The stress field and energy of screw dislocation in smectic A liquid crystals and the mistakes of the classical solution

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The mistakes in the classical solution of a screw dislocation in smectic A liquid crystals are pointed out. A serious problem with the well-known theory is pointed, which may be named de Gennes–Kleman–Pershan paradox and has existed for many decades in the scientific community of liquid crystal study. The correct solution is given in this paper by a simplest, elementary, and straight forward method. In connection with this, the stress field and energy of dislocation are discussed in detail. The present article provides the correct stress field and dislocation energy as well.

Keywords: liquid crystals, dislocation, exact solution

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1. Introduction

As is well known, liquid crystals and quasicrystals are the important phases in condensed matter, and fascinating from a fundamental point of view. Liquid crystals are also significant due to a number of current and potential applications. Liquid crystal is an intermediate phase between isotropic liquid and solid. The mechanical properties of the phase are very interesting, and have extensively been studied, such as by de Gennes and Prost,[1] Kleman,[2] Kleman and Oswald,[3] Oswald and Pieranski,[4] and others. However, the needs of basic research and engineering applications promotes further study, especially, in defects, three-dimensional elasticity, plasticity, and dynamics. Among the defects, the dislocations and focal conics have been investigated.[1–6] In addition, recently Brostow *et al*.[7] have carried out numerical simulation on crack formation and propagation in polymer liquid crystal. Liquid crystals including smectic ones can be classified as monomer liquid crystals (MLCs) no matter whether or not they can polymerize polymer liquid crystals (PLCs). That classification was given by Samuski[8] and has been used by a number of authors.[9,10] The present model is applicable to MLCs, smectic A phase in particular. People have been studying dislocations in liquid crystals A for at least the last several decades. In the work on the solution of screw dislocation of smectic A liquid crystals, there has been a long-standing puzzle. Kleman[2] and Pershan[11] separately found the solution

$$u = \frac{b\theta}{2\pi}, \tag{1}$$

which is well known and important for the study and it belongs to a classical work in this discipline, according to the de Gennes' equation of elasticity of smectic A liquid crystals (i.e., Eq. (5) in the following), one of the most famous and important results in the liquid crystal study (see e.g. Refs. [1], [2], and [4]). In Eq. (1), u is the displacement along the direction of z axis, i.e., the direction normal to the layers of smectics A, b the magnitude of the Burgers vector of the screw dislocation, and θ the polar angle of the position vector in the xy plane. The result is widely cited by many others, e.g. Ref. [5], etc. Though certain researchers, e.g., Pleiner,[12] criticized the de Gennes–Kleman–Pershan's solution, he still confirmed that solution (1) holds in the region outside the dislocation core. Unfortunately the idea has been widely accepted. Further discussion on the solution is necessary. The above solution is a solution out of the core of the dislocation. Kralj and Sluckin[13,14] studied the core structure of a screw dislocation in smectic A liquid crystal, which is very interesting and important. The core structure naturally influences the solution out of the core. But at present our attention is focused on the solution out of the core, if we can correctly explore the solution, this may help us to reveal the core structure.

2. Basis of discussion

Many investigations have been conducted from different angles so far, such as the magnetism analogue,[1,11] the differential geometry,[15] the dynamics,[16] the structure of dislocation core,[13,14,17] etc. Although these different points of view are beneficial, they bring some difficulties to the readers. To guarantee that the discussion can arrive at a unanimous result, a basis in common followed by the individual participants is necessary.

The basis of elasticity of smectic A liquid crystals was established first by de Gennes and Prost,[1] then Landau and Lifshitz[5] outstandingly simplified the formulation. Though

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the theory and formulation are well known, it is very beneficial to recall them once again for the discussion.

