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# On the Stability of Topologically Non-Trivial Point Defects

Hiroyuki MORI and Hiizu NAKANISHI

*Department of Physics, Faculty of Science and Technology, Keio University, Hiyoshi, Kohoku-ku, Yokohama 223*

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We demonstrate that a topologically non-trivial point defect can be energetically unstable against expanding into a ring defect by taking nematic liquid crystal as an example.

## §1. Introduction

The theory of topological classification of defects in ordered media has been developed.[1-4] In the theory, line and point defects are classified by using the first and the second homotopy group, respectively. Each topological class of defects consists of several energetically metastable defect configurations which can be transformed continuously into one another with finite energy barrier. On the other hand, the defects which belong to different topological classes cannot be transformed by continuous deformation, therefore topologically non-trivial point or line defects are considered quite stable and require a large amount of energy (proportional to the system size) to disappear unless they go out of the system through the surface.

It has been pointed out that besides the line and point defects there is another type of defect, a ring defect, which has rather interesting features. The local structure of the ring defects is identical with that of the line defects while the ring defects are localized in finite volume like the point defects. The classification of the ring defects has been first analized by Mineev[3] and the general homotopy theory for that has been developed by Nakanishi, Hayashi and Mori.[5] They found that the topological types of ring defects are characterized by the automorphism classes of the semidirect product of the first and the second homotopy group $\pi_1(X) \square \pi_2(X)$, where $X$ stands for an order parameter space.[5] Namely, each ring defect can be classified by a set $(\gamma, n)$ which is a representative of an automorphism class, where $\gamma \in \pi_1(X)$ and $n \in \pi_2(X)$. It has been also shown that the ring defect $(\gamma, n)$ has a local line defect structure of $\gamma$ and becomes a point defect $n$ when it shrinks.[5]

Some ring defects can be transformed into point defects continuously by reducing their radii to zero. This process suggests a possibility of the reverse process that a topologically non-trivial point defect may be energetically unstable against expanding into a ring defect. This is quite contrary to the general belief that topologically non-trivial point defects are inevitably physically stable.[6] We study this problem by taking nematic liquid crystal as an example.

In the next section, basic facts of nematic liquid crystal are described and the free energy for simple point and line defects are estimated. In §3 the distortion energy of a ring defect is estimated by two ways, which agree quite well. Discussion and summary are given in §4.

## §2. Nematic Liquid Crystal

The order parameter of nematic liquid crystal is the direction of molecules and a configuration of the nematics is represented by a field of a unit vector $n$ (director). Since the head and tail of the molecule are not distinguishable, $n$ and $-n$ represent the same local state and hence the order parameter space is the projective plane $RP^2$. The first and the second homotopy group of $RP^2$, by which the line and point defects of nematics are

classified respectively, are

$$\pi_1(RP^2)=Z_2\equiv\{0, 1\}, \tag{1}$$

and

$$\pi_2(RP^2)=Z\equiv\{0, \pm1, \pm2, \cdots\}. \tag{2}$$

Since 0 represents the uniform configuration, we can see from eq. (1) that there is only one topologically non-trivial line defect, which is represented by 1. As for the point defect, it is known that $+i$ and $-i$ ($i=1, 2, 3, \cdots$) represent the same defect and thus a topological class of point defects may be labeled by a positive integer.[1)]

The distortion energy of the nematic ordered state is given by[7)]

$$F_{\text{dist}}=\int dV\{1/2\cdot K_1\cdot(\text{div } \boldsymbol{n})^2+1/2\cdot K_2 \cdot(\boldsymbol{n}\cdot\text{rot } \boldsymbol{n})^2+1/2\cdot K_3\cdot(\boldsymbol{n}\times\text{rot } \boldsymbol{n})^2\}, \tag{3}$$

where $K_1$, $K_2$, and $K_3$ are the elastic constants corresponding to the distortion energy of splay, twist, and bend deformation respectively. In equilibrium configurations, the director $\boldsymbol{n}$ is arranged to minimize the distortion energy (3) under given boundary conditions and consequently $\boldsymbol{n}$ must be at each point parallel to the molecular field $\boldsymbol{h}$,[7)]

$$\boldsymbol{n}/\!/\boldsymbol{h}=K\nabla^2\boldsymbol{n}, \tag{4}$$

where we have assumed $K_1=K_2=K_3=K$ (one constant approximation) in the expression of $\boldsymbol{h}$.

