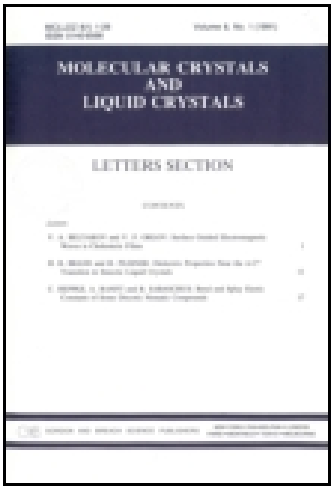

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Vortex Dynamics in a Smectic Liquid Crystal and Its Stochastic Aspect

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The dynamics and stochastic aspect of the vortices that occur in a smectic-A liquid crystal close to its nematic-smectic A transition point is investigated. Using the analogy between our target system and the superfluid system, we discuss following two topics: The first topic is the formulation of the equation of motion of the vortex center, and the other one is the analysis of the random behavior of the vortices.

Keywords vortex dynamics; liquid crystal; superfluid; nonlinear Schröedinger equation; Langevin equation; Fokker-Planck equation; path integral

PACS numbers: 42.70.Df, 61.30.Dk, 61.30.Jf

1. Introduction

Liquid crystals are the unique materials which exhibit a variety of condensed phases inherent in their anisotropic nature arising from the direction of the constituent molecules [1–3]. It is also known that the dynamics of a liquid crystal can be formulated in the framework of elasticity [4].

Among a variety of aspects of the liquid crystals, the analogy with the superconductor is amazing [1]. Using such analogy, we can elegantly describe the peculiar nature of the phase transition between nematic and smectic A phases (in brevity, NS phase transition).

Besides this we expect a close analogy with the vortices in nematic and smectic-A liquid crystals and those in superconductivity or superfluid He [5, 6]. In the latter case, the vortices are described by the nonlinear Schröedinger equation for the order parameter characterizing the quantum condensates.

In this article we explore the typical aspects of the vortecis in liquid crystal (which are abbreviated as LCV in what follows) occurring in smectic-A phase in the vicinity of the NS phase transition.

The advantage of this study is that, to the best of our knowledge, it is the first attempt to formulate the motion of vortices occurring in a smectic liquid crystal in terms of the nonlinear Schröedinger equation of (2+1) version. The height z is treated as time variable, whereas (x, y) that are perpendicular to z axis are treated as space coordinates. Then

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following the procedure used in the superfluid theory, we can develop the dynamics of a vortex and its stochastic aspect. We here emphasize that such an attempt as a transcription of the formulation that has been used in one type of condensed state to another kind of condensed state (liquid crystal) may uncover a novel aspect that has not yet been explored sufficiently. This study is a first step toward such a direction.

2. Superfluid Analogy of Free Energy Functional for NS Phase Transition

Let us introduce a coordinate system that describes the ordered state of smectic-A liquid crystal. Smectic-A phase is characterized by the periodically-arranged layered structure in one direction. In this paper, we set the z axis normal to the plane of the layers (FIG. 1). Besides this direction, we have two degrees that are attributed to the parallel direction along the layer, i.e. the directions $(x, y) = \mathbf{x}$. Now the smectic phase can be described by the density profile [1]:

$$\rho(\mathbf{r}) = \rho_0 + \rho_1(\mathbf{r})\cos(qz + \phi(\mathbf{r})), \tag{1}$$

where ρ_0 is the average density of the media, ρ_1 is the amplitude of the modulation of the density, $q = \frac{2\pi}{L_0}$ is the fixed wave number with L_0 being the period of the periodic layers, ϕ is the phase modulation, and $\mathbf{r} = (\mathbf{x}, z)$. Here it is plausible to assume that the wave number is much larger than the modulation; namely, $q >> |\frac{\partial\phi}{\partial z}|$. Let us define the order parameter in a complex form:

