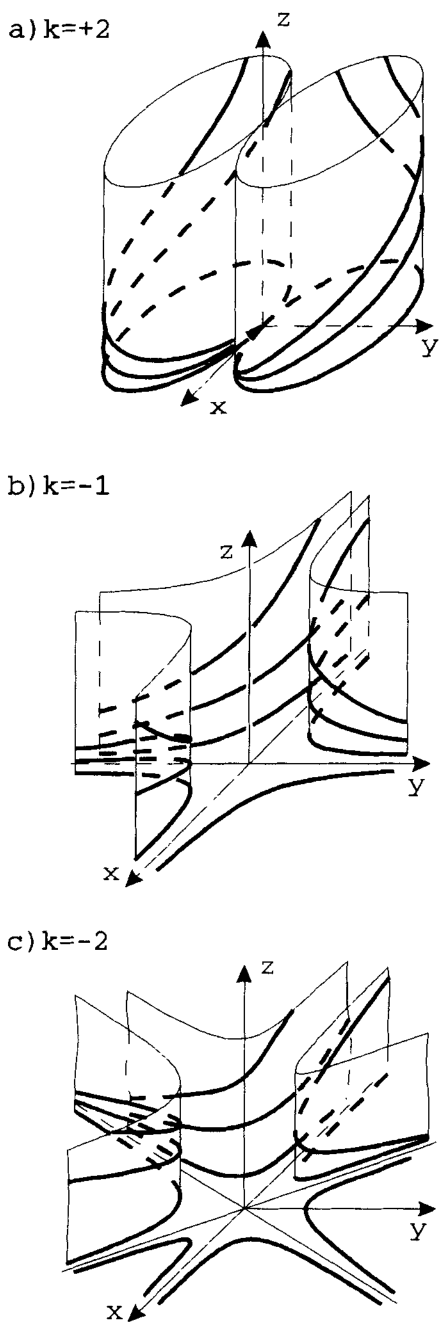

FIGURE 2 Integral defects of cylindrical type

this such a structure can be labeled as a defect of cylindrical type. Eq.(7) is invariant with respect to the conversion y→-y, hence the director fields are symmetric about xz-plane, to say the least. Moreover, at C = 1 there is a symmetry about xy-plane. In the subsequent discussion such structures will be referred to as mirror-symmetric ones.

FIGURES 1 and 2 depict structures of cylindrical type with mirror symmetry for some values k; they have been obtained by the numerical integration of Eq.(7).

For k=(2n+1)/2 the director field has a single symmetry plane xz, with the solutions α_k^+ and α_k^- corresponding to the different structures - with minimum or maximum on the director lines intersected the symmetry plane xz. Another plane of symmetry (xy) arises at C = 1 (FIGURE 1); in this case these structures differ from the corresponding Frank disclinations by only small-scale symmetric "escaping" of director along z-axis.

For k=n the director lines are not closed. For k > 0 vector lines emerge out of the origin of coordinates and, in going through one complete revolution around the cylinder $\rho_k(\varphi, C_1)$, go to infinity along the z-axis in the manner shown in FIGURE 2a for C = 1. For k < 0 vector lines present hyperbolae; at C = 1 one end of the line asymptotically approaches xy-plane, but the second one moves away to great distance from it (FIGURE 2b,c). In this case solutions α_k^+ and α_k^- correspond to the same structures, which differ from each other only by the rotation about z-axis.

Number of cylindrical surfaces $\rho_k(\varphi, C_1)$ increases by two units as the parameter $|k|$ increases by a unit; the resulting added plane of symmetry goes through z-axis.

In this way the integral structures of cylindrical type have the symmetry group $\mathbf{C}_{|k-1|v}$. It includes $|k-1|$ symmetry planes intersecting along the z-axis at $\pi/|k-1|$-angles. For C = 1 one gets an orthogonal symmetry plane xy so that the defects of mirror symmetry have the symmetry group $\mathbf{D}_{|k-1|h}$. At k = 1 that group degenerates into the group $\mathbf{D}_{\infty h}$; this corresponds to the axially symmetric point defects.