The simplest configurations with the point and line defect are given in Fig. 1. They are represented by $1\in\pi_2$ and $1\in\pi_1$ respectively. The distortion energies (3) are easily estimated and the free energies for these configurations are

$$F_{\text{point}}\sim 8\pi K_1 R+F_{\text{p,core}}, \tag{5}$$

and

$$F_{\text{line}}\sim(\pi/8)\cdot(K_1+K_3)\cdot L\cdot\log(D/\xi)+F_{\text{l,core}}, \tag{6}$$

respectively, where $R$ is a radius of the system, $L$ is a length of the line defect, and $D$ is a radius of the system cross section normal to the line defect. $F_{\text{p,core}}$ and $F_{\text{l,core}}$ are the core energies which come from the singular regions. These terms will be of order

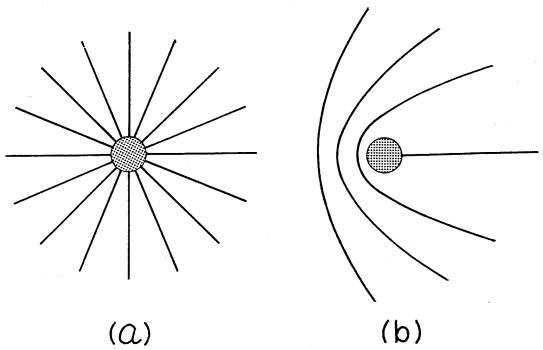


Fig. 1. (a) The configuration with the point defect of $1\in\pi_2$. (b) The configuration with the line defect of $1\in\pi_1$. The cross section normal to the line defect is shown.

$$F_{\text{p,core}}\sim\xi^3\cdot\Delta f, \tag{7}$$

$$F_{\text{l,core}}\sim\xi^2\cdot L\cdot\Delta f, \tag{8}$$

where $\xi$ is coherence length and $\Delta f$ is condensation energy density. It should be noted that $F_{\text{line}}$ is greater than $F_{\text{point}}$ even without the core energy if $R\sim L\sim D\gg\xi$.

## §3. Ring Defect in Nematics

Now we consider the ring defect represented by (1, 1) with a radius $a$, where the first $1\in\pi_1=Z_2$ indicates that its local line structure is the same with that of the line defect of $1\in\pi_1$ and the second $1\in\pi_2=Z$ means that the ring defect becomes the point defect represented by $1\in\pi_2$ when its radius goes to zero.[3,5)]

One of the possible configurations which converges to the configuration Fig. 1(a) for $|\boldsymbol{r}|\to\infty$ is shown in Fig. 2. Rough estimate of the free energy for this configuration is obtained as follows. Imagine a sphere of radius $\alpha a$ which encloses the ring defect (Fig. 2. $\alpha$ is a constant of order 1). Outside the sphere, the configuration can be seen as that of the point defect 1. Accordingly, the free energy which comes from this region is expected to be about $8\pi K_1(R-\alpha a)$ from eq. (5). Inside the sphere, the configuration might be regarded as that of the line defect 1 which is bent to be a ring. The distortion energy from this region should be around $(\pi/8)\cdot(K_1+K_3)\cdot 2\pi a\cdot\log(\alpha a/\xi)$ since $L$ and $D$ in eq. (6) should be taken as $2\pi a$ and $\alpha a$ respectively in this case. Therefore the difference of the free energy between the ring and the point defect $\Delta F(\text{a})=F_{\text{ring}}(a)-F_{\text{point}}$