As is well known, the discussion is in the macroscopic scope, i.e., in the continuum frame of liquid crystals. The Landau–Ginzburg–de Gennes free energy of the deformation of the smectic A liquid crystals is[5]

$$\begin{aligned} F_{\rm d} &= F - F_0(T) = \frac{1}{2}(A/\rho_0)(\rho-\rho_0)^2 \\ &\quad + C(\rho-\rho_0)\frac{\partial u}{\partial z} + \frac{1}{2}B\rho_0\frac{\partial^2 u}{\partial z^2} + \frac{1}{2}K_1\left(\nabla^2 u\right)^2 \\ &= \frac{1}{2}\rho_0 B'\frac{\partial^2 u}{\partial z^2} + \frac{1}{2}K_1\left(\nabla^2 u\right)^2, \\ \nabla^2 &= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}, \quad \rho-\rho_0 = -\rho_0 m\frac{\partial u}{\partial z}, \\ m &= \rho_0\frac{C}{A}, \quad B' = B - \frac{C^2}{A}, \end{aligned}$$

in which $\rho_0 B'$ and K_1 are Young's modulus and splay modulus, respectively, and there is no deformation of twisting nor bending (i.e., $K_2 = 0$ and $K_3 = 0$).

This is the starting point of the following discussion.

Consider a smectic A liquid crystal, in which there is a screw dislocation along the direction of z axis. The physical model can be formulated by the following boundary conditions:

$$\begin{cases} (x^2+y^2)^{1/2} \to \infty: \quad \sigma_{ij} = 0, \\ \sigma_{zz}(x,0) = 0, \\ \int_\Gamma {\rm d}u = b, \end{cases} \tag{2}$$

in which σ_{ij} denotes the stress tensor, recalling u the displacement along the direction of z axis, b the magnitude of the Burgers vector, in addition, Γ a contour enclosing the dislocation core. A quantitative description of the problem needs to introduce relevant basic equations.

According to de Gennes and Prost[1] or Landau and Lifshitz,[5] the stress tensor for smectic liquid crystal (exactly speaking for smectics A) is

$$\begin{cases} \sigma_{xx} = \sigma_{yy} = K_1\nabla^2\dfrac{\partial u}{\partial z}, \\ \sigma_{zz} = \rho_0 B'\dfrac{\partial u}{\partial z}, \\ \sigma_{zx} = \sigma_{xz} = -K_1\nabla^2\dfrac{\partial u}{\partial x}, \\ \sigma_{zy} = \sigma_{yz} = -K_1\nabla^2\dfrac{\partial u}{\partial y}, \\ \sigma_{xy} = \sigma_{yx} = 0, \end{cases} \tag{3}$$

in which $u \equiv u_z$ is the displacement of the z component, $B' = B - C^2/A$, A, B, C, and K_1 are material constants, see Refs. [1] and [5], recalling that physically the constant $\bar{B}$ describes material modulus relating to the deformation arising from displacements, while K_1 describes material modulus relating to the deformation arising from curvature. It is evident in the stress tensor (3) only the symmetry part, according to the theory of Landau and Lifshitz,[5] is considered, and the viscous part is omitted here by following the method adopted in the community of liquid crystals.

Substituting Eq. (3) into the equilibrium equations

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0 \tag{4}$$

yields the final governing equation

$$\rho_0 B'\frac{\partial^2 u}{\partial z^2} - K_1\nabla^2\nabla^2 u = 0, \tag{5}$$

which was derived from the energy minimization by de Gennes and Prost.[1] In Eq. (5),

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}.$$

The solution of the dislocation is reduced to solving Eq. (5) under boundary conditions (2), which can be called the boundary value problem "(5), (2)".

Because we assume that the problem is uniform along the z axis, any field variable is independent of self-variable z, i.e.,

$$\frac{\partial(\ )}{\partial z} = 0, \tag{6}$$

where ( ) represents any field function. So, equation (5) is reduced to

$$\nabla^2\nabla^2 u = 0. \tag{7}$$

In this case, the boundary value problem "(5), (2)" is replaced by the boundary value problem "(7), (2)".

