INTERACTION OF AN ELONGATED PARTICLE SUSPENDED IN A NEMATIC WITH A (1/2) DISCLINATION LINE

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An elongated particle suspended in a nematic is described with the help of a localized system of defects. Elastic interaction of such a particle with a plane disclination with a strength of (1/2) is considered. It is demonstrated that, in the vicinity of a disclination, the system of defects of the particle undergoes essential changes that depend on the distance d between the particle and the disclination and the orientation of the particle with respect to the special disclination line. In this case, the interaction force is of attractive character and depends only on the distance d.

1. Introduction

Suspensions of colloid particles in liquid crystals represent very perspective materials from the viewpoint of their use in current information processing and display systems. In such suspensions, anisotropic optical properties of the carrier matrix are combined with specific (for example, dielectric [1] or magnetic [2,3]) properties of the disperse phase. Due to this fact, it is possible to synthesize new liquid crystal materials that essentially differ from pure systems in a number of physical parameters.

Materials of such a kind include, in particular, the so-called ferronematics (FNs) – suspensions of single-domain ferro- or ferrimagnetic particles in nematic liquid crystals (NLC) [2–5]. In the given systems, the use of the anisometric (for example, elongated) form of magnetic grains gives a possibility to realize the strong orientational connection between the directions of the long axes of ferroparticles (that is, their magnetic moments) and the director **n** of a nematic matrix. This allows one to increase the magnetic susceptibility of the suspension by 2–4 orders of magnitude as compared to pure NLC and to control the orientational structure of FN with the help of weak (up to 10 Oe) magnetic fields.

In the synthesized thermotropic FNs [2], the elongated grains of the disperse phase were characterized by the length $L \sim 0.5$ μm and radius $R \sim L/14$. As the characteristic dimensions of ferroparticles essentially exceed the length a of NLC molecules ($a \sim (2 \div 5) \times 10^{-3}$ μm), we described theoretically the internal structure of the suspension, by considering particles of the disperse phase as macroscopic objects suspended in the nematic matrix [4–6]. Every object of such a kind forms an orientational distortion around itself which can be identified in many cases with some system of linear defects. In this case, it is natural to expect that particles will interact with linear defects of the liquid crystal matrix itself. Such disclination approaches were earlier used in the literature for the description of the director field in the vicinity of spherical [7] and elongated [8] particles as well as for description of the interaction between two particles of either spherical [9] or elongated [10] form. Furthermore, there exist the theoretical and experimental investigations of the interaction of a spherical particle with disclination lines [11]. However, the problem of the interaction of an elongated particle with linear defects wasn't discussed till now.

In the given paper, we'll take the first step to the solution of this problem by investigating the character of the elastic interaction between a particle and a disclination line with the strength (topological charge) $m_d = 1/2$. As was shown in [12], in the case where the elastic moduli of a nematic K_{11}, K_{22}, and K_{33} are close, this kind of plane disclinations is resistant to the escape to the third dimension.

Implying thermotropic FNs [2], let's specify homeotropic boundary conditions for the NLC director on the surfaces of elongated particles. As was shown in the experiments, the long axes of such particles in the suspended state are oriented normally to the director. The axis of an external disclination must be also oriented in the same direction. That's why we'll consider below the most real situation where an elongated particle is parallel to the disclination line.

2. Disclination Methods of Description of a Particle

We now derive the equation of equilibrium for an NLC and present a particle in the form of a localized system of defects.

We assume that the elongated particle has a cylindrical form and the anchoring of the director with its surface is rigid (the surface anchoring energy is infinitely large). Let's introduce a Cartesian coordinate system with the z-axis directed in the line of the long axis of the particle. Taking into account that the particle length L is much higher than its radius R, possible distortions close to the cylinder ends can be neglected. In this case, the expected NLC orientational structures will have a form of plane deformations with the director $\mathbf{n} = [\cos\Phi, \sin\Phi, 0]$, where $\Phi = \Phi(x, y)$. The equilibrium distribution of the director field, that is, the equilibrium value of the angle $\Phi = \Phi(x, y)$ can be found from the minimum condition of the NLC free energy. In the case of plane deformations and in the so-called two-constant approach $K_{11} = K_{22} = K$, the free energy functional F has the form

$$F = \frac{KL}{2}\int\limits_V \left[(\mathrm{div}\mathbf{n})^2 + (\mathrm{rot}\mathbf{n})^2\right] dV = \frac{KL}{2}\int\limits_V (\nabla\Phi)^2 dV. \quad (1)$$