The characteristic feature of the mirror symmetric director fields of cylindrical type is only a slight variation of their structures from the corresponding planar disclinations near xy-plane ($\lim\limits_{z\to 0} \alpha_k^{\pm}(\rho, z) = \frac{\pi}{2}$). However as it moves away from xy-plane the function $\alpha_k^{\pm}(\rho, z)$ converges fast to 0 or π; that corresponds to director orientation along z-axis. So, the considerable distortions take place around the origin (FIGURE 3). It should be mentioned that the surfaces $\alpha_k^+(\rho, z)$ and $\alpha_k^-(\rho, z)$ are symmetric about the plane z = 0 and for the different k they do not differ from each other qualitatively. Moreover, from the relation $\lim\limits_{\rho\to 0} \alpha_k^{\pm}(\rho, z) = \pm\frac{\pi}{2}\left(1 - \mathrm{sign}(z)\right)$ it follows that director field $\vec{\mathbf{n}}_k(\vec{\mathbf{r}})$ is not defined at $\vec{\mathbf{r}}=0$ at all k. This means that in the director field there is a point defect.

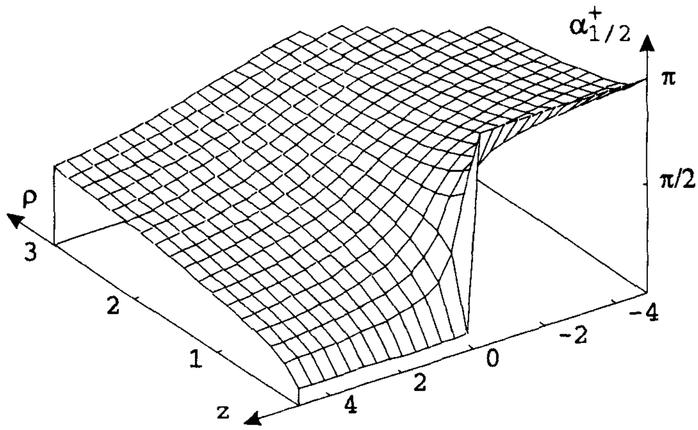

FIGURE 3

From FIGURE 3 it will be obvious that there exists a continuous mapping of $\alpha^{\pm}_k(\rho, z)$ onto a horizontal plane $\alpha = \pi / 2$. Taking into consideration that $\vec{\mathbf{n}}_k(\vec{\mathbf{r}})$ is a continuous function of $\alpha^{\pm}_k(\rho, z)$ one can conclude that it is possible for planar disclinations (2) and defects of cylindrical type of the same k to transform into each other as the energetic considerations require.

TOPOLOGICAL ANALYSIS

Degree of mapping for the structures under consideration is defined as

$$N = \frac{1}{4\pi}\iint_S \left|\vec{\mathbf{n}}\left[\frac{\partial\vec{\mathbf{n}}}{\partial\xi}, \frac{\partial\vec{\mathbf{n}}}{\partial\eta}\right]\right| d\xi d\eta = \frac{|k|}{2}\int_{\alpha(0)}^{\alpha(\pi)} \sin\alpha \, d\alpha = |k|, \qquad (8)$$

where (ξ, η) are arbitrary coordinates on the spherical surface S with a defect at the centre. It is seen from (8) that the degree of mapping does not depend on parameter C, and classes of topologically equivalent configurations are labeled by a set of integer and half-integer $|k|$.

The type of topological defect in nematics is known to be specified[5] by the kind of a compact set of points on the surface of a unit sphere $S^2\backslash Z_2$ with identified antipodal points (or projective plane RP^2 what is the same). This set is covered by the "arrow" of directors (if they are put from the sphere centre $S^2\backslash Z_2$) when the point or line defect is gone around over a closed surface or a loop. Such a set can be one of the three types:

1) a closed surface Σ_N, which covers RP^2 N times; it corresponds to a point defect of a strength N;

2) a nonshrinkable closed loop $\gamma_{1/2}$, which connects two antipodal points of RP^2; it corresponds to the stable half-integral line disclinations;

3) a nonclosed surface Σ_0 (or a nonclosed contour γ_0), which is continuously shrinkable to a point; it corresponds to a topologically unstable point (or line) defect with the director field that can be continuously deformed into the homogeneous one.