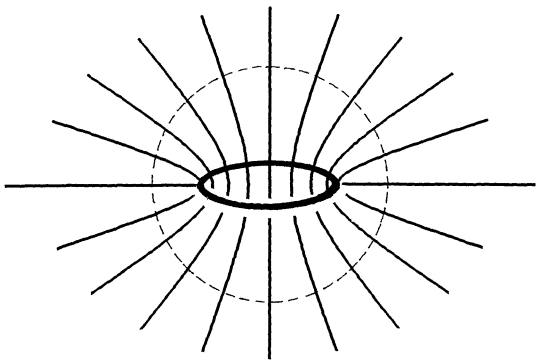

Fig. 2. The configuration forming the ring defect of (1, 1) is shown. Outside the dotted sphere, the configuration may be considered as that of the point defect.

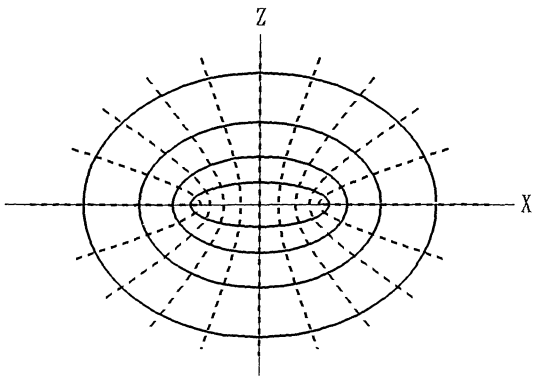


Fig. 3. The ellipsoids of revolution (10) are shown in the $x$-$z$ plane (solid lines). The dashed lines denote the hyperbola which are normal to the ellipsoids. The molecules are assumed to be normal to the ellipsoids of revolution.

can be roughly estimated as

$$\begin{aligned}\Delta F(a) \sim & -8\pi K_1 \alpha a + (\pi/8)\cdot(K_1+K_3)\cdot 2\pi a \\ & \cdot \log(\alpha a/\xi) + 2\pi a \xi^2 \Delta f - \xi^3 \Delta f \\ = & 2\pi a \cdot \{-4\alpha K_1 + \xi^2 \Delta f + (\pi/8) \\ & \cdot (K_1+K_3)\cdot \log(\alpha a/\xi)\} - \xi^3 \Delta f. \end{aligned} \tag{9}$$

The third and forth terms in the first line are the core energy. The energy reduction $-8\pi K_1 \alpha a$ is due to the relaxation of the spray distortion inside the ring. If $(-4\alpha K_1 + \xi^2 \Delta f)$ is negative, the energy difference (9) can have a minimum with finite $a$ $(>\xi)$, and the point defect is unstable against expanding into the ring defect.

Our estimate (9) can be confirmed by more elaborate calculation. Assume the configuration where the molecules of liquid crystal are normal to the surfaces of the ellipsoids of revolution

$$\frac{x^2+y^2}{a^2\cosh^2 u} + \frac{z^2}{a^2 \sinh^2 u} = 1, \tag{10}$$

where $u$ is a positive parameter (Fig. 3). Note that this configuration satisfies the boundary condition that $\boldsymbol{n} \to \boldsymbol{r}/|\boldsymbol{r}|$ for $|\boldsymbol{r}| \to \infty$ but does not satisfy equilibrium condition (4), therefore the distortion energy obtained from this should give the upper limit of minimum energy for that of the ring defect (1, 1) with the boundary condition.

Using the spheroidal coordinates $(u, v, \phi)$, which are related to the Cartesian coordinates by

$$\begin{cases} x = a\cdot\cosh u \cdot \cos v \cdot \cos\phi, \\ y = a\cdot\cosh u \cdot \cos v \cdot \sin\phi, \\ z = a\cdot\sinh u \cdot \sin v, \end{cases} \tag{11}$$

we can calculate analytically the distortion energy for this configuration. We have to remove the core region around the ring singularity where the nematic order is destroyed. To simplify the calculation, we take the core region as the region which is enclosed by the ellipsoid of revolution

