# Stability of a hyperbolic disclination ring in a nematic liquid crystal

Jun-ichi Fukuda[1] and Hiroshi Yokoyama[1,2]
[1]*Yokoyama Nano-structured Liquid Crystal Project, ERATO, Japan Science and Technology Corporation, 5-9-9 Tokodai, Tsukuba 300-2635, Japan*
[2]*Nanotechnology Research Institute, AIST, 1-1-4 Umezono, Tsukuba 305-8568, Japan*
(Received 13 February 2002; published 29 July 2002)

The stability of a hyperbolic disclination ring in a nematic liquid crystal is considered by extending the argument for a radial disclination ring due to Mori and Nakanishi. The ring configuration is indeed stable in the presence of the saddle-splay elasticity (characterized by $K_{24}$). The ring radius is estimated to be $a\sim 2.9r_c$, with $r_c$ being the core radius when $K_{24}\simeq K/2$, where $K$ is the Frank elastic constant in the one-constant approximation.

DOI: 10.1103/PhysRevE.66.012703 PACS number(s): 61.30.Cz, 61.30.Jf

Nematic liquid crystals [1,2] have attracted a great deal of interest as an experimentally accessible system showing topological defects [3–5], which include point and line singularities. One of the interesting properties of a topological defect in a nematic liquid crystal is that a radial (hyperbolic) point defect with topological charge $+1(-1)$ (termed also as a "hedgehog") can be transformed continuously into a disclination ring of strength $+1/2(-1/2)$ (for illustration of these defects, see Fig. 1). This was experimentally observed by Lavrentovich and Terentjev [6] as a pathway of the transition between radial and hyperbolic hedgehogs. The possibility of continuous transformation between a point defect and a disclination ring is closely associated with the head-tail invariance of the liquid crystal molecule (or the equivalence of $\boldsymbol{n}$ and $-\boldsymbol{n}$ in terms of the director), which allows half-integer defects. However, topological theories do not provide any answer to the energetic stability of a point defect against transformation to a disclination ring and there have been many theoretical attempts [7–16] to investigate which configuration is energetically favorable. Main focus of the previous studies is the stability of a radial hedgehog [Fig. 1(a)] and most of the previous papers have concluded that a radial point defect is intrinsically metastable or unstable to open up a disclination ring [Fig. 1(b)], although the possibility that the presence of the saddle-splay elasticity makes a ring shrink to a point has also been pointed out [10]. The aim of this paper is to investigate, by extending a previous approach by Mori and Nakanishi [7], the stability of a hyperbolic point defect [Fig. 1(c)] versus a hyperbolic disclination ring [Fig. 1(d)], which, to our knowledge, almost no previous theoretical studies have paid attention to.

This work is motivated by our recent numerical study [17] on a defect structure in liquid crystal colloids. Recently, liquid crystal colloids and particles (or isotropic liquid droplets) dispersed in a nematic host fluid, have been providing fascinating problems concerning topological defects, because the configuration of topological defects is significantly influenced by various factors such as the size of the particles or the anchoring properties on the particle surface [18–21]. One of the interesting and nontrivial configurations is a hyperbolic hedgehog that lies close to a particle. This hedgehog is small enough to be regarded as pointlike in observations by optical methods and the theoretical studies [22–25], concerning this hyperbolic hedgehog does not go into its detailed structure and most of them have assumed that it is a point. In the recent simulations performed by the present authors [17], however, the observation of a detailed structure of the topological defect was achieved by utilizing an adaptive mesh refinement scheme and it was shown that the hyperbolic hedgehog takes the form of a ring, not a point. Although this paper deals with a different situation of an isolated hyperbolic hedgehog, considering the lack of fundamental understanding of the fine structure of a hyperbolic hedgehog, we believe that it should be worthwhile to present a theoretical study on the intrinsic nature of a hyperbolic hedgehog defect.

