Large-scale continuous theory of cholesterics

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A continual theory of cholesterics is constructed using larger scales than those of the pitch of a helix. The free energy is expressed in terms of the unit vector of the normal to the cholesteric planes and the distortion v_s analogous to the superfluid velocity of He^3-A.

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The continuous theory of cholesterics (see the review article of de Gennes[1]) is based on the fact that a cholesteric is a nematic at smaller distances than the pitch of the helix $1/q_0$. The distortion energy of the cholesteric

$$F_d = \frac{1}{2} K_1 (\vec{\nabla} \mathbf{n})^2 + \frac{1}{2} K_2 (\mathbf{n} \operatorname{rot} \mathbf{n} + q_0)^2 + \frac{1}{2} K_3 [\mathbf{n} \operatorname{rot} \mathbf{n}]^2 \tag{1}$$

is the distortion energy of the nematic to which is added the linear term $K_2 q_0 \mathbf{n}$ rot $\mathbf{n}$ with respect to the gradients. This term accounts for the existence of the helical cholesteric structure, since the inhomogeneous state $\mathbf{n} = \text{const}$, which gives $F_d = \frac{1}{2} K_2 q_0^2$, has minimum energy F_d and the state

$$\mathbf{n}(\mathbf{r}) = \vec{\alpha} \cos (q_0 \mathbf{l} \mathbf{r}) + \vec{\beta} \sin (q_0 \mathbf{l} \mathbf{r}) \tag{2}$$

(α, β, and $\mathbf{l} = [\alpha,\beta]$ are three unit vectors and $\mathbf{l}$ indicates the direction of the axis of the helix) which gives $F_d = 0$.

The next step is the construction of a large-scale continuous theory of cholesterics, which can be used for much larger scales than the pitch of the helix. Such a theory was proposed by Lyubenskiĭ and de Gennes (see Ref. 1). This theory, however, proved to have its flaws such as the omission of the dependence of the free energy on K_1. Our aim is to obtain a correct large-scale theory of cholesterics.

For large scales the cholesteric states are given by the orientation of the three unit vectors α, β, and $\mathbf{l}$, which is the order parameter in the cholesterics [note that the superfluid helium He^3-A the order parameter is also represented by three unit vectors, if the spin-orbit interaction is taken into account (see, for eaxmple, Ref. 2)]. If the cholesteric structure is slightly distorted, then α, β, and $\mathbf{l}$ will depend on the coordinates. It is required that the energy (1) be averaged over the rapidly varying field $\mathbf{n}(\mathbf{r})$ in such a way that it would retain the quadratic dependence on the gradients of the slowly varying variables α; β, and $\mathbf{l}$. As seen from the dimensional considerations, the quantity q_0 should not be included in the final expression for the free energy.

We write the distribution of the field $\mathbf{n}(\mathbf{r})$ in an arbitary, slightly distorted cholesteric structure in the following form:

$$\mathbf{n}(\mathbf{r}) = \vec{a}\cos\phi + \vec{\beta}\sin\phi . \tag{3}$$

In this formula a superfluous function ϕ was added to the three variables $\alpha,\cdot\beta,\mathbf{1} = [\alpha,\beta]$. This function can be chosen by requiring that

$$\vec{\nabla}\phi = q_0 \mathbf{l} . \tag{4}$$

By substituting Eq. (3) into Eq. (1) we can show that this choice of ϕ eliminates in the free energy the linear terms with respect to the gradients of the order parameter, leaving only the quadratic dependence on these gradients:

$$F_d = \frac{1}{2} K_1 (\vec{\nabla}.\vec{a}\cos\phi + \vec{\nabla}\vec{\beta}\sin\phi)^2 + \frac{1}{2} K_2 (\vec{a}\,\mathrm{rot}\,\vec{a}\cos^2\phi + \vec{\beta}\,\mathrm{rot}\,\vec{\beta}\sin^2\phi$$

$$+ \sin\phi\cos\phi(\vec{a}\,\mathrm{rot}\,\vec{\beta} + \vec{\beta}\,\mathrm{rot}\,\vec{a}))^2 + \frac{1}{2} K_3([\vec{a}\,\mathrm{rot}\,\vec{a}]\cos^2\phi$$

$$+ [\vec{\beta}\,\mathrm{rot}\,\vec{\beta}]\sin^2\phi + \sin\phi\cos\phi([\vec{a}\,\mathrm{rot}\,\vec{\beta}] + [\vec{\beta}\,\mathrm{rot}\,\vec{a}]))^2 . \tag{5}$$

Expression (5) can be easily averaged over the rapidly varying function ϕ, if we assume that $\langle\sin\phi\rangle = 0$, $\langle\cos^2\phi\rangle = 1/2$, $\langle\cos^4\phi\rangle = 3/8$, etc. As a result, introducing instead of α and β the variable $\mathbf{v}_s$ according to the formula

$$v_s^i = -\vec{\beta}\nabla^i\vec{a}, \tag{6}$$

we obtain for the energy of the cholesteric the following expression:

$$\langle F_d \rangle = \frac{1}{16}(K_2 + 3K_3)(\vec{\nabla}\mathbf{l})^2 + \frac{1}{2} K_2 (\mathbf{l}\,\mathbf{v}_s)^2 + \frac{1}{4}(K_1 + K_3)[\mathbf{l}, \mathbf{v}_s]^2 . \tag{7}$$