$$\frac{x^2+y^2}{(a+\xi)^2} + \frac{z^2}{2a+\xi} = 1, \tag{12}$$

and the hyperboloid of revolution of one sheet

$$\frac{x^2+y^2}{(a-\xi)^2} - \frac{z^2}{2a-\xi} = 1, \tag{13}$$

(Fig. 4). After some calculation, we get for $R \to \infty$ and $a \gg \xi$

$$\Delta F(a) = \Delta F_{\text{dist}}(a) + \Delta F_{\text{core}}(a), \tag{14}$$

$$\begin{aligned}\Delta F_{\text{dist}}(a) \sim & 2\pi a \cdot \{-(5/4\cdot\pi - 1/2\cdot I)\cdot K_1 \\ & -(1/4\cdot\pi - 1/2\cdot I)K_3 + (\pi/8) \\ & \cdot (K_1+K_3)\cdot \log(a/2\xi)\}, \end{aligned} \tag{15}$$

$$\Delta F_{\text{core}}(a) \sim 2\pi a \xi^2 \Delta f - \xi^3 \Delta f, \tag{16}$$

where

$$I \equiv \int_0^1 dx \tan^{-1} x/x = 0.915965\cdots.$$

Only the expression for $a \gg \xi$ is given in eq.

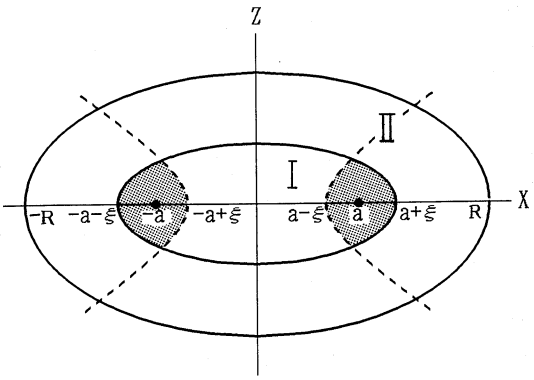


Fig. 4. The core region is shown by shaded area, which is enclosed by the ellipsoid of revolution of eq. (12) and the hyperboloid of revolution of one sheet of eq. (13). I and II denote the regions of integral in eq. (A·6).

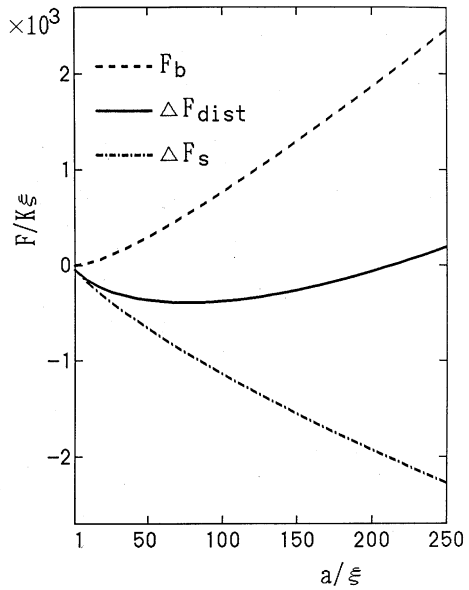


Fig. 5. Distortion energy of the ring defect as a function of radius $a$. The dotted dash, dashed, and solid line denote the spray, bend, and total distortion energy $\Delta F_s$, $F_b$, and $\Delta F_{dist}$ respectively. For $a/\xi<1$ the expression (A·10)–(A·13) cannot be used.

(15) because the general expression for $a>\xi$ is rather lengthy. The full expression is given in the appendix.

We can see that eq. (14) agrees with eq. (9) quite well, which shows the picture given earlier in this section is good. $\Delta F_{dist}$ given by (A·10)–(A·13) and (A·15) as a function of the ring radius $a$ is shown in Fig. 5, where we have taken $K_1=K_3=K$. $\Delta F_{dist}$ is negative for $a$ smaller than a certain value and has a minimum around $a\sim 80\xi$. This means that the point defect is unstable against expanding into the ring defect if the condensation energy density $\Delta f$ is small enough.