The minimization of this functional gives the Laplace equation for the angle Φ:

$$\Delta\Phi = \frac{\partial^2\Phi}{\partial x^2} + \frac{\partial^2\Phi}{\partial y^2} = 0. \quad (2)$$

The solution $\Phi(x, y)$ of the given equation must satisfy the homeotropic boundary conditions on the surface of the particle, that is, the director $\mathbf{n}$ corresponding to this solution must be oriented normally to the side face of the cylinder. Let's demonstrate the ways of constructing the solutions for a separate elongated particle suspended in a nematic.

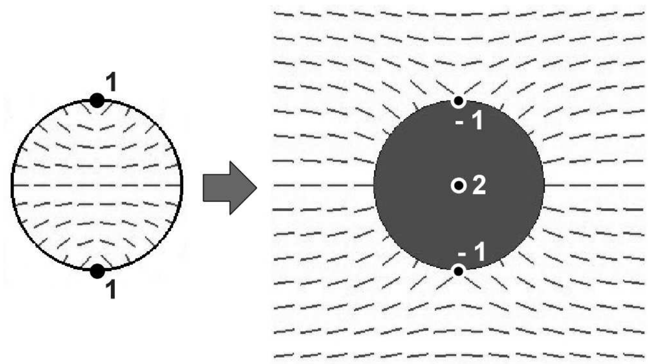


Fig. 1. Particle with the charge $q = 0$ in a nematic matrix: the inversion of a planar polar structure in a cylindrical capillary

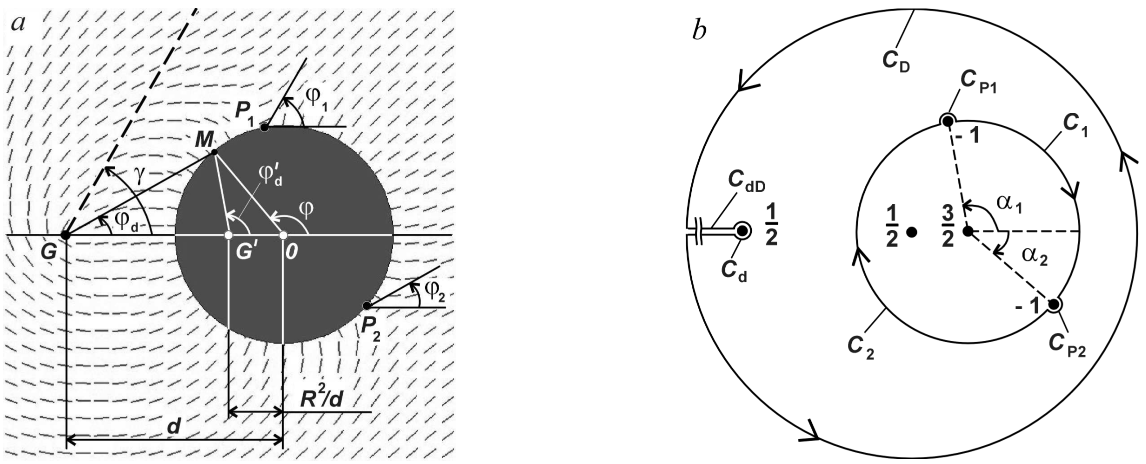
It's well known [13–15] that the solution of the equation of equilibrium (2) can be presented by any superposition of distortions specified by plane disclinations with arbitrary topological charges multiple of (1/2). This fact allows one to describe an elongated particle with the help of a localized system of defects using at least two different methods.