We first review briefly the calculation of Mori and Nakanishi [7] who discussed the energetic stability of a radial disclination ring [Fig. 1(b)]. They constructed an ansatz configuration of the director $\boldsymbol{n}$ by assuming that $\boldsymbol{n}$ is normal to the surfaces of the ellipsoids of revolution,

$$\frac{\rho^2}{a^2(1+\xi^2)}+\frac{z^2}{a^2\xi^2}=1, \tag{1}$$

where $a$ is the radius of the ring disclination and $\xi$ is a positive parameter characterizing the ellipsoid. We have employed the cylindrical coordinate $(\rho,z,\phi)$ with $\rho^2=x^2+y^2$. The resultant form of $\boldsymbol{n}$ is

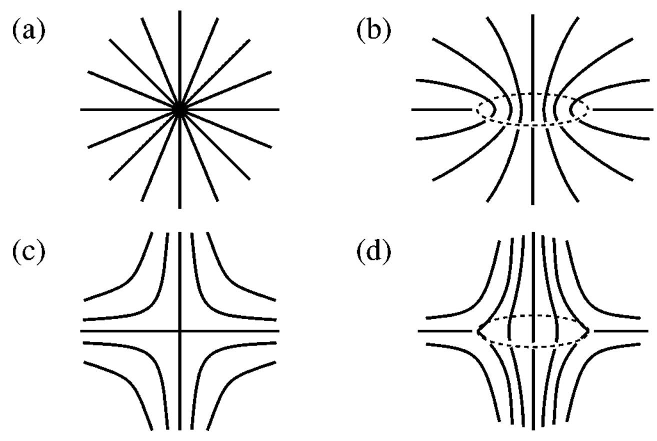


FIG. 1. Schematic illustration of (a) a radial point defect (hedgehog), (b) a radial disclination ring, (c) a hyperbolic point defect (hedgehog), and (d) a hyperbolic disclination ring.

 

$$n_\rho = \frac{\rho\xi^2}{\sqrt{\rho^2\xi^4 + z^2(1+\xi^2)^2}},$$

$$n_z = \frac{z(1+\xi^2)}{\sqrt{\rho^2\xi^4 + z^2(1+\xi^2)^2}}, \tag{2}$$

$$n_\phi = 0.$$

This ansatz configuration reduces to that of a radial point disclination in the limit $a \to 0$. Note that this ansatz configuration satisfies only the boundary condition $\boldsymbol{n} \to \boldsymbol{r}/|\boldsymbol{r}|$ at $|\boldsymbol{r}| \to \infty$ and does not satisfy the equilibrium condition even in the case of one constant approximation. Therefore, the distortion energy calculated below should give the upper limit of the minimum energy of the ring defect.

The distortion energy due to the radial disclination ring is evaluated by substituting the ansatz director field (2) to the Frank elastic energy

$$F = \frac{1}{2}\int d\boldsymbol{r}\{K_1(\nabla\cdot\boldsymbol{n})^2 + K_2(\boldsymbol{n}\cdot\nabla\times\boldsymbol{n})^2 + K_3|\boldsymbol{n}\times(\nabla\times\boldsymbol{n})|^2\}$$
$$-\int d\boldsymbol{r}K_{24}\nabla\cdot[\boldsymbol{n}\times(\nabla\times\boldsymbol{n}) + \boldsymbol{n}(\nabla\cdot\boldsymbol{n})]. \tag{3}$$