According to this classification the director fields of cylindrical type with the integer degrees of mapping N, correspond to surfaces Σ_N. Therefore they have point defects both in terms of topology and in terms of analysis of singular points of the corresponding vector function $\vec{\mathbf{n}}_k(\vec{\mathbf{r}})$.

Director fields of cylindrical type with the half-integer degrees of mapping N=n+1/2, correspond to surfaces Σ_N, covered RP^2 n+1/2 times. Such a surface is not shrinkable to a point, but it is topologically equivalent to a loop $\gamma_{1/2}$. This means that a half-integral defect of cylindrical type is topologically equivalent to the half-integral stable disclination. Formally a shrinking of Σ_N to $\gamma_{m+1/2}$ is equivalent to a continuous mapping the function $\alpha_k^{\pm}(\rho, z)$ to $\alpha = \pi / 2$. In this case the half-integral defect of cylindrical type transforms into a planar Frank's disclination of the corresponding strength.

ENERGY OF DEFECTS OF CYLINDRICAL TYPE

Let us calculate the free energy of elastic distortion arising in the nematic sample if there are defects of cylindrical type.

Free energy density of nematic distortions in one-constant approximation of the continuum theory $K_i = K$ ($i = 1,2,3$) takes the form

$$f = \frac{K}{2}\left\{(\mathrm{div}\ \vec{\mathbf{n}})^2 + (\mathrm{rot}\ \vec{\mathbf{n}})^2\right\}.$$

Substituting of Eq.(4) into this relation and integrating it over the spherical volume of radius R give the following expression for the distortion energy

$$E_k(\alpha_k^{\pm}, C) = \frac{E_R}{2}|k|\left\{1 + C^2 k J_{|k|}(C)\right\}. \qquad (9)$$

Here $E_R = 8\pi KR$ is the energy of the radial hedgehog[1];

$$J_{|k|}(C) = \int_0^{\infty} \frac{x^{|k|-1}\left(1 - C^2 x^{|k|}\right)}{\left(1 + C^2 x^{|k|}\right)^3}\,\frac{1 - x}{1 + x}\,dx. \qquad (10)$$

As the integral function $J_{|k|}(C) > 0$, one can see from Eq.(9) that the positive defects of cylindrical type always have more energies than the negative defects. Also $E_k(C)$ and $E_{-k}(C)$ are symmetric about $E_k^* = \frac{E_R}{2}|k|$, and have the extreme values at $C = 1$ (maximum for $k > 0$ and minimum for $k < 0$). The difference in energy between positive and negative defects of mirror symmetry is to $\Delta E_k(C = 1) = 8\pi KRk^2 J_k$ and it converges to the constant limit $\Delta E_{k\,lim} = 4\pi KR$ (at $k \geq 10$ $|\Delta E_k - \Delta E_{k\,lim}| \leq 0{,}033\pi KR$) rather rapidly. Hence $J_{|k|}(C = 1) \approx 1/2k^2$ and Eq.(9) can be written as the simple analytic formula for reasonably large k

$$E_k(C = 1) \approx 4\pi KR\left(|k| + \frac{1}{2}\,\mathrm{sign}(k)\right),\quad k \neq 1. \qquad (11)$$

Thus, if the value of parameter C is not fixed then only negative defects of mirror symmetry of the type sketched in FIGURE 1e,f and 2b,c will be energetically stable. For the positive defects a relaxation into the symmetric states with $C \to 0$ and $C \to \infty$ with energy E_k^* are energetically favourable.