(Note that the last term is missing in the theory of Lyubenskiĭ and de Gennes.) The variable $\mathbf{v}_s$ is based on the condition arising from Eq. (6)

$$(\mathrm{rot}\,\mathbf{v}_s)_i = \frac{1}{2} e_{ijk}\mathbf{l}\left[\frac{\partial\mathbf{l}}{\partial x_j}, \frac{\partial\mathbf{l}}{\partial x_k}\right] . \tag{8}$$

This Mermin-Ho relation[2] was obtained for He^3-*A*, where the variable $\mathbf{v}_s$ is the superfluid velocity. In the presence of vortices in the $\mathbf{v}_s$ field, the δ-function terms should be added on the right-hand side of Eq. (8). As is evident from Eq. (4), the variable **l** is also based on the condition

$$\mathrm{rot}\,\mathbf{l} = 0 . \tag{9}$$

This condition indicates that equidistance between the cholesteric layers is a strict requirement. It fully determines the distribution of the field **l** for the given boundary

conditions, in contrast to He^3-A, in which the field **l** is determined from the equation obtained by minimizing the energy functional such as (7). The vector field $\mathbf{v}_s$ is determined by minimizing $\langle F_d \rangle$ for the given field **l** and for condition (8).

Let us briefly discuss the singularities of the cholesterics. Volovik and Mineev[3] and Mineev[4] discussed the classification of the singularities in terms of the topological structure of the region of variation of the cholesteric order parameter ignoring condition (9). Allowance for this condition complicates the classification. The characteristics now must include the singularities for solution of Eq. (9) for caustics and focal surfaces, and all the χ^N lines (vortices in the field $\mathbf{v}_s$ with N circulation quanta, the circulation quantum is equal to π) and even the monopole which, in contrast to that in He^3-A (see Ref. 5) are stable. Let us examine, for example, the solution for the monopole. The monopole in a cholesteric is a system of concentric spherical layers whose center generates a vortex with $N = 4$ (see Fig. 1). In fact, the system of spherical layers

$$\mathbf{l}(\mathbf{r}) = \hat{\mathbf{r}} \tag{10}$$

($\hat{\mathbf{r}}$, $\hat{\boldsymbol{\theta}}$, and $\hat{\boldsymbol{\phi}}$ are unit vectors of the spherical coordinates system) satisfies Eq. (9); condition (8) has the form

$$\mathbf{rot}\, \mathbf{v}_s = \mathbf{r}/r^3. \tag{11}$$

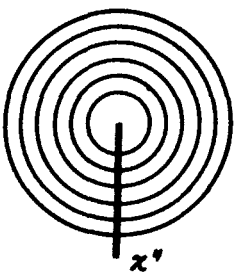

FIG. 1. Monopole in the cholesteric-hedgehog in the vector field normal to the cholesteric layers **l**, whose center generates χ^4 disclination.

The equation obtained by varying functional (7) under condition (11) has the solution

$$\mathbf{v}_s = \hat{\boldsymbol{\phi}} \frac{1 - \cos\theta}{r \sin\theta} . \tag{12}$$

The solution was chosen in such a way that the vortex (χ^4 disclination) generated from the monopole is situated on the lower axis $z < 0$, as shown in Fig. 1. In this case, the term $4\pi\theta(-z)\delta(\boldsymbol{\rho})$ should be added on the right-hand side of Eq. (11). The field $\mathbf{v}_s$(12) coincides exactly with the vector-potential field of the Dirac monopole.[6] The vortex with $N = 4$ can break up into two vortices with $N = 2$, but the configuration of the layers does not change as a result of this, since it is defined by Eq. (9), regardless of the distribution of the field $\mathbf{v}_s$. The next problem is to construct nonlinear dynamics of the cholesteric for the variables **l** and $\mathbf{v}_s$ and for the ordinary hydrodynamic variables.

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[1]P.G. de Gennes, Fizika zhidkikh kristallov (Physics of Liquid Crystals), Mir, M., 1977, ch. 6.
[2]N.D. Mermin and T.L. Ho, Phys. Rev. Lett. **36**, 594 (1976).
[3]G.E. Volovik and V.P. Mineev, Zh. Eksp. Teor. Fiz. **72**, 2256 (1977) [Sov. Phys. JETP **45**, 1186 (1977)].
[4]V.P. Mineev, J. de Phys. Lett. (in press).
[5]S. Blaha, Phys. Rev. Lett. **36**, 874 (1976).
[6]P.A. Dirac, Proc. Roy. Soc. **A133**, 60 (1931).