The first method is rather evident: the system of defects has the total topological charge $q = 1$ and consists of one disclination line oriented along the cylinder axis. The distortion is specified by the angle $\Phi = \varphi = \arctan(y/x)$, which corresponds to the homeotropic cohesion, while the energy of the particle obtained from (1) has a form

$$F_{\mathrm{part}}(q = 1) = \pi K L \ln(D/R),$$

where D is the characteristic dimension of the sample. This method of description has an essential disadvantage: a particle with the charge $q = 1$ doesn't match the uniform distribution of the director field. In practice, a suspension with such particles can be realized only in inhomogeneous liquid crystal systems with a large number of defects. Energetically, this situation is extremely disadvantageous.

In the other method of description, the localized system of defects consists of three disclination lines, while its total topological charge $q = 0$. The arrangement and charges of the disclination lines can be easily obtained if we apply the inversion transformation to the well-known planar polar NLC structure in a cylindrical capillary [15, 16] (see Fig. 1). As was shown in [15], this structure is specified by two disclination lines with the charges $m'_1 = m'_2 = 1$. The disclinations pass through



a **b**

Fig. 2. Particle close to a disclination: a – the diagram of constructing the solution, b – charge distribution and integration contour

diametrically opposite points of the circle that specifies the side face of the cylinder in the (x, y) plane. The inversion transformation with respect to the circle of radius R which is equivalent to the substitution

$$r = \sqrt{x^2 + y^2} \to R^2/r, \varphi = \arctan(y/x) \to -\varphi,$$

conserves the homeotropic type of anchoring on the surface of the particle but changes the charge of the disclination lines to the opposite one, i.e. $m_1' = m_2' = 1 \to m_1 = m_2 = -1$. In addition, a disclination line is formed at the axis of the particle that has the topological charge $m_0 = 2$ and represents the image of a fictitious distortion with the charge $m_\infty = -2$ spread at infinity (or an image of the disclination with $m_\infty = -2$ that passes through an infinitely remote point of the Riemannian sphere). Thus, at $q = 0$, the particle is described by the localized system of disclination lines $\{-1, 2, -1\}$, while the uniform distribution of the director corresponds to the function $\Phi = 2\varphi - \varphi_1 - \varphi_2$, where the angles φ_1, φ_2 are specified by surface defects. The energy of such a particle obtained from (1) coincides with the energy of the planar polar structure and has the form [4, 15]

$$F_{\text{part}}(q = 0) = \pi K L \ln (R/2\rho), \quad (3)$$

where ρ is the radius of the disclination core. It's worth noting that, at $q = 0$, the particle matches the uniform distribution of the director field, i.e. it doesn't violate the long-range orientational order of the liquid crystal suspension. Moreover, for the real suspensions with $\rho \sim a \sim (2 \div 5) \times 10^{-3}$ μm, $R \sim 3.5 \times 10^{-1}$ μm, and the samples with the characteristic dimension $D \sim 10^1 \div 10^3$ μm, we obtain $F_{\text{part}}(q = 0) < F_{\text{part}}(q = 1)$, i.e. the $q = 0$ state is more energetically advantageous than the $q = 1$ one. That's why we consider below that the particle has the total topological charge $q = 0$.

3. Reconstruction of the System of Defects of a Particle in the Vicinity of a Disclination

Let's consider a cylindrical particle with the charge $q = 0$ suspended in a nematic that is localized in the vicinity of a disclination line with the strength $m_d = 1/2$. The axis of the disclination passes in parallel to the cylinder axis at the distance $d \geq R$. Let's find the director distribution, i.e. the function $\Phi(x, y)$ that satisfies Eq.(2) and the homeotropic boundary conditions on the surface of the particle.

It is known [13, 14] that a disclination line is characterized by a nonuniform distribution of the director field that corresponds to the function

$$\Phi_d = \frac{\varphi_d}{2} + \beta, \quad (4)$$

where β is the initial phase of the disclination. This orientational distortion violates the condition of homeotropic anchoring on the surface of the particle. In order to satisfy the specified boundary conditions, it's necessary to reconstruct the initial system $\{-1, 2, -1\}$ of localized defects of the particle.