## §4. Discussion and Summary

A topological defect has been considered to keep its identity quite well. The homotopy theory tells us that the topological defect cannot be transformed into the other classes of defect continuously. Accordingly, the topological defect can be said to be persistent and never changes its type unless it goes out of the system through the surface. On the other hand, the theory also gives the combination rule of defects. For instance, the point defect represented by $2\in \pi_2=Z$ in the nematics can split into two point defects represented by $1\in \pi_2$. This process should occur with finite energy barrier of order $\xi^3\Delta f$ and can be considered as physically local and continuous. In this sense the topological defects may change but the processes conserve "the topological charge". The conventional homotopy theory, however, does not assume the possibility that a point defect may change into a line defect or others.

Such processes are possible by going through the ring defects. Some ring defects turn into point defects when their radii go to zero. If their radii become infinite, the topological charge diffuses and the system will be left with non-singular texture. Thereby a configuration with a point defect can be transformed continuously into a non-singular configuration through a ring defect. If a part of the ring defect goes out of the system, the ring defect becomes a line defect, which shows that a point defect can be transformed into a line defect. Therefore it is physically important to examine the possibility that a topologically stable point defect may be unstable energetically.

We have examined the possibility by taking the point defect in the nematic liquid crystal as an example. Assuming the configuration with the ring defect which can be transformed into the point defect continuously, we have estimated the distortion energy. The resulting

energy are found to consist of two terms which depend on the ring radius $a$; the one is proportional to $-a$ and the other is to $a\cdot\log a$. The first term comes from the relaxation of distortion inside the ring and the second term is the contribution from the line defect of length $2\pi a$. The total distortion energy of the ring defect is actually found to get smaller than that of the point defect for certain $a$. This means that the point defect is unstable if the condensation energy which comes from the singular region is small enough, namely, if $(-4\alpha K_1+\xi^2\Delta f)$ is negative, the point defect is unstable against expanding into the ring defect. For large $a$, the $a\cdot\log a$ term exceeds the first two terms in eq. (9) and the free energy has a minimum at finite $a$.

Let us examine the order of magnitude of the constants which appear in the expression. The elastic constant $K$'s are of order $U/d$,[7] where $U$ is a typical interaction energy between molecules and $d$ is a molecular dimension. We expect the condensation energy per volume $\Delta f$ to be of order $U/d^3$, therefore when the coherence length $\xi$ is of order $d$, $\xi^2\Delta f$ and $K$'s are of the same order and thus $(-4\alpha K_1+\xi^2\Delta f)$ may well be negative.

Actually the existence of the ring defects has been suggested for the nematic liquid crystal MBBA in a capillary with a homeotropic boundary.[8] The radius of the ring defect was estimated about 1 $\mu$m. If we neglect the core energy and compare this with our theoretical estimate $80\xi$, the coherence length $\xi$ should be about 120 Å, which is of order of the molecular size.

## Appendix

In the appendix, we derive eq. (15). For the configuration we have assumed, the distortion energy density for spray, twist and bend are given by

$$\mathscr{F}_s=1/2\cdot K_1\frac{\tanh^2u\cdot(\sinh^2u+\cosh^2u+\sin^2v)^2}{a^2(\sinh^2u+\sin^2v)^3}, \tag{A·1}$$

$$\mathscr{F}_t=0, \tag{A·2}$$

$$\mathscr{F}_b=1/2\cdot K_3\frac{\sin^2v\cdot\cos^2v}{a^2(\sinh^2u+\sin^2v)^3}, \tag{A·3}$$

in the spheroidal coordinates respectively. The volume integral for the spheroidal coordinates is

$$\int dV\cdots=\int d\phi\int dv\int du\mathscr{J}(\phi,v,u)\cdots, \tag{A·4}$$

$$\mathscr{J}(\phi,v,u)\equiv a^3(\sinh^2u+\sin^2v)\cdot\cosh u\cdot\cos v. \tag{A·5}$$