Equations (2)–(7) are the basis in common in the discussion. If the discussion and dialog follow the basis, many confusions in methodology and logics can be avoided.

3. The simplest and most direct solving way

To enable readers to understand the discussion easily, we suggest taking the simplest, elementary, and straight forward method to solve the boundary value problem "(7), (2)" without using the magnetism analogue, Fourier transform, Green function, etc. Some references made the problem complicated by using complicated mathematical methods. In contrast, we take an alternative way, in which the analysis is extremely simplified.

Introducing polar coordinate system (r,θ), equation (7) is rewritten as

$$\begin{aligned} &\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}\right) \\ &\times\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}\right)u(r,\theta) = 0. \end{aligned} \tag{7a}$$

A suitable solution of Eq. (7a) through the method of separation of variables, i.e., $u(r,\theta)=f(r)\Theta(\theta)$, takes the following form

$$\begin{aligned} u = \frac{b}{2\pi}\big[&(Dr^2+Er^2\ln r+F+G\ln r)\theta \\ &+(D_1 r+E_1 r\ln r)\,\theta\sin\theta \\ &+(F_1 r+G_1 r\ln r)\,\theta\cos\theta\big], \end{aligned}$$

where we have neglected the terms which are independent of the solution of the dislocation. In other words, those terms that only cause an increment in angle when going along a circuit around the dislocation core are retained. Making use of the conditions (2), we find that the parts related to D, E, and G give rise to an increment dependent on r when running around the dislocation core. So the above solution further takes the following form

$$\begin{aligned} u = \frac{b}{2\pi}\big[&F+(D_1 r+E_1 r\ln r)\sin\theta \\ &+(F_1 r+G_1 r\ln r)\cos\theta\big]\theta, \end{aligned} \tag{8}$$

in which E_1 and G_1 are the unknown constants, and they vanish by considering stress continuity. So, finally, solution (8) is

$$u=\frac{b}{2\pi}\left[F+D_1 r\sin\theta+F_1 r\cos\theta\right]\theta. \tag{8a}$$

Furthermore, using conditions (2) one can determine $F=1$ and $F_1=0$. However, the unknown constant D_1 still cannot be determined. To determine the value of D_1, the stress field must be given. This can be done by substituting Eq. (8a) into Eq. (3), yielding

$$\begin{cases} \sigma_{zx}=\dfrac{b}{2\pi}\dfrac{2K_1D_1\left(x^2-y^2\right)}{\left(x^2+y^2\right)^2}, \\ \sigma_{zy}=\dfrac{b}{2\pi}\dfrac{4K_1D_1yx}{\left(x^2+y^2\right)^2}. \end{cases} \tag{9}$$

In Ref. [18] we developed the mathematical theory of dislocations in quasicrystals, in which the problems of crystals are naturally included (because if the phason field is absent, the quasicrystals are reduced to crystals). The theory demonstrated that the higher partial differential equations describing dislocations need appropriate additional boundary conditions besides the dislocation condition, otherwise the boundary value problem will not be well-conditional. This is valid for boundary value problem "(7), (2)" too. Expression (2) includes two conditions for determining the unknown constants F and D_1 besides the condition at infinity. Because condition $\sigma_{zz}(x,0)=0$ is automatically satisfied, we must now search an additional condition determining solution. We here use the minimization of dislocation energy, i.e.,

$$\frac{\partial U}{\partial D_1}=0, \tag{10}$$

where the energy will be given in the following (i.e., Eqs. (17)–(19)). From this condition we have

$$D_1=\frac{-8\pi\alpha/3}{(R_0+r_0)\left(\dfrac{\pi}{4}\alpha\beta+\dfrac{b^2K_1}{8\pi}\right)\ln\dfrac{R_0}{r_0}+\dfrac{\pi}{320}\alpha\gamma(R_0-r_0)}, \tag{11}$$

in which

$$\begin{cases} \alpha=\left(\dfrac{b}{2\pi}\right)^4\rho_0 B', \\ \beta=2+\dfrac{32\pi^2}{3}, \\ \gamma=75-160\pi^2+256\pi^4. \end{cases} \tag{12}$$