$$\Psi = \psi(\mathbf{r})\exp[iqz] \tag{2}$$

with the modified amplitude,

$$\psi(\mathbf{r}) \equiv n_1(\mathbf{r})\exp[i\phi(\mathbf{r})], \tag{3}$$

$$|n_1(\mathbf{r})|^2 = \rho_1(\mathbf{r})\cos(qz + \phi(\mathbf{r})) \tag{4}$$

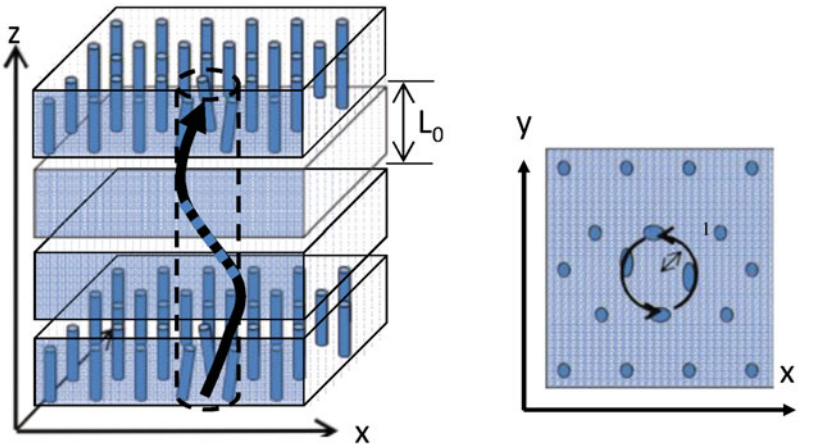

Figure 1. The setting of our target system. The left figure shows a typical smectic-A structure. The thickness of one layer is L_0. The right figure shows a view from the z-direction. If the liquid crystal molecules are tilted slightly from the z-direction, they can construct a vortex structure.

We now use the Frank-Oseen free energy that is written in the following Landau-Ginzburg form [1, 5]:

$$\mathcal{F} = \frac{1}{2}\int \left[C_l \left| \frac{\partial \Psi}{\partial z} \right|^2 + C_t \left| \nabla_\perp \Psi \right|^2 + a \left| \Psi \right|^2 + \frac{g}{2} |\Psi|^4 \right] d\mathbf{x} dz,$$
$$\simeq \frac{1}{2}\int \left[-iqC_l \left(\psi^* \frac{\partial \psi}{\partial z} - \text{c.c} \right) + C_t |\nabla_\perp \psi|^2 + (a + C_l q^2)|\psi|^2 + \frac{g}{2}|\psi|^4 \right] d\mathbf{x} dz. \tag{5}$$

Here C_t and C_l are called the transversal and longitudinal elastic constants. The parameter a is defined as $a = a_0(T - T_c)$ with $a_0 > 0$ in the vicinity of the NS transition temperature T_c. Furthermore, g is prescribed to be positive. Stepping to the second line from the first line, we use the approximation such that $|\frac{\partial \psi}{\partial z}| << q$.

We now substitute the relation (3) into (5) and rewrite $\mathcal{F}$ using a fluid-dynamical form [7]:

$$\mathcal{F} = \int (L_C - H) dz. \tag{6}$$

The first term L_C is called the canonical term, and is defined as follows

$$L_C = \gamma \int n_1^2 \frac{\partial \phi}{\partial z} d^2x, \tag{7}$$

with $\gamma = qC_l$. The second term in (5) is the Hamiltonian term which consists of the kinetic energy term H_K and the nonlinear interaction potential V:

$$H = H_K + V, \tag{8}$$
$$H_K = -\frac{C_t}{2}\int \nabla_\perp \psi^\dagger \nabla_\perp \psi d\mathbf{x} = -\frac{C_t}{2}\int \left[(\nabla_\perp n_1)^2 + n_1^2 (\nabla_\perp \phi)^2 \right] d\mathbf{x}, \tag{9}$$
$$V = \frac{1}{2}\int \left(m n_1^2 - \frac{g}{2} n_1^4 \right) d\mathbf{x}, \tag{10}$$

where we set the notation:

$$m \equiv -a - C_l q^2 = -a_0(T - T_c). \tag{11}$$

Here, m is the effective mass, and the second term on the last line of (9) is nothing but the fluid kinetic energy, if we define the "velocity field " $\mathbf{v}$ through $\mathbf{v} \equiv \nabla\phi$. The double well potential (10) has the minimum point at $|n_1| = \sqrt{m/g}$. When the system temperature goes up to T_c from below, the phase transition from smectic-A to nematic occurs. At this transition, the periodic structure in the z-direction disappears, and this means that the wave number q in (1) goes to 0. By combining the above-mentioned two conditions $T \nearrow T_C$ and $q \nearrow 0$, we realize that m goes to 0 at the critical point.