We note that the saddle-splay elasticity is taken into account later by Lavrentovich *et al.* [10]. We also note that the splay-bend elasticity, whose elastic constant is $K_{13}$, is dropped here [26]. We introduce the ellipsoidal coordinate $(\xi,\eta,\phi)$ with

$$\rho^2 = a^2(1+\xi^2)(1-\eta^2),$$

$$z = a\xi\eta. \tag{4}$$

The volume of integration is taken as $0 \leqslant \xi \leqslant \sqrt{(R/a)^2-1}$, which, in real space, corresponds to the region inside the ellipsoid of revolution $\rho^2/R^2 + z^2/(R^2-a^2) = 1$. The volume of integration, however, should not include the core region where the elastic energy density diverges. We take, as the excluded volume, the region that satisfies $\xi^2 < p^2$ and $\eta^2 < q^2$, where $p^2 = 2r_c/a + r_c^2/a^2$ and $q^2 = 2r_c/a - r_c^2/a^2$, and $r_c$ characterizes the size of the core region. The volume of integration in real space is illustrated in Fig. 2. We note that this geometry is well defined when $a > r_c$, because the two core regions touch each other when $a = r_c$. After some calculation, we obtain for $R/a \to \infty$ and $r_c/a \to 0$,

$$F = 8\pi(K_1 - K_{24})R + \mathcal{O}(a/R) + 2\pi a\left\{-\left(\frac{5}{4}\pi - \frac{1}{2}I\right)K_1 - \left(\frac{1}{4}\pi - \frac{1}{2}I\right)K_3 + \pi K_{24} + \mathcal{O}(\sqrt{r_c/a})\right\}$$
$$+\frac{\pi^2}{4}(K_1+K_3)a\ln\frac{a}{2r_c} + 2\pi a\mathcal{E}_c, \tag{5}$$

where $I$ is the Catalan's constant defined as

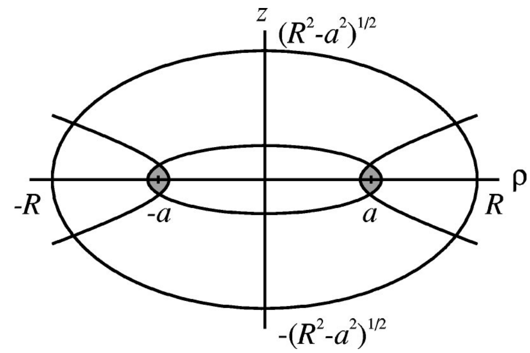


FIG. 2. The volume of integration for the evaluation of the elastic energy is taken inside the outer ellipsoid. The shaded regions indicate the excluded core regions.

$$I \equiv \int_0^1 dx\frac{\tan^{-1}x}{x} \simeq 0.916. \tag{6}$$

The first term of Eq. (5) is equal to the distortion energy of a radial point disclination. The third term proportional to $2\pi a$ corresponds to the line tension of the ring disclination and the fourth terms arises from the cutoff of the core region. The last term is the core energy, with $\mathcal{E}_c$ being its line density.

We can readily apply the argument above to the case of a hyperbolic disclination ring [Fig. 1(d)] by employing the configuration

$$n_\rho = -\frac{\rho\xi^2}{\sqrt{\rho^2\xi^4 + z^2(1+\xi^2)^2}},$$

$$n_z = \frac{z(1+\xi^2)}{\sqrt{\rho^2\xi^4 + z^2(1+\xi^2)^2}}, \tag{7}$$

$$n_\phi = 0.$$

The difference between this configuration (7) and the original one (2) for the radial disclination ring is just the sign of $n_\rho$. It can be shown easily that the configuration (7) reduces to that of a hyperbolic point disclination in the limit $a \to 0$ and therefore can be used as an ansatz configuration for a hyperbolic disclination ring. After some calculation, we obtain

$$(\nabla\cdot\boldsymbol{n})^2 = \frac{\xi^2}{a^2(\xi^2+\eta^2)^5(1+\xi^2)}\{(\xi^2+\eta^2)^2 + (1+\xi^2) \times[(2\eta^2-1)(\xi^2+\eta^2) + 4\eta^2(1-\eta^2)]\}^2, \tag{8}$$

$$\boldsymbol{n}\cdot\nabla\times\boldsymbol{n} = 0, \tag{9}$$

$$|\boldsymbol{n}\times\nabla\times\boldsymbol{n}|^2 = \frac{\eta^2(1-\eta^2)}{a^2(\xi^2+\eta^2)^5}[(2\xi^2+1)(\xi^2-\eta^2+1)-1]^2, \tag{10}$$

