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Stability of Saturn-Ring and Dipole Defects Around Microspheres Suspended in Nematic Liquid Crystals

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Abstract: The stability of Saturn-ring and dipole defects in nematic liquid crystals is studied. Two structures are possible around microspheres suspended in nematic liquid crystals: a Saturn-ring and a dipole, which are investigated by calculating their Frank free energy. As a result, if $k_{24} < k\left(1 - \frac{1}{2} \ln \frac{R_1}{r_c}\right)$, the Saturn-ring is the preferred configuration which does not depend on the particle size, where R_1 is the length of liquid crystal molecule, k and k_{24} are the elastic constants, and r_c is the radius of the disclination line core. If $k_{24} > k\left(1 - \frac{1}{2} \ln \frac{R_1}{r_c}\right)$, for small particles the Saturn-ring defect is more stable, and contrarily for large particles the dipole defect is more stable. The results demonstrate that a transition from the Saturn-ring defect to the dipole defect is induced either by increasing the particle size, the saddle-splay elastic constant k_{24} or by decreasing k .

Key words: director field; Saturn-ring defect; free energy

悬浮在向列相液晶中球形微粒周围的土星环和偶极子缺陷的稳定性

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摘 要: 在向列相液晶中悬浮的球形微粒周围可能存在两种类型的缺陷: 土星环结构和偶极子结构。文章通过计算它们的自由能, 研究了向列相液晶中两种类型缺陷的稳定性。计算结果表明: 当 $k_{24} < k\left(1 - \frac{1}{2} \ln \frac{R_1}{r_c}\right)$ 时, 土星环缺陷是稳定的, 并且和球形微粒的半径无关, 其中 R_1 是液晶分子的长度, k 和 k_{24} 是弹性常数, r_c 是向错线核心的半径; 当 $k_{24} > k\left(1 - \frac{1}{2} \ln \frac{R_1}{r_c}\right)$ 时, 对于半径较小的球形微粒土星环缺陷比较稳定, 但是对于较大的球形微粒偶极子缺陷比较稳定。进而可得, 通过增加粒子半径、鞍形展曲弹性常数 k_{24} 或者减小弹性常数 k 的方法可以实现土星环缺陷向偶极子缺陷的转变。

关 键 词:指向矢量;土星环缺陷;自由能

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1 Introduction

Colloidal dispersions^[1] can be found and are extensively used in our daily life such as foods, paints, and drugs, they are of considerable technological importance. Colloidal systems with a liquid crystal as a host fluid are of special interest. In the bulk, insertion of a spherical particle into a nematic solvent with strong homeotropic anchoring at its surface yields two possible director configurations: In the dipole configuration the particle is accompanied by a topological point defect^[1-4], whereas in the Saturn-ring configuration the particle is surrounded by a 1/2 disclination ring at the equator. In the experiments of Poulin and co-workers^[5,6], the dipole configuration is always observed. The Saturn-ring defects around solid microspheres is observed by Yuedong Gu et al^[7]. Of course, the disclination ring can be moved upward or downward, and by shrinking it to the topologically equivalent hyperbolic point defect, the Saturn-ring is continuously transformed into the dipole configuration. The defect state can be modified by external electric or magnetic fields. Since the way a droplet scatters light depends on its director configuration, different topological states will scatter light differently. It is thus possible to control the amount of light scattering from an array of droplets with modest electric field. This is the basis for a display technology. In this paper, we will discuss the relation between two director configurations and the radii of the spherical particles by calculating the free energy of the defects.

This paper is organized as follows. In Sec. 2, the Frank free energy density of nematic liquid crystals is introduced. The free energy of Saturn-ring defects is calculated in Sec. 3. In Sec. 4, we

give our numerical results. The conclusions of this paper are given in Sec. 5.

2 Frank Free Energy

In the continuum theory of nematic liquid crystals, the free energy density F can be expanded in a power series of the director field n . The result is the total Frank free energy density^[8]:

$$F = \frac{1}{2} \{ k_1 (\nabla \cdot n)^2 + k_2 [n \cdot (\nabla \times n)]^2 + k_3 [n \times (\nabla \times n)]^2 \} + \frac{1}{2} k_{24} \nabla \cdot [(n \cdot \nabla)n - n(\nabla \cdot n)] \quad (1)$$