3. Vortex Dynamics

3.1. The Profile of LCV

On the basis of the above setting, we apply the analysis to the profile of the vortex in the (x, y) plane. We consider the special case where the center of the vortex $\mathbf{X}(z) = (X(z), Y(z))$ is located at the origin of the space, $\mathbf{X}(z) = (0, 0)$. Let us introduce an ansatz for the phase function: We choose $\phi = \tan^{-1}(\frac{y}{x})$. Under this ansatz, it is natural to assume that the density profile is a function of $r = \sqrt{x^2 + y^2}$; $n_1 = n_1(r)$. Thus the Hamiltonian is written as

$$H = -\frac{\pi}{2}\int\left[C_t\left(\left(\frac{dn_1}{dr}\right)^2 + \frac{n_1^2}{r^2}\right) - mn_1^2 + \frac{g}{2}n_1^4\right]rdr. \tag{12}$$

By using the variation equation $\delta H = 0$, we have the following equation for n_1.

$$\frac{d^2n_1}{dr^2} + \frac{1}{r}\frac{dn_1}{dr} - \frac{n_1}{r^2} + \frac{m}{C_t}n_1 - \frac{g}{C_t}n_1^3 = 0. \tag{13}$$

From this equation, we obtain an asymptotic form for $n_1(r)$ as $n_1^2(\infty) = \frac{m}{g}$. The derivation of this asymptotic form is carried out by imposing the boundary condition at the origin $n_1(0) = 0$. This equation (13) has the same form as the Gross-Pitaevskii equation. We show some examples of changes of the asymptotic value of n_1 obtained by simulation (FIG. 2). We can easily see that $n_1 \to 0$ as $m \to 0$, when the system temperature is close to the NS phase transition temperature.

3.2. Evolution Equation for the Center of LCV

We now consider the evolutional behavior of the center of a single LCV with respect to the propagation to z direction [8]. The solution is parameterized by the coordinate of the $\mathbf{X}(z)$, such that $n_1(\mathbf{x} - \mathbf{X}(z))$ and $\phi(\mathbf{x} - \mathbf{X}(z))$. By using this parameterization, the canonical term

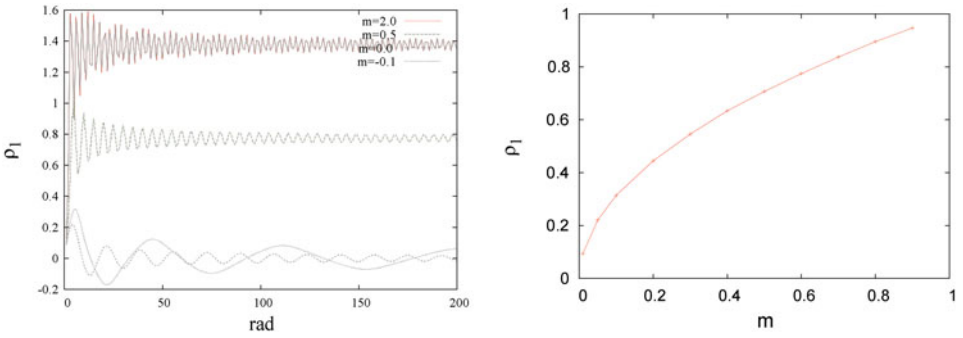

Figure 2. Left: The simulation results of The LCV profiles for various effective mass. The mass is changed as 2.0, 0.5, 0.0, and −0.1. The other parameters are set to 1, such that $C_t = C_l = g = a = q = 1$. Right: Points are the simulation results of the n_1 at rad=200 for various mass, and line is the theoretical result $n_1 = \sqrt{m}$