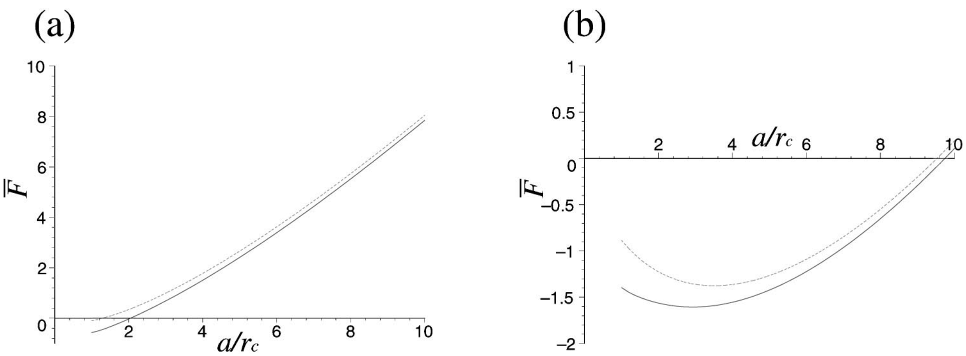


FIG. 3. The reduced elastic energy of a disclination ring $\overline{F}=\lim_{R\to\infty}[F-8\pi(K+K_{24})R/3]/4\pi K r_c$ as a function of $a/r_c$ for (a) $K_{24}=0$ and (b) $K_{24}=K/2$. Dotted lines represent the results obtained by using Eq. (12) as $F$ after truncating the contribution of $a\times\mathcal{O}(\sqrt{r_c/a})$. Notice again that our model geometry is well defined when $a/r_c>1$.

$$\nabla\cdot[\boldsymbol{n}\times(\nabla\times\boldsymbol{n})+\boldsymbol{n}(\nabla\cdot\boldsymbol{n})] =\frac{2\xi^2}{a^2(\xi^2+\eta^2)^3}[(2\eta^2-1)(\xi^2+\eta^2)+4\eta^2(1-\eta^2)], \tag{11}$$

where $\xi$ and $\eta$ are the ellipsoidal coordinates introduced in Eq. (4). The integration of the elastic energy density can be performed straightforwardly by substituting Eqs. (8), (9), (10), and (11) to Eq. (3) and when the volume of integration is taken same as that in the preceding argument (Fig. 2), the result is in the limit of $R/a\to\infty$ and $r_c/a\to 0$,

$$F=\frac{8\pi}{15}(3K_1+2K_3+5K_{24})R+\mathcal{O}(a/R) +2\pi a\left\{-\left(\frac{1}{4}\pi-\frac{1}{2}I\right)(K_1+K_3)-\pi K_{24}+\mathcal{O}(\sqrt{r_c/a})\right\} +\frac{\pi^2}{4}(K_1+K_3)a\ln\frac{a}{2r_c}+2\pi a\mathcal{E}_c. \tag{12}$$

The first term is again the distortion energy of a hyperbolic point disclination and the remaining terms are the energy attributed to the ring disclination. Using the result obtained above, we can estimate the equilibrium radius of a hyperbolic ring disclination as a function of the elastic constants and the core energy. We simplify the situation by adopting the one constant approximation $K_1=K_3=K$. Then the equilibrium radius becomes

$$a=2r_c\exp\left\{\frac{4}{\pi}\left(\frac{K_{24}}{K}\pi-\frac{\mathcal{E}_c}{K}+\frac{\pi}{4}-I\right)\right\} =2r_c\exp\left(4\frac{K_{24}}{K}-\frac{4}{\pi}\frac{\mathcal{E}_c}{K}-0.166\right). \tag{13}$$