At the first stage of constructing the solution, we used the image method [14]. We assume that the external disclination line passes through the point $G = [-d, 0]$

of the (x, y) plane (see Fig. 2,*a*). Let's put a fictitious disclination having the same charge $m'_d = 1/2$ to the point $G' = [-R^2/d, 0]$ conjugate with respect to the circle of radius R. In this case, for an arbitrary point M lying on the circle of radius R, the triangles OMG and OMG' are similar, as they have a common angle, while two sides adjacent to it are proportional. Taking into account this fact, one can express the distortion specified on the surface of the particle by two considered disclination lines in terms of the angle φ:

$$(\Phi_d + \Phi'_d)_R = \left(\frac{\varphi_d + \varphi'_d}{2}\right)_R = \frac{\varphi}{2},$$

where $\beta = 0$. In order to compensate the obtained distortion, we put an additional fictitious disclination with the charge $m'_0 = -1/2$ at the axis of the particle.

We now pass to the second step of constructing the solution, namely we will compensate an additional turn of the director on the surface of the particle that takes place at the expense of the non-zero initial phase β of the external disclination. It is achieved by means of a change of the mutual orientation of the linear defects $\{-1, 2, -1\}$ that describe the particle. It follows from Fig. 1 that, in the uniform matrix of a nematic, defects are localized on the same line. In the vicinity of the external disclination, linear defects that have the charges $m_1 = m_2 = -1$ and are moved by the surface of the particle can shift from the diametrically opposite points of the circle that specifies the side face of the cylinder. The magnitude and direction of a displacement of each linear defect must depend on both the distance d between the particle and the external disclination and the azimuth orientation of the particle with respect to the special disclination line. We recall that, by the special line, we imply the direction of the rectilinear radial "line of flow" of the distribution $\mathbf{n}(x, y)$ of a separate disclination [13]. In our case, this line is oriented at the angle $\gamma = 2\beta$ to the direction that joins the axes of the particle and the disclination, i.e., to the reference direction of the angle φ (see Fig. 2,*a*).

Let's assume that the surface disclinations with the charges $m_1 = m_2 = -1$ are localized at the points $P_1 = [\cos(\alpha_1), \sin(\alpha_1)]$ and $P_2 = [\cos(\alpha_2), \sin(\alpha_2)]$, where the angles α_1 and α_2 are shown in Fig. 2,*b*, while the anticlockwise direction is accepted for the positive reference direction. In this case, it's easy to demonstrate geometrically (as was done, e.g., in [15]) that, on the surface of the particle, the director will deviate from the initial radial direction by the angle $\Phi_0 = -\frac{\alpha_1+\alpha_2}{2}$. In order to recover the homeotropic orientation of the director, it's necessary to add the phase $(-\Phi_0)$ to the distribution formed by the disclination lines. In this case, the full expression for the angle $\Phi(x, y)$ will have the form

$$\Phi = \frac{\varphi_d + \varphi'_d}{2} + \frac{3\varphi}{2} - \varphi_1 - \varphi_2 + \frac{\alpha_1 + \alpha_2}{2}. \quad (5)$$

As the charge of the particle remains equal to zero, the field of the director at large distances $D \gg d$ must correspond to the distortion specified by the external disclination line, that is, function (4). This fact allows one to establish the relation between α_1, α_2, and β:

$$\beta = -\Phi_0 = \frac{\alpha_1 + \alpha_2}{2}. \quad (6)$$

In a real system, the phase β is specified, while the angles α_1 and α_2 must represent functions of β. That's why we need two additional conditions that link the parameters α_1, α_2, and β. The first condition is presented by relation (6) that lets two parameters be independent, for example, β and α_1. The other condition is that of minimum of the free energy functional $F(\beta, \alpha_1)$ with respect to α_1, i.e. $\partial F(\beta, \alpha_1)/\partial\alpha_1 = 0$. Let's derive the free energy of the system and determine the functions $\alpha_1(\beta)$ and $\alpha_2(\beta)$.