L_C is rewritten as

$$L_C = -\gamma \int n_1^2 \mathbf{v} \cdot \dot{\mathbf{X}} d^2x. \tag{14}$$

with $\dot{\mathbf{X}} \equiv \frac{d\mathbf{X}}{dz}$. From the Euler-Lagrange equation, we get the equation of motion for the center of the vortex:

$$\begin{aligned} \frac{d}{dt}\left(\frac{\partial L_c}{\partial \dot{X}}\right) - \frac{\partial L_c}{\partial X} &= -\gamma \int \left\{ \frac{\partial}{\partial x}\left(n_1^2 v_y\right) - \frac{\partial}{\partial y}\left(n_1^2 v_x\right) \right\} d\mathbf{x}\dot{Y} \\ &= -\gamma n_1^2 \left(\int \{\nabla \times \mathbf{v}\} d\mathbf{x} \right) (\mathbf{k} \times \dot{\mathbf{X}}). \end{aligned}$$

Besides the canonical term, by adding the term comming from the hamiltonian $\tilde{H}$, which describes the interaction between the voltexis and other objects, we arrive at the *Kirchhoff* equation of motion [9]:

$$\mu\left(\mathbf{k} \times \dot{\mathbf{X}}\right) = -\frac{\partial \tilde{H}}{\partial \mathbf{X}}. \tag{15}$$

By operating $\mathbf{k}\times$ to (15) from the left side, we obtain

$$\mu \dot{\mathbf{X}} = \mathbf{k} \times \frac{\partial \tilde{H}}{\partial \mathbf{X}}, \tag{16}$$

where $\mathbf{k}$ is the unit vector perpendicular to (x, y) plane and $\mu \equiv n_0^2 \gamma \sigma$. σ is defined as

$$\sigma = \int \left(\frac{\partial v_y}{\partial x} - \frac{\partial v_x}{\partial y} \right) d\mathbf{x}, \tag{17}$$

which gives the winding number that characterizes the topological nature of the vortex.

Here we consider the expression $\tilde{H}$. If impurities are distributed randomly in the medium, the motion of LCV is trapped locally or pinned. Let V_{pin} be the pinning potential; $V_{pin} = v_0 \delta(\mathbf{r} - \mathbf{a})$, with $\mathbf{a}$ the pinning center. Then, we obtain,

$$\tilde{H} \equiv V_{pin} = \int |\psi|^2 v_0 \delta(\mathbf{r} - \mathbf{a}) d\mathbf{x} = v_0 f(|\mathbf{X} - \mathbf{a}|). \tag{18}$$

4. The Stochastic Theory

4.1. The Langevin Equation and Functional Integral

The two different forms of the equation of motion for the single LCV, i.e. (15) and (16) still have a room for an extention to incorporate some additional effects; i.e. dissipative force and the random fluctuation force [10, 11]. These effects can be included in the model by the following replacement: $\tilde{H} \to \tilde{H} + Z$, here the random term Z is a functional of (ψ, ψ^*), and this is equivalent to substituting the following relation: $\frac{\partial \tilde{H}}{\partial \mathbf{X}} \to \frac{\partial \tilde{H}}{\partial \mathbf{X}} + \zeta$, where $\zeta = \frac{\partial Z}{\partial \mathbf{X}}$. Finally, by adding the dissipative term $\eta \dot{\mathbf{X}}$: $\frac{\partial \tilde{H}}{\partial \mathbf{X}} + \zeta \to \frac{\partial \tilde{H}}{\partial \mathbf{X}} + \eta \dot{\mathbf{X}} + \zeta$, we arrive at

the Langevin equation:

$$\frac{d\mathbf{X}}{dz} + A(\mathbf{X}) = \mathbf{c}, \tag{19}$$

where $\mathbf{A}$ and $\mathbf{c}$ are defined by:

$$\mathbf{A} = \frac{1}{\mu^2 + \eta^2}\left\{\eta\frac{\partial \tilde{H}}{\partial \mathbf{X}} - \mu\left(\mathbf{k} \times \frac{\partial \tilde{H}}{\partial \mathbf{X}}\right)\right\}, \tag{20}$$

$$\mathbf{c} = -\frac{1}{\mu^2 + \eta^2}\left(\eta\zeta - \mu\mathbf{k} \times \zeta\right). \tag{21}$$