The core energy is roughly estimated as $\mathcal{E}_c/r_c^2\sim U/\xi_N^3$, where $U$ is a characteristic microscopic interaction energy and $\xi_N$ is the nematic correlation length. The radius of the defect core $r_c$ is of the order of $\xi_N$ and the elastic constant is roughly given as $K\sim U/\xi_N$, which yields $\mathcal{E}_c\sim K$. When we set $\mathcal{E}_c=K$ and the saddle-splay elasticity is absent ($K_{24}=0$), we obtain $a\simeq 0.474r_c$, which implies that the disclination ring is unstable to shrink to a point because $a<r_c$. The saddle-splay elastic constant $K_{24}$, however, has been shown experimentally [27] to be of the order $K$ and it follows from the Cauchy relationship [28] that

$$K_{24}=\frac{1}{4}(K_{11}+K_{22}). \tag{14}$$

In the one constant approximation, Eq. (14) reads $K_{24}=K/2$ and Eq. (13) yields $a\simeq 3.50r_c$. Therefore, in the presence of saddle-splay elasticity, a hyperbolic point disclination can be unstable to form a disclination ring.

However, this result may cast a doubt to the self-consistency of the treatment above where we have dropped the contribution of $a\times\mathcal{O}(\sqrt{r_c/a})$ in $F$. Therefore, we evaluate the full elastic energy numerically with the aid of the algebraic program MAPLE™ 6.01. In Fig. 3, we plot the reduced elastic energy of the disclination ring $\overline{F}=\lim_{R\to\infty}[F-8\pi(K+K_{24})R/3]/4\pi K r_c$ as a function of $a/r_c$ under the one-constant approximation $K_1=K_3=K$ and $\mathcal{E}_c=K$. Figure 3 indicates that the qualitative feature of the elastic energy is the same as that in the previous treatment, although the equilibrium ring radius in the presence of saddle-splay elasticity is slightly changed to $a\simeq 2.92r_c$.

Finally, we briefly comment on the contribution of the saddle-splay elasticity and the core energy to the stability of a hyperbolic disclination ring. As can be seen in the first term of Eq. (12), the saddle-splay term gives a positive contribution to the elastic energy in the case of a hyperbolic hedgehog. The relaxation of the hyperbolic configuration by the transformation from a point disclination to a ring thus reduces the elastic energy and the saddle-splay elasticity favors the formation of a ring. We note that this contribution of the saddle-splay elasticity has already been argued in a qualitative manner or as a rough estimate in previous studies [10,23,17] and our quantitative analysis presented here confirms the importance of the saddle-splay elasticity. Although the estimated value of $a$ is rather small, it follows from Eq. (13) that $a$ depends sensitively on the core energy $\mathcal{E}_c$ and that the smaller $\mathcal{E}_c$ yields larger $a$. It has been shown [29,30] that the disclination core is not an isotropic liquid and relaxes the distortion energy by taking a biaxial structure, which might lead to a smaller $\mathcal{E}_c$ than the value used in the estimation above and therefore a larger $a$. A more elaborate treatment of the core properties such as a Landau-de Gennes approach in terms of a second-rank tensor order parameter [1,8,12,13,15,16,30] might be necessary to determine precisely the equilibrium ring radius.

In summary, we have shown that the argument of Mori and Nakanishi, which is devoted to the discussion on the energetic stability of a radial disclination ring in a nematic liquid crystal, can be easily extended to the case of a hyperbolic disclination ring. It has also been shown that a hyperbolic disclination ring can be stable in the presence of the saddle-splay elasticity. The ring radius $a$ is estimated to be $a \sim 2.9 r_c$, with $r_c$ being the radius of the defect core, although $a$ is sensitively dependent on the elastic constants and the core energy.