where k_1, k_2, k_3 and k_{24} are, respectively, the splay, twist, bend and saddle-splay elastic constants. For simplicity and without loss of generality, suppose the director field lies in the planes which are locally vertical to the disclination lines at their intersection points. In this case, the director field can be viewed as a 2-dimensional vector field and can be expressed as $n^a = n^a(x^1, x^2)$ ($a=1, 2$), where $x=(x^1, x^2)$ is the local coordinate system on a fixed plane. (The parallel component n^3 of the director field along the disclination lines has no contribution to the winding numbers, i. e., the disclination strengths. So it will not affect the free energy density of disclination lines and we can set $n^3 = \text{constant}$ or 0.) To keep our calculations as simple as possible, we will use the one-constant limit ($k_1 = k_2 = k_3 = k$) of the Frank free energy density^[2-3,9]:

$$F = F_d + F_m \quad (2)$$

where

$$F_d = \frac{1}{2} k \partial_i n^a \partial_i n^a, \quad i, a = 1, 2 \quad (3)$$

$$F_m = \frac{1}{2} (k - k_{24}) \epsilon^{ij} \epsilon_{\alpha\beta} \partial_i n^a \partial_j n^\beta, \quad i, j, \alpha, \beta = 1, 2 \quad (4)$$

F_d is the distorted energy density of director field

around the disclination lines. F_m is the free energy density of the disclination lines themselves^[9].

It has been calculated that the distorted energy and the free energy of the disclination lines themselves per unit length of disclination line are given by^[9]:

$$\int F_d dV = \int_c^d \frac{1}{2} k m^2 \frac{1}{r^2} 2\pi r dr = k\pi m^2 \ln\left(\frac{d}{r_c}\right) \quad (5)$$

$$\begin{aligned} \int F_m dV &= (k - k_{24})\pi \sum_{l=1}^N \beta_l \eta_l = \\ &= (k - k_{24})\pi m = (k - k_{24})\pi \chi \end{aligned} \quad (6)$$

where m is the disclination strength, r_c is the radius of the disclination line core which is of order 10 nm^[10], d is the least distance of disclination line to other defects^[11], χ is the Euler characteristic of liquid crystals.

3 Free Energy of Saturn-ring Defects

Now, let us discuss the free energy of Saturn-ring defects which disclination strength m is $-1/2$ (Fig. 1). Imagine a sphere of radius R_0 that encloses a Saturn-ring defect and a spherical particle whose radius is a (Fig. 2). Outside of the sphere, the configuration can be seen as a point defect. Accordingly, if there are no defects in the sphere, the free energy of which is expected to be about^[12]

$$F_0 = 8\pi(k - k_{24})(R_0 - a) \quad (7)$$

similarly, the free energy that comes from the spherical region, which radius is from a to $(a + 2R_1)$, is expressed by:

$$F_1 = 16\pi R_1(k - k_{24}) \quad (8)$$

Inside the sphere of radius R_0 where there

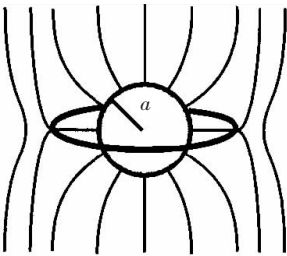


Fig. 1 Saturn-ring configuration with a disclination ring encircling the particle at its equator

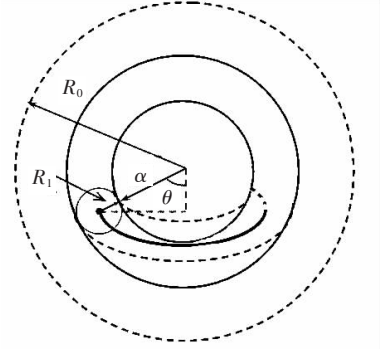


Fig. 2 Coordinates (α, θ) for a disclination ring with a general position around the spherical particle.

are no defects, the free energy of a toroidal region of cross section πR_1^2 has the form:

$$F_2 = \frac{F_1}{\frac{4}{3}[(a + 2R_1)^3 - a^3]} 2\pi^2 R_1^2 (a + R_1) \sin\theta \quad (9)$$

According to Eqs. (5) and (6), the free energy of a Saturn-ring is

$$\begin{aligned} F_3 &= 2\pi(a + R_1) \sin\theta \left[\int F_d dV + \int F_m dV \right] = \\ &= 2\pi(a + R_1) \sin\theta \left[k\pi m^2 \ln\left(\frac{R_1}{r_c}\right) + (k - k_{24})\pi m \right] \end{aligned} \quad (10)$$

So the total free energy in the sphere of radius R_0 takes the form:

$$\begin{aligned} F &= F_0 - F_2 + F_3 = 8\pi(k - k_{24})(R_0 - a) + \\ &+ \frac{1}{2}\pi^2(a + R_1) \sin\theta f(a) \end{aligned} \quad (11)$$

where

$$\begin{aligned} f(a) &= k \ln\left(\frac{R_1}{r_c}\right) - 2(k - k_{24}) - \\ &- \frac{48R_1^2(k - k_{24})}{(a + 2R_1)^3 - a^3} \end{aligned} \quad (12)$$

4 Results and Discussions

In this section we present the results of our numerical calculation. There are two important cases of Eq. (12):

Case 1 For $k \ln\left(\frac{R_1}{r_c}\right) < 2(k - k_{24})$, that is

$$k_{24} < \left(1 - \frac{1}{2} \ln \frac{R_1}{r_c}\right) k \quad f(a) < 0 \quad (13)$$

From Eqs. (11) and (12) we see that, with the

increasing of θ , the total free energy F is reduced. This means the Saturn-ring defect, in this case, is more stable and the director configuration does not depend on the particle size.