A consist of two terms: The first term is described the dissipation, and the other the gyration, which is analogous to the Lorentz force acting on a charged particle in a uniform magnetic field $\mathbf{k}$. The meaning of $\mathbf{c}$ is the reduced random force. We adopt the Gaussian white noise for the random force [12, 13];

$$\langle c_i(z)\rangle = 0,\ \langle c_i(z)c_j(z+u)\rangle = h\delta_{ij}\delta(u). \tag{22}$$

By assuming the variance of $\mathbf{c}$ as $\langle \mathbf{c}^2\rangle = h$, the probability distribution of $\mathbf{c}$ can be given by

$$P[\mathbf{c}(z)] = \exp\left[-\frac{1}{2h}\int_0^z \mathbf{c}^2(z)dz\right]. \tag{23}$$

Using this distribution, the propagator $\mathcal{K}$ between two points $\mathbf{X}(z)$ and $\mathbf{X}(0)$ at two different heights, is given by the functional integral:

$$\mathcal{K}[\mathbf{X}, z|\mathbf{X}, 0] = \int \prod_z \delta\left(\left(\frac{d\mathbf{X}}{dz} + A(\mathbf{X})\right) - \mathbf{c}(z)\right) \times \exp\left[-\int \frac{\mathbf{c}^2(z)}{2h}dz\right] \mathcal{D}\mathbf{X}\mathcal{D}\mathbf{c}(z), \tag{24}$$

with the Dirac δ functional. By carrying out the Gaussian integral over the field $\mathbf{c}(t)$, and putting $z = i\tau$, we get

$$\mathcal{K} = \int \exp\left[\frac{i}{h}\int\left(\frac{1}{2}\left(\frac{d\mathbf{X}}{d\tau}\right)^2 + i\mathbf{A}\cdot\frac{d\mathbf{X}}{d\tau} - V\right)d\tau\right]\mathcal{D}[\mathbf{X}], \tag{25}$$

where we define $V = \frac{1}{2h}\mathbf{A}^2$. This equation is nothing but the path integral for a particle in a vector potential $\mathbf{A}$ and a scalar potential V.

4.2. The Fokker-Planck Equation

The probability distribution $P(\mathbf{X})$ for the vortex center vector $\mathbf{X}$ satisfies the following integral equation:

$$P(\mathbf{X}, \tau) = \int \mathcal{K}(\mathbf{X}, \tau|\mathbf{X}', 0)P(\mathbf{X}', 0)d\mathbf{X}.$$

Following the standard procedure of path integral, we find the Schröedinger type equation for a particle moving in a vector potential and a scalar potential $(-i\mathbf{A}, V)$

$$ih\frac{\partial P}{\partial \tau} = \left[\frac{1}{2}\left(-ih\frac{\partial}{\partial \mathbf{X}} - i\mathbf{A}\right)^2 + V\right]P. \tag{26}$$

Now going back to the real variable, by noting the relation; $i\frac{\partial}{\partial\tau} = -\frac{\partial}{\partial z}$, we get

$$\frac{\partial P}{\partial z} = \frac{h}{2}\frac{\partial^2 P}{\partial \mathbf{X}^2} - \frac{1}{2}\frac{\partial(\mathbf{A}P)}{\partial \mathbf{X}}. \tag{27}$$

This is the Fokker-Planck equation (for brevity FP eq.) of the standard form.

4.3. An Example of the Specific Potential

To construct a special solution of the equation of motion (27), let us consider the case that the pinning center is placed at the origin, $\mathbf{a} = \mathbf{0}$. As a functional form of the pinning potential $f(r)$, we adopt a simulated form that is described by the function:

$$f(r) = C(1 - \exp[-\alpha r]). \tag{28}$$

Using this, we can construct some solution of the equation of motion (19) numerically (FIG. 3).