It should be noted that the degenerate case $k = +1$ satisfies (11) only at $C_0 = \pi/2$ and $C = 1$ when director lies in the concentric circular cylinders. Hence such a structure is a defect of cylindrical type as well (FIGURE 4). But unlike the corresponding planar disclination of the strength +1, vector lines of this structure are spatial spirals with an exponentially increasing pitch as the curve moves away from xy-plane; the sign of a spiral is defined by the choosing of a solution (4a) (α^+ or α^-).

a) $\vec{n}\left(\alpha_1^+, \beta_1 = \varphi + \frac{\pi}{2}\right)$ b) $\vec{n}\left(\alpha_1^-, \beta_1 = \varphi + \frac{\pi}{2}\right)$

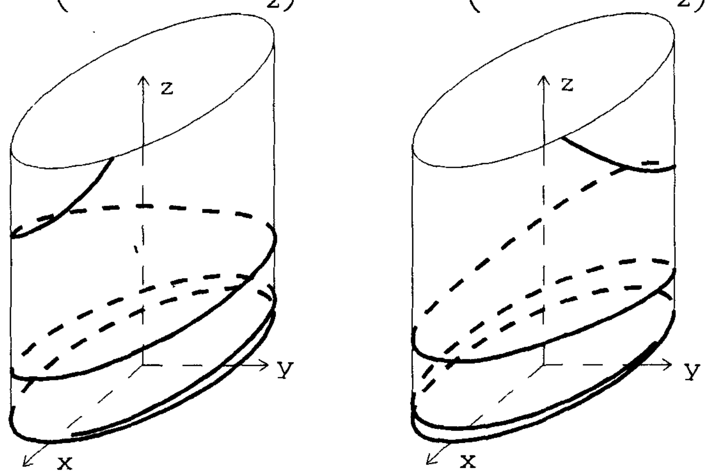

FIGURE 4

DISCUSSION AND CONCLUSIONS

Therefore the solutions of nematic equilibrium equations permit integral and half-integral singularities of different topological types and symmetries.

Point defects of cylindrical type (P^c) differ essentially from axially symmetric ones[2] (P^a) both in structure, symmetry and energy. These two classes of point defects have two common defects, namely, the radial and hyperbolic hedgehogs that possess the features characterized by both the classes simultaneously.

Half-integral defects of cylindrical type (L^c) are topologically equivalent to the stable Frank's disclinations of the half-integral strength (L^p) and differ from the latter

TABLE I

Type	Solutions of equilibrium equations	Features	Topological invariants
Planar disclinations[1] L_k^p	$\alpha = \frac{\pi}{2}$ $\beta_k(\varphi) = k\varphi$	director field is orthogonal to the disclination line	N=0 when k=n; N=1 when k=n+1/2, n is integer
Defects of cylindrical type a) $L^c_{k=n+1/2}$ (linear) b) $P^c_{k=n}$ (point)	$\alpha_k^{\pm}(C,\theta) = 2\mathrm{atan}\left(C\tan^{\pm\lvert k\rvert}\frac{\theta}{2}\right)$ $\beta_k(\varphi) = k\varphi$	1) the director has projection on a plane normal to the disclination line which coincides with the director field of L_k^p; 2) director lies on the cylindrical surfaces $\rho_k(\varphi, C_1)$ (6)	a) N=|k|=n+1/2, defects are topologically equivalent to the disclinations b) N=|k|=n; they are point defects
Defects of cylindrical type with mirror symmetry (C=1) a) $L^{c(m)}_{k=n+1/2}$; b) $P^{c(m)}_{k=n}$	$\alpha_k^{\pm}(\theta) = \pm 2\mathrm{atan}\left(\tan^{\pm\lvert k\rvert}\frac{\theta}{2}\right)$ $\beta_k(\varphi) = k\varphi$	3) In addition to 1) and 2) they are symmetric about the xy-plane	a) linear (FIGURE 1); b) point (FIGURE 2)
Axially symmetric point defects[2] P_k^a	$\alpha_k(\theta) \approx k\theta$, $\beta = \varphi$	there are 2|k-1| sectors bounded by the director straight lines and a symmetry axis C_∞	N=|k|, k=n

TABLE I (continue)