4. Calculation of the Free Energy

First of all, let's determine uniquely the function $\Phi(x, y)$ from (5). For this purpose, let's cut the (x, y) plane, as it is shown in Fig. 2,*b*. The free energy functional (1) can be obtained with the help of the Gauss theorem as

$$F = \frac{KL}{2}\int_V (\nabla\Phi)^2 dV =$$

$$= \frac{KL}{2}\left[\int_V \nabla(\Phi\nabla\Phi)dV - \int_V \Phi\Delta\Phi dV\right] =$$

$$= \frac{KL}{2}\left[\int_{C_{\rm ex}} \Phi\nabla\Phi d\mathbf{c} + \int_{C_{\rm in}} \Phi\nabla\Phi d\mathbf{c}\right]. \quad (7)$$

Here, we take into account that, according to (2), $\Delta\Phi = 0$; the integration contour that consists of the external $C_{\rm ex} = C_D + C_{dD} + C_d$ and internal $C_{\rm in} = C_1 + C_2 + C_{P1} + C_{P2}$ regions is shown in Fig. 2,*b*. Taking into consideration that the gradient of the function $\Phi(x, y)$ consists of the components of the $\nabla\varphi$ type, each of them representing a circular vector [13, 14], we obtain that the integral over the remote circle C_D is equal to zero. Based on the same considerations, one can conclude that the disclinations localized at the centers of small contours C_d, C_{P1}, and C_{P2} of radius ρ don't contribute to the corresponding integrals, that's why the order of the latter doesn't exceed (ρ/R). As $\rho \ll R$, these integrals can be neglected.

Let's consider the integral over the cut C_{dD} which can be easier calculated using polar coordinates. The jump of function (5) across this cut is equal to π. In the upper half of the cut, $\nabla_\varphi \Phi \uparrow\uparrow d\mathbf{c}$, the quantity $dc = -dr$, while the integral is taken between the limits D and $\rho+d$. In this case, by changing the range of integration and neglecting the terms of the order of (ρ/R) and higher, we obtain

$$F_{dD} = \frac{\pi KL}{2} \int\limits_{D}^{d+\rho} dr \left[\frac{1}{2(r-d)} + \frac{d}{2(rd-R^2)} + \frac{3}{2r} - \right.$$

$$\left. - \frac{R\cos\alpha_1 + r}{R^2 + 2rR\cos\alpha_1 + r^2} - \frac{R\cos\alpha_2 + r}{R^2 + 2rR\cos\alpha_2 + r^2} \right] =$$

$$= F_{dis} + \frac{\pi KL}{4} \times$$

$$\times \ln \frac{\left(R^2 + 2dR\cos\alpha_1 + d^2\right) \cdot \left(R^2 + 2dR\cos\alpha_2 + d^2\right)}{d^2\left(d^2 - R^2\right)}, \tag{8}$$

where $F_{\text{dis}} = (\pi KL/4) \ln (D/\rho)$ is the energy of the external disclination line.

Let's pass to the integration over the regions C_1 and C_2 on the surface of the particle. In these regions, function (5) takes the values φ and $(\varphi + \pi)$, correspondingly, while the radial component of the vector $(\nabla\Phi)$ is equal to

$$\nabla_r \Phi = \frac{\sin(\alpha_1) + \sin(\varphi)}{2R\left(\cos(\alpha_1) - \cos(\varphi)\right)} + \frac{\sin(\alpha_2) + \sin(\varphi)}{2R\left(\cos(\alpha_2) - \cos(\varphi)\right)} +$$

$$+ \frac{d\sin(\varphi)}{d^2 + 2dR\cos(\varphi) + R^2}.$$

Taking into account that $\nabla_r \Phi \uparrow\downarrow d\mathbf{c}$, $dc = -Rd\varphi$, and the integration is carried out over the surface of the particle except for the cut (with the sector $2\alpha_\rho = 2\arctan(\rho/R)$) points P_1 and P_2, we obtain, in the $\rho \ll R$ approximation,

$$F_{C_1+C_2} = -\frac{KL}{2} \left[\int\limits_{\alpha_2+\alpha_\rho}^{\alpha_1-\alpha_\rho} R\varphi \nabla_r \Phi d\varphi + \right.$$

$$\left. + \int\limits_{\alpha_1+\alpha_\rho}^{2\pi+\alpha_2-\alpha_\rho} R\left(\varphi+\pi\right) \nabla_r \Phi d\varphi \right] =$$

$$= \frac{\pi KL}{4} \ln \frac{(R^2 + 2dR\cos\alpha_1 + d^2)(R^2 + 2dR\cos\alpha_2 + d^2)}{d^2} +$$

$$+ F_{\text{part}}(q = 0,\, \alpha_1,\, \alpha_2). \tag{9}$$

Here, $F_{\text{part}}(q = 0, \alpha_1, \alpha_2)$ is the energy of the particle with asymmetric arrangement of the disclination lines $\{-1, 2, -1\}$:

$$F_{\text{part}}\left(q = 0, \alpha_1, \alpha_2\right) = \pi KL \ln \frac{R}{\rho\sqrt{2\left(1 - \cos(\alpha_1 - \alpha_2)\right)}}. \tag{10}$$