[1] P.G. de Gennes and J. Prost, *The Physics of Liquid Crystals*, 2nd ed. (Oxford University Press, New York, 1993).

[2] S. Chandrasekhar, *Liquid Crystals*, 2nd ed. (Cambridge University Press, Cambridge, UK, 1992).

[3] N.D. Mermin, Rev. Mod. Phys. **51**, 591 (1979).

[4] H.-R. Trebin, Adv. Phys. **31**, 195 (1982).

[5] P. M. Chaikin and T.C. Lubensky, *Principles of Condensed Matter Physics* (Cambridge University Press, Cambridge, UK, 1995).

[6] O.D. Lavrentovich and E.M. Terentjev, Zh. Éksp. Teor. Fiz. **91**, 2084 (1986) [Sov. Phys. JETP **64**, 1237 (1986)].

[7] H. Mori and H. Nakanishi, J. Phys. Soc. Jpn. **57**, 1281 (1988).

[8] E. Penzenstadler and H.-R. Trebin, J. Phys. (France) **50**, 1027 (1989).

[9] S. Kralj and S. Žumer, Phys. Rev. A **45**, 2461 (1992).

[10] O.D. Lavrentovich, T. Ishikawa, and E.M. Terentjev, Mol. Cryst. Liq. Cryst. Sci. Technol., Sect. A **299**, 301 (1997).

[11] E.M. Terentjev, Phys. Rev. E **51**, 1330 (1995).

[12] A. Sonnet, A. Kilian, and S. Hess, Phys. Rev. E **52**, 718 (1995).

[13] E.C. Gartland, Jr. and S. Mkaddem, Phys. Rev. E **59**, 563 (1999); S. Mkaddem and E.C. Gartland, Jr., *ibid.* **62**, 6694 (2000).

[14] C. Chiccoli, P. Pasini, F. Semeria, T.J. Sluckin, and C. Zannoni, J. Phys. II **5**, 427 (1995).

[15] R. Rosso and E.G. Virga, J. Phys. A **29**, 4247 (1996).

[16] S. Kralj and E.G. Virga, J. Phys. A **34**, 829 (2001).

[17] J. Fukuda, M. Yoneya, and H. Yokoyama, Phys. Rev. E **65**, 041709 (2002).

[18] P. Poulin, H. Stark, T.C. Lubensky, and D.A. Weitz, Science **275**, 1770 (1997).

[19] P. Poulin and D.A. Weitz, Phys. Rev. E **57**, 626 (1998).

[20] O. Mondain-Monval, J.C. Dedieu, T. Gulik-Krzywicki, and P. Poulin, Eur. Phys. J. B **12**, 167 (1999).

[21] Y. Gu and N.L. Abbott, Phys. Rev. Lett. **85**, 4719 (2000).

[22] R.W. Ruhwandl and E.M. Terentjev, Phys. Rev. E **56**, 5561 (1997).

[23] T.C. Lubensky, D. Pettey, N. Currier, and H. Stark, Phys. Rev. E **57**, 610 (1998).

[24] S.V. Shiyanovskii and O.V. Kuksenok, Mol. Cryst. Liq. Cryst. Sci. Technol., Sect. A **321**, 45 (1998).

[25] H. Stark, Eur. Phys. J. B **10**, 311 (1999); Phys. Rep. **351**, 387 (2001).

[26] H. Yokoyama, Phys. Rev. E **55**, 2938 (1997), and references therein.

[27] G.P. Crawford and S. Žumer, Int. J. Mod. Phys. B **9**, 2469 (1995), and references therein.

[28] J. Nehring and A. Saupe, J. Chem. Phys. **54**, 337 (1971).

[29] I.F. Lyuksyutov, Zh. Éksp. Teor. Fiz. **75**, 358 (1978) [Sov. Phys. JETP **48**, 178 (1978)].

[30] N. Schopohl and T.J. Sluckin, Phys. Rev. Lett. **59**, 2582 (1987).