In the case without dissipation $\eta = 0$, we can construct as exact solution and (20) is given as

$$\mathbf{A} = \frac{\alpha C}{\mu}\exp[-\alpha r]\left(\mathbf{k} \times \frac{\mathbf{X}}{|\mathbf{X}|}\right).$$

In this case, the vortex center may be written as the circular orbit : $\mathbf{X} = (R_c \cos\Phi,\ R_c \sin\Phi)$ with R_c constant. Therefore, the equation of motion is simply written as $\dot{\Phi} = \kappa$ with $\kappa \equiv \frac{\alpha C}{R_c \mu}\exp[-\alpha R_c]$. The corresponding functional integral is reduced to the form:

$$\mathcal{K} = \int \exp\left[-\frac{1}{2}\int_0^z R_c^2\left(\dot{\Phi} - \kappa\right)^2 dz\right]\mathcal{D}(\Phi),$$

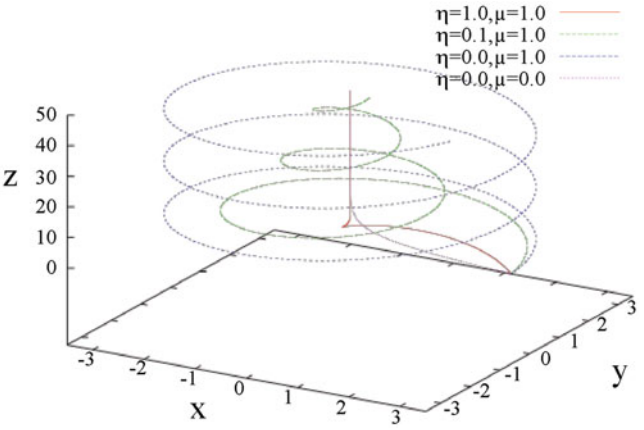

Figure 3. The simulation results for various dissipation constant η. We set (η, μ)=(1.0,1.0), (0.1,1.0),(0.0,1.0) and (0.0,0.0). The case η=0.0 is a special case without dissipation, and observed uniform rotation.

which is a path integral for a *free particle* on a circle. The corresponding FP eq. is given by the diffusion-type equation.

$$\frac{\partial P}{\partial z} = \frac{1}{R_c^2}\frac{\partial^2 P}{\partial \Phi^2} - \kappa \frac{\partial P}{\partial \Phi}. \tag{29}$$

By taking into account of the periodic boundary condition and using the theta function [14, 15], we obtain the solution [11]:

$$P(\Phi, z) = \sum_{n=-\infty}^{\infty} \exp\left[-\left(\frac{h}{R_c^2}n^2 + in\kappa\right)z\right]\exp[in\Phi].$$

The expectation value of $\mathbf{X}$ is calculated as

$$< \mathbf{X} >= \int_0^{2\pi} \mathbf{X} P(\Phi, z) d\Phi = \pi R_c \exp\left[-\frac{h}{R_c^2}z\right] \times (\cos(\kappa z), -\sin(\kappa z)). \tag{30}$$

5. Summary

In this note, using an analogy between the liquid crystals and the superfluid systems, we have attempted to develop a formulation of the dynamics as well as the stochastic aspects of the vortices that are expected to occur in a liquid crystal of smectic phase close to the smectic A-nematic phase transition. The nonlinear Schröedinger type equation describes the vortex motion. This equation can be converted to a Langevin-type equation in the presence of the random fluctuations.

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Appendix A: Spatial Symmetry

The variation equation of the free energy functional (5) with respect to ψ leads to the nonlinear Schrödinger type equation,

$$i\gamma \frac{\partial \psi}{\partial z} = \left(-C_t \nabla^2 - m + \frac{g}{2}|\psi|^2\right)\psi = \hat{H}\psi \tag{A1}$$

Here we set the Hamiltonian, $\hat{H} = -C_t\nabla^2 - m + \frac{g}{2}|\psi|^2$. In this equation, γ plays a role of the Planck constant and the longitudinal coordinate z plays a role of time variable. The *wave function* ψ are determined by an equation where the imaginary unit i appears in the coefficient. This equation retains the same form if we replace z in (31) by $-z$ and at the same time take the complex conjugate [16].

In the classical mechanics point of view, the equations are unchanged by the replacement of the space direction $\mathbf{x}$ to $-\mathbf{x}$. In the system of this paper (FIG. 1), the symmetry with respect to the two direction of z and $-z$ is expressed in the invariance of the above

Schröedinger equation (31) when the sign of z is changed to $-z$ and ψ is simultaneously replaced by ψ.

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