It's worth noting that, in the uniform matrix of a nematic, relation (10) passes into expression (3) that corresponds to the energy minimum at $\alpha_2 = \alpha_1 \pm \pi$. In addition, formula (10) also gives a correct result in the case of the coalescence of the surface disclination lines with the charges $m_1 = m_2 = -1$. In this case, the particle is described by the localized system of linear defects $\{-2, 2\}$. The coalescence takes place at $|\alpha_1 - \alpha_2| \sim \arctan(\rho/R)$, which corresponds to the energy $F_{\text{part}}\left(q = 0, \alpha_1 = \alpha_2\right) = 2\pi KL \ln(R/\rho)$. In the uniform matrix of a nematic, such a situation is metastable. However, coalescence is possible in the vicinity of an external disclination, where fictitious disclinations having the strength $(\pm 1/2)$ are added to the system of defects of the particle. This result will be demonstrated in the next chapter.

Let's return to the free energy functional. Substituting the values of integrals (8) and (9) into (7) and expressing the angle α_2 in terms of α_1 and β with the help of (6), we obtain

$$F = F_{\text{dis}} + F_{\text{part}}\left(q = 0\right) + F_{\text{inter}}(\beta, \alpha_1), \tag{11}$$

where the relation

$$F_{\text{inter}}(\beta, \alpha_1) = \frac{\pi KL}{2} \ln(2(R^2 + 2dR\cos\alpha_1 + d^2) \times$$

$$\times(R^2 + 2dR\cos(2\beta - \alpha_1) + d^2))/$$

$$/(d^3\sqrt{d^2 - R^2}(1 - \cos(2\alpha_1 - 2\beta))) \quad (12)$$

describes the intermediate functional of the energy of interaction between the particle and the disclination.

5. Arrangement of Surface Defects and Force of the Particle–Disclination Interaction

Let's find the arrangement of surface linear defects. Minimizing the interaction energy (12) with respect to α_1, we obtain the equation for the function $\alpha_1(\beta)$:

$$\frac{dR\sin a_1}{R^2 + 2dR\cos\alpha_1 + d^2} - \frac{dR\sin(2\beta - \alpha_1)}{R^2 + 2dR\cos(2\beta - \alpha_1) + d^2} +$$

$$+\frac{\sin(2\alpha_1 - 2\beta)}{1 - \cos(2\alpha_1 - 2\beta)} = 0.$$

This equation has two real roots that determine the equilibrium positions of the surface disclinations in terms of the angles α_1 and α_2:

$$\alpha_{1,2} = 2\mathrm{arctan}\Big(\big(\left(d^2 + R^2\right)\tan\beta\pm$$

$$\pm\sqrt{(d^2 + R^2)^2 tg^2\beta + (d^2 - R^2)^2})/((d - R)^2)\Big). \quad (13)$$

The character of reconstruction of the system of defects that describe the particle as a function of its position with respect to the special line of the external disclination is shown in Fig. 3, where $d = 2.5R$. At large distances $d \gg R$, the surface defects are arranged at the angles $\alpha_{1,2} = \beta\pm\pi/2$. At $d = R$, the external disclination coincides with its image and the nearest surface linear defect (two surface defects at β=0, see Fig. 3). Due to the annihilation of disclinations of opposite charges $m_d + m'_d + m_1 = 0$ or $m_d + m'_d + m_2 = 0$, one disclination line remains on the surface of the particle and its position is determined by the angle $\alpha = 2\beta$.