From Eqs. (8) and (1), one can find that the solution given by Kleman[2] and Pershan[11] is only one of terms of the present solution. It can also be said that the classical solution is the zero-order approximation of the present solution. In particular, in their solution there exists neither stress nor dislocation that causes stress-free state, while in our solution, there exists the stress field, and it exhibits a square singularity near the dislocation core. This singularity is also different from the stress field induced by a screw dislocation in conventional crystals. For the latter, the stress field has an r^{-1} singularity, rather than r^{-2} singularity.

4. Mathematical mistakes of the classical solution

In solid crystal elasticity (or classical elasticity) the screw dislocation problem is formulated by

$$\begin{cases} (x^2+y^2)^{1/2}\to\infty: \quad \sigma_{ij}^{(\mathrm{c})}=0, \\ \int_\Gamma \mathrm{d}u_z^{(\mathrm{c})}=b^{(\mathrm{c})}, \end{cases} \tag{13}$$

and

$$\nabla^2 u_z^{(\mathrm{c})}=0, \tag{14}$$

in which

$$\begin{cases} \sigma_{zx}^{(\mathrm{c})}=\sigma_{xz}^{(\mathrm{c})}=\mu\dfrac{\partial u_z^{(\mathrm{c})}}{\partial x}, \\ \sigma_{zy}^{(\mathrm{c})}=\sigma_{yz}^{(\mathrm{c})}=\mu\dfrac{\partial u_z^{(\mathrm{c})}}{\partial y}. \end{cases} \tag{15}$$

Here, super-index (c) represents the crystal, μ the shear modulus of the crystals.

The solution (1) is only the solution of boundary value problem "(14), (13)". According to the theory of partial differential equations or mathematical theory of elasticity,[19,20] the solution (1) of boundary value problem "(14), (13)" cannot be the solution of boundary value problem "(7), (2)" at the same time. The problem cannot be solved by the so-called smallest surface concept, provided Eqs. (3) and (5) are invalid. We believe that equations (3) and (5) (and its reduced form (7)) are valid, and the single straight screw dislocation along the z axis must be obtained from Eq. (7) under boundary condition (2). The solution (8) is the unique solution of boundary value problem "(7), (2)".

5. Physical mistakes of the classical solution

The solution (1) leads to some physical mistakes too.

(i) It leads to zero stress field

Substituting solution (1) into Eq. (3) leads to

$$\sigma_{ij} = 0, \quad i,j = 1,2,3. \tag{16}$$

This is completely wrong physically.

(ii) It leads to wrong energy formula

The energy induced by the dislocation is one of important aspects of the problem. On the calculation of energy induced by the dislocation, there are many contradictions among Refs. [1], [4], [15], and [17], even if in the monograph[4] there is logic contradiction itself. This shows the difficulty of the problem. According to our understanding, the point of view of Kleman[15] is correct, though his calculation is not complete, in which there are some mistakes because he used solution (1). Adopting the point of view of Kleman, the energy consists of splay, bulk deformation, and the dislocation core energy, i.e.,

$$\begin{cases} U_1 = \iint_A \dfrac{1}{2} K_1 \left(\nabla^2 u\right)^2 \mathrm{d}x\mathrm{d}y, \\ U_2 = \iint_A \dfrac{1}{2} \rho_0 B' \left[\left(\dfrac{\partial u}{\partial x}\right)^2 + \left(\dfrac{\partial u}{\partial y}\right)^2\right]^2 \mathrm{d}x\mathrm{d}y, \\ U_3 = \dfrac{1}{2} \iint_\Omega \left(\sigma_{zx}\dfrac{\partial u}{\partial x} + \sigma_{zy}\dfrac{\partial u}{\partial y}\right) \mathrm{d}x\mathrm{d}y \\ \quad = \dfrac{1}{2} \displaystyle\int_{r_0}^{R_0} \int_0^{2\pi} r\left(\sigma_{zx}\dfrac{\partial u}{\partial x} + \sigma_{zy}\dfrac{\partial u}{\partial y}\right) \mathrm{d}r\mathrm{d}\theta, \end{cases} \tag{17}$$

