Configuration of a chiral smectic-C film with a circular inclusion

— Pathological contribution of spontaneous bend? —

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キラルスメクチックC液晶からなる2次元薄膜中に円形のコロイド粒子が含まれる時の，液晶のc-ディレクタの構造，および粒子表面に生じる欠陥の配置を解析的に考察する．液晶のキラリティに起因する自発的な曲げ変形の存在により，キラルでないスメクチック液晶の場合に期待される四重極の対称性を持った構造とは異なり，より対称性の低い双極子の対称性を持った，表面欠陥を伴う構造が形成される．液晶の自由エネルギーを最小にする表面欠陥の位置は，自発的な曲げ変形の強さ，コロイド粒子の半径のみならず，液晶薄膜の外側の境界の形，および境界条件に（たとえ境界が無限遠にあっても）依存するという，直観的には理解しがたい結果が導き出される．上記の結果は，自発的な曲げ変形に関する自由エネルギーの寄与が原因となっている．

Colloidal dispersions with liquid crystal (LC) hosts have attracted great interest for the last decade, and recent attention has been focused on quasi-two-dimensional (2D) thin films with colloidal inclusions as well as three-dimensional systems. Here we consider a chiral smectic-C (SmC) LC film as the host fluid of the 2D colloidal system. Recently Dolganov et al.[1] showed experimentally that the c-director profile of the chiral SmC film around a circular inclusion adopts dipolar rather than quadrupolar configuration observed in achiral SmC films. They also argued that it might be attributed to spontaneous bend inherent in 2D chiral LC systems. Later, Bohley and Stannarius[2] carried out numerical calculations to show that the presence of the spontaneous bend term in the elastic energy of the c-director indeed brings about dipolar configurations. The aim of the present study is to give an analytic argument on how spontaneous bend influences the c-director configuration and the position of surface defects in a chiral SmC film with a circular inclusion that imposes tangential anchoring[3].

The free energy of the chiral SmC film in terms of c-director with $\boldsymbol{c} = (\cos\phi(x,y), \sin\phi(x,y))$ is written formally as $F = F_{\text{el}} + F_{\text{Ch}}$, where the usual elastic energy F_{el} is given by

$$F_{\text{el}} = \frac{K}{2}\int_{\Omega} dxdy\,[(\nabla\cdot\boldsymbol{c})^2 + (\nabla\times\boldsymbol{c})^2] = \frac{K}{2}\int_{\Omega} dxdy\,(\nabla\phi)^2 = \frac{K}{2}\int_{C_{\text{inclusion}}+C_{\text{outer}}} dl\,\phi\boldsymbol{\nu}\cdot\nabla\phi, \quad (1)$$

and the contribution from the spontaneous bend in a chiral SmC film, F_{Ch}, is

$$F_{\text{Ch}} = -Kq\int_{\Omega} dxdy\,\nabla\times\boldsymbol{c} = -Kq\int_{C_{\text{inclusion}}+C_{\text{outer}}} d\boldsymbol{l}\cdot\boldsymbol{c}. \quad (2)$$

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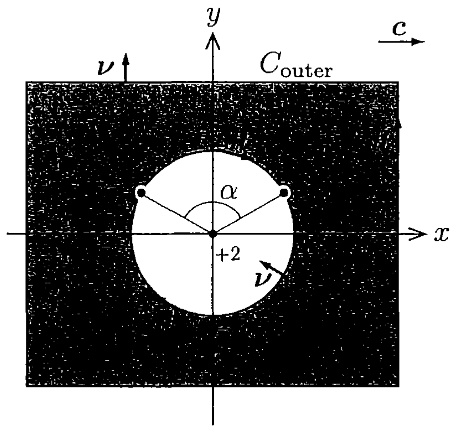

Figure 1: Geometry of our system.

Here K is the elastic constant assumed to be equal for splay and bend deformations, and q characterizes the sign and strength of spontaneous bend. See Fig. 1 for the illustration of the geometry of our system and the definition of the other undefined symbols.

We consider a circular inclusion of radius R whose center is located at the origin. We assume $\boldsymbol{c} = (1, 0)$ at infinity, and rigid tangential anchoring at the inclusion boundary ($r = R$). It is easily shown that the profile $\phi(x, y) = 2\tan^{-1}\frac{y}{x} - \tan^{-1}\frac{y-R\cos(\alpha/2)}{x-R\sin(\alpha/2)} - \tan^{-1}\frac{y-R\cos(\alpha/2)}{x+R\sin(\alpha/2)}$ satisfies the Euler-Lagrange equation in the bulk, $\nabla^2\phi = 0$, as well as the boundary conditions at the inclusion boundary and at infinity. Two surface defects of strength $-1/2$ are located at $(\pm R\sin(\alpha/2), R\cos(\alpha/2))$.

From the above profile of ϕ, $F_{\rm el}$ can be readily calculated and one finds $F_{\rm el} = -\pi K \ln\sin(\alpha/2)$, apart from an uninteresting singular contribution independent of α. On the other hand, the evaluation of $F_{\rm Ch}$ suffers from indefiniteness in the contribution from the outer boundary $C_{\rm outer}$. Indeed, when we consider, as $C_{\rm outer}$, a rectangle whose sides along the x and the y direction are l_1 and l_2, respectively, the above profile of ϕ yields $F_{\rm Ch}$ dependent on l_2/l_1:

$$\lim_{l_1, l_2 \to \infty, l_2/l_1:\text{fixed}} F_{\rm Ch} = -2KqR\left(\alpha - \pi + 4\tan^{-1}\frac{l_2}{l_1}\cos\frac{\alpha}{2}\right). \tag{3}$$

One can also imagine fixing $\boldsymbol{c}$ at $C_{\rm outer}$ first, and pushing $C_{\rm outer}$ away to infinity. This treatment corresponds to choosing $l_2/l_1 = 0$ in eq. (3). Therefore $F_{\rm ch}$ depends not only on α, R and the material parameters, but also on the shape (l_2/l_1) of $C_{\rm outer}$ and how $\boldsymbol{c}$ is treated at $C_{\rm outer}$.

We consider two cases, $l_2/l_1 = 0$ and $l_2/l_1 = 1$, to discuss how the position of surface defects, α, depends on q and R[3]. The former yields results similar to that of numerical calculation in Ref. [2]; α depends monotonically on qR, $d\alpha/d(qR) > 0$, and $\lim_{qR\to\pm\infty} = 2\pi(+)$ or $0(-)$, corresponding to the dipolar profile with one surface defect with strength -1. On the other hand, the latter results in non-trivial behavior; for $|qR| > 4.66$, we find a metastable configuration as well as a stable one. The stable branch satisfies $d\alpha/d(qR) < 0$, and α does not go to 2π or 0 when $qR \to \pm\infty$, in sharp contrast to the former. The present result indicates, against intuition, that the $\boldsymbol{c}$-director configuration depends substantially on the shape and the treatment of the outer boundary of the film, even when it is at infinity.

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