Case 2 For $k\ln\left(\frac{R_1}{r_c}\right) > 2(k - k_{24})$, that is $k_{24} > \left(1 - \frac{1}{2}\ln\frac{R_1}{r_c}\right)k$. If $f(a) < 0$, from Eq(12), we have

$$a < \left[\sqrt{\frac{8(1-y)}{2y + \ln\frac{R_1}{r_c} - 2}} - \frac{1}{3} - 1 \right] R_1 \quad (14)$$

where $y = \frac{k_{24}}{k}$. Similarly, from Eqs. (11), (12) and (14), we can see that the Saturn-ring defect is more stable. If a is larger than the right term of Eq. (14), we would obtain $f(a) > 0$, then the total free energy F is decreased with the decreasing of θ . This means the Saturn-ring defect is unstable and could evolve to a more stable state of the dipole configuration.

In the nematic liquid crystals, the length of bar-like molecules R_1 should be of order 30 nm^[11], r_c is about 10 nm. In Fig. 3, we plot the radius of the spherical particle a as a function of the ratio of k_{24} to k . Fig. 4 presents the radius of the spherical particle a as a function of the ratio of k_{24} to k and the length of molecules R_1 . It can be seen that the Saturn-ring configuration is more stable below the curve in Fig. 3(the curved surface is in Fig. 4) and the dipole configuration is more stable above the curve (curved surface). From these figures we can see that the stability of the defects around the spherical particle is effected by the radius of the spherical particle a and the elastic constants. For small particles the Saturn-ring is the relatively stable configuration. For large particles, the dipole is the preferred configuration. If $k_{24} = 0.451k$ and the radius of the spherical particle is smaller than 251 nm, the Saturn-ring configuration is more stable than dipole configuration. Meanwhile, we see that, with the increasing of k_{24} or the decreasing of k , the dipole configuration is more stable.

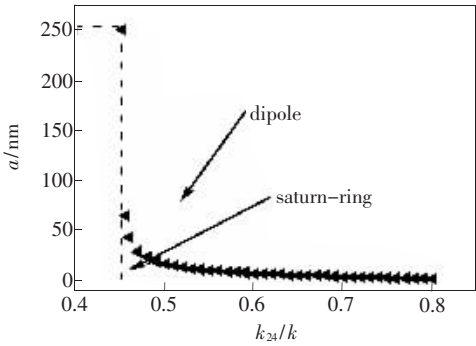


Fig. 3 Radius of the spherical particle as a function of k_{24}/k

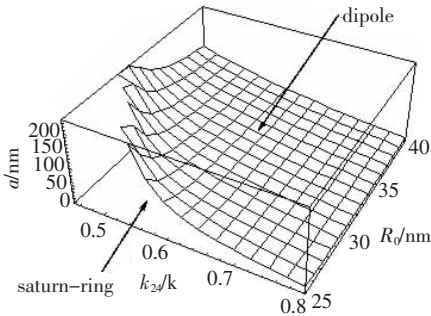


Fig. 4 Radius of the spherical particle as a function of k_{24}/k and R_0

5 Conclusion

In summary, we have studied the stability of Saturn-ring and dipole defects around microspheres suspended in nematic liquid crystals by calculating their Frank free energy. According to our calculations, the saddle-splay elastic constants and the radius of the particle play important roles for the stability of the defects. For different k_{24} , the stable configurations are different. If $k_{24} < \left(1 - \frac{1}{2}\ln\frac{R_1}{r_c}\right)k$, the Saturn-ring is the preferred configuration. If $k_{24} > \left(1 - \frac{1}{2}\ln\frac{R_1}{r_c}\right)k$ and a satisfy Eq. (14), the Saturn-ring configuration is stable too. If $k_{24} > \left(1 - \frac{1}{2}\ln\frac{R_1}{r_c}\right)k$ and a is larger than the right term of Eq. (14), the dipole configuration is stable. One can conclude that a transition from the Saturn-ring defect to the dipole defect can be achieved either by increasing a , k_{24} or by decreasing k .

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