$$U = U_1 + U_2 + U_3, \tag{18}$$

where A represents the integration domain — the total xy-plane, and R_0 and r_0 are the conventional notations in calculating dislocation energy.

If substituting solution (1) into energy equation (18), one can obtain the wrong results only.

According to the Landau–Ginzburg–de Gennes free energy, the first term on the right-hand side of Eq. (18) always vanishes. Substituting Eq. (8) into the first, second, and third terms, we obtain $U_1 = 0$, and

$$\begin{aligned} U_2 &= \frac{\pi}{8}\left(\frac{b}{2\pi}\right)^4 \rho_0 B' \left[\frac{1}{r_0^2} - \frac{1}{R_0^2}\right] \\ &\quad + \frac{\pi}{8}\left(\frac{b}{2\pi}\right)^4 \rho_0 B' D_1^2 \left[2 + \frac{32\pi^2}{3}\right] \ln\frac{R_0}{r_0} \\ &\quad + \frac{D_1}{240}\frac{\pi}{8}\left(\frac{b}{2\pi}\right)^4 \rho_0 B' \left[\frac{5120}{R_0 + r_0}\right. \\ &\quad \left. + 3D_1\left(75 - 160\pi^2 + 256\pi^4\right)\right]\left(R_0^2 - r_0^2\right), \\ U_3 &= \frac{b^2 K_1 D_1^2}{16\pi} \ln\frac{R_0}{r_0}. \end{aligned} \tag{19}$$

From solution (1) we cannot obtain these energy expressions. Solution (1) does not hold for smectic A liquid crystals, even if under the condition of continuum model. The invalidity is present not only in the region inside the core of dislocation, but also in the region outside the core of dislocation.

6. Meaning of present solution

Solution (8) overcomes the mistakes of well-known classical solution (1) mentioned above, from which we obtain some meaningful and useful results. For example, we evaluate the dislocation core energy of smectic A, and find that the dislocation energy is correlated to both Young's modulus and splay modulus. Another finding may be the stresses obtained from solution (8) and they are expressed as

$$\sigma_{xz}, \sigma_{yz} \sim r^{-2}, \quad r \to 0. \tag{20}$$

This presents a different singularity from that in quasicrystals[18] apart from crystals.

7. Conclusion and discussion

In this article, by taking the fundamental physical framework as the basis in common of the discussion, according to the existence and uniqueness principle of partial differential equations, we adopt the simplest, elementary, and straight forward method to demonstrate the mistakes of the well-known solution (1), which has spread for almost four decades, and to derive the correct solution. This proves that the classical solution is only the zero-order approximation of the present correct solution. The discussion may provide a solution to the long-standing puzzle in studying the screw dislocation in smectic A liquid crystals. Due to the difficulty of the problem we cannot say that in this paper all aspects of the long-standing puzzle have been solved. In addition, the stress singularity of dislocation in the phase that reveals the difference between crystals and quasicrystals may be a meaningful finding. The discussion on the core structure of dislocation is left for further study. We believe that a correct solution out of the core may be a basis

for discussing core structure. The present work focuses on the discussion about smectic A liquid crystals, which belong to one kind of the material. The problem concerning other kinds of liquid crystals, e.g. nematic liquid crystals, is very important too, and there are some studies in relevant areas, see Refs. [21]–[26], etc. The dislocations in this kind of liquid crystal need to be further discussed.

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