Symmetry	**Energy of a single defect**	**Interaction (Energy and Force)**
1) translations along the discli nation line; 2) $C_{2\|k-1\|v}$: $2\|k-1\|$ symmetry planes intersect on symmetry axis $C_{2\|k-1\|}$ at $\pi/2\|k-1\|$-angles	per unit length of disclination: $E_k = \pi K k^2 \ln \frac{R}{r_c} + E_c,$ E_c and r_c are core energy and core radius respectively	$E_{k_1 k_2}(a) =$ $= \pi K (k_1 + k_2)^2 \ln \frac{R}{r_c} -$ $-2\pi K k_1 k_2 \ln \frac{a}{2r_c},$ $F_{k_1 k_2}(a) = \frac{2\pi K k_1 k_2}{a}$
a) generally there is one plane of symmetry (xz) passing through the disclination line b) $C_{\|k-1\|v}$: $\|k-1\|$ symmetry planes intersected on axis $C_{\|k-1\|}$	$E_k(C) = 4\pi KR\|k\|\left(1 + C^2 k J_{\|k\|}(C)\right)$ $J_{\|k\|}(C) = \int_0^\infty \frac{x^{\|k\|-1}\left(1 - C^2 x^{\|k\|}\right)}{\left(1 + C^2 x^{\|k\|}\right)^3} \times$ $\times \frac{1-x}{1+x} dx$	
a) there are two normal symmetry planes xy and xz b) $D_{\|k-1\|h}$: $\|k-1\|$ symmetry planes intersect on axis $C_{\|k-1\|}$ at $\pi/\|k-1\|$-angles and perpendicular symmetry plane xy; for even $\|k-1\|$ there is an inversion	$E_k = 4\pi KR\|k\|\left(1 + k I_{\|k\|}\right)$ $I_{\|k\|} = J_{\|k\|}(C = 1) \approx 2/k^2,$ $E_k = f(k)$	
$D_{\infty h}$: a symmetry axis C_∞ and symmetry planes passing through C_∞	$E_k \approx 2\pi KR\left\{\frac{k^2(2k+1)}{2k-1} + \right.$ $\left. + \sum_{n=1}^{\|k\|} \frac{1}{2n-1}\right\},$ $E_k = f(k^2)$	$E_{k_1k_2}(a) = E_{k_1+k_2} + \pi K I_0 a \times$ $\begin{cases} -k_1k_2, & k_1 \neq -k_2 \\ k^2 + 4\|k\|, & k_1 = -k_2 = k \end{cases}$ $F_{k_1k_2}(a) = \pi K I_0 \times$ $\begin{cases} k_1k_2, & k_1 \neq -k_2 \\ -k^2 - 4\|k\|, & k_1 = -k_2 = k \end{cases}$ $I_0 = \frac{\pi^2}{4}$

by 3D-distortions of director lines. These distortions are the small-scale "escape" from the planes orthogonal to z-axis. Formally this is reflected in the fact that the Cartesian components of director depend more on the spatial coordinate (z). Also L^c are more energetically favourable to the planar structures L^p because of the linear dependence of energy on topological invariant k and because of an absence of a divergence of the integral (9) at x=y=0.

Hence defects of cylindrical type are the "escaped" structures of classic disclinations of the corresponding strength. Planar disclinations of half-integral strengths k, that are slightly distorted by the "escape", remain topologically as the disclinations. Planar disclinations of integral strengths k "escape" completely and transform into a point defect. Retention of a point singularity within xy-plane is caused by equiprobability of the "escape" in both the positive and negative directions along z-axis as it is dictated by the symmetry of nematic equilibrium equations.

It should be noted that in the hyperbolic hedgehog, which is labeled by both k = +1 and k = -1, one can consider an "escape" of radial or hyperbolic planar disclination respectively according to its orientation.

Therefore all the singularities of nematic director field in 3D-space are divisible into four classes: planar and non-planar disclinations, axially symmetric point defects and point defects of cylindrical type.

The main results about structures, symmetry, topological invariants, energy of single defect and interaction of two defects are summarized in TABLE I.

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