The energy of interaction between the particle and the external linear defect can be derived by the substitution of (13) into (12):

$$F_{\mathrm{inter}} = \frac{3\pi KL}{4}\ln\frac{\left(d^2 - R^2\right)}{d^2}. \quad (14)$$

The given relation demonstrates that the interaction energy doesn't depend on the phase β: the initial system of localized defects of the particle is reconstructed in the field of the director of the external disclination line in such a way that the vector of the force of the particle–disclination interaction has no azimuth component. This vector is radial and its value amounts to

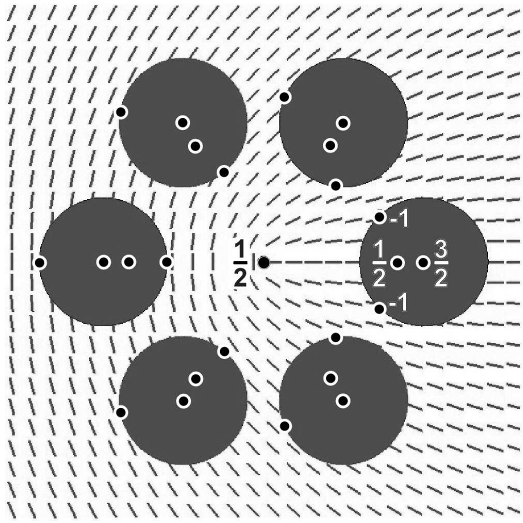


Fig. 3. Arrangement of defects of a particle depending on its position with respect to the special disclination line at $d = 2.5R$

$$f = -\frac{\partial F_{\mathrm{inter}}}{\partial d} = -\frac{3\pi KLR^2}{2d\left(d^2 - R^2\right)}. \quad (15)$$

As $f < 0$, the interaction between the particle and the disclination line is of attractive character. At $d \gg R$, the attractive force decreases with distance as $(1/d^3)$. The minimum of the free energy (11) is reached at $d = R$; in this case, the particle "attaches" the disclination line, and the above-described annihilation of defects happens. Moreover, the function $\Phi(x, y)$ from (5) corresponds to the distortion specified by two linear defects: the disclination with the charge (3/2) that passes along the particle axis and that with the charge (−1) localized on the surface of the particle. The energy of such a configuration can be obtained from relations (11) and (14) at $d \sim R + \rho/2$; this gives $F = (\pi KL/4)\ln\left(DR/\rho^2\right)$.

6. Conclusions

In the given paper, we have demonstrated that a distortion formed by an elongated particle suspended in a nematic can be described with the help of a localized system of three linear defects with the charges $\{-1, 2, -1\}$. In the vicinity of an external disclination with the strength (1/2), this system is transformed into a system of four defects with the charges $\left\{-1, \frac{1}{2}, \frac{3}{2}, -1\right\}$. The relative position of the indicated defects and the force of interaction between the particle and the disclination line are determined. It is shown that this force corresponds to the attraction and depends on the distance d between the particle and the disclination as $(1/d^3)$.

The given result obtained for the homeotropic type of anchoring can be generalized to the case of circular anchoring where the director is normal to the particle axis and tangent to its side face. In the case of circular anchoring, the function $\Phi(x, y)$ differs from (5) by the additional phase $(\pm\pi/2)$, which corresponds to the turn of the special disclination line (see Fig. 3) by the angle $(\pm\pi)$. Such a turn doesn't result in a change of the interaction energy (14) and force (15) of the particle–disclination interaction.

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ВЗАЄМОДІЯ ЗАВИСЛОЇ В НЕМАТИКУ ГОЛКОПОДІБНОЇ ЧАСТИНКИ З ДИСКЛІНАЦІЙНОЮ ЛІНІЄЮ СИЛИ (1/2)

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Р е з ю м е

Представлено опис завислої в нематику голкоподібної частинки за допомогою локалізованої системи дефектів. Розглянуто пружну взаємодію такої частинки із плоскою дисклінацією сили (1/2). Показано, що поблизу дисклінації система дефектів частинки зазнає істотних змін, які залежать від відстані d між частинкою й дисклінацією та від орієнтації частинки відносно особливої лінії дисклінації. При цьому сила взаємодії має характер притягання та залежить тільки від відстані d.