In order to exclude the core region which is enclosed by surfaces (12) and (13), we devide the integral into two regions I and II (Fig. 4) as

$$F_{\text{dist}}=\left(\int_{\text{I}}dV+\int_{\text{II}}dV\right)(\mathscr{F}_s+\mathscr{F}_b), \tag{A·6}$$

$$\int_{\text{I}}dV\cdots=2\int_0^{2\pi}d\phi\int_0^{\pi/2}dv\int_{\cosh^{-1}\left(\frac{a+\xi}{a}\right)}^{\cosh^{-1}(R/a)}du\mathscr{J}(\phi,v,u)\cdots, \tag{A·7}$$

$$\int_{\text{II}}dV\cdots=2\int_0^{2\pi}d\phi\int_{\cos^{-1}\left(\frac{a-\xi}{a}\right)}^{\pi/2}dv\int_0^{\cosh^{-1}\left(\frac{a+\xi}{a}\right)}du\,\mathscr{J}(\phi,v,u)\cdots, \tag{A·8}$$

where we restrict the integral region inside the ellipsoid of revolution

$$\frac{x^2+y^2}{R^2}+\frac{z^2}{R^2-a^2}=1. \tag{A·9}$$

After subtracting the distortion energy of point defect (5), we take the limit $R\to\infty$. Calculation is straightforward and we get,

$$\int_{\text{I}}dV\mathscr{F}_s-8\pi K_1R=2\pi aK_1\{-\pi/2-9p/2+\tan^{-1}p+(p^2+1)/2\cdot\tan^{-1}(1/p)+1/2\cdot J_1-7/2J_2\}, \tag{A·10}$$

$$\int_{\mathrm{II}} dV\mathscr{F}_s = 2\pi a K_1 \{(4p - \tan^{-1}p)(1-q) + p/2 - (p^2+1)/2 \cdot \tan^{-1}(1/p) - pq/2 + (p^2+1)/2 \cdot \tan^{-1}(q/p) + 1/2 \cdot I_1(q) - 7/2 \cdot I_2(q)\}, \quad (A \cdot 11)$$

$$\int_{\mathrm{I}} dV\mathscr{F}_b = 2\pi a K_3 \{p/2 - (p^2+1)/2 \cdot \tan^{-1}(1/p) + 1/2 \cdot J_1 - 1/2 \cdot J_2\}, \quad (A \cdot 12)$$

$$\int_{\mathrm{II}} dV\mathscr{F}_b = 2\pi a K_3 \{p/2 \cdot (q-1) + (p^2+1)/2 \cdot (\tan^{-1}(1/p) - \tan^{-1}(q/p)) + 1/2 \cdot I_1(q) - 1/2 \cdot I_2(q)\}, \quad (A \cdot 13)$$

where

$$p = \sqrt{(1+\xi/a)^2 - 1}, \quad q = \sqrt{1-(1-\xi/a)^2},$$

$$J_1 = \int_0^1 ds \cdot 1/s \cdot (\pi/2 - \tan^{-1}(p/s)), \quad J_2 = \int_0^1 ds \cdot s \cdot (\pi/2 - \tan^{-1}(p/s)),$$

$$I_1(q) = \int_q^1 ds \cdot 1/s \cdot \tan^{-1}(p/s), \quad I_2(q) = \int_q^1 ds \cdot s \cdot \tan^{-1}(p/s).$$

The distortion energy,

$$\Delta F_s = \int_{\mathrm{I}} dV\mathscr{F}_s + \int_{\mathrm{II}} dV\mathscr{F}_s, \quad F_b = \int_{\mathrm{I}} dV\mathscr{F}_b + \int_{\mathrm{II}} dV\mathscr{F}_b, \quad (A \cdot 14)$$

$$\Delta F_{\mathrm{dist}} = \Delta F_s + F_b, \quad (A \cdot 15)$$

are shown in Fig. 5 as a function of $a/\xi$. When $a \gg \xi$, eqs. (A·10)-(A·13) and (A·15) lead to eq. (15).

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