ISSN 0021-3640, JETP Letters, 2007, Vol. 86, No. 6, pp. 389–392. © Pleiades Publishing, Ltd., 2007.
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On the Asymptotic Nonlinearity in Smectics

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Received August 9, 2007

Isolated sources of deformation in smectics for which the problem of determining the displacement field is significantly nonlinear at arbitrarily long distances even for a small action amplitude are indicated. Nonlinear asymptotic expressions can be determined in some cases.

PACS numbers: 61.30.-v

DOI: 10.1134/S0021364007180099

Perturbation fields of the order parameter far from point or linear defects in condensed media are usually low, and linear theory can be used to find their asymptotic behavior. However, as shown in our study [1], a specific situation arises in smectics: nonlinearity significantly changes the deformation field of the edge dislocation. Although the problem is nonlinear, their analytical solution has been determined. Ishikawa and Lavrentovich [2] observed the indicated effect when investigating a defect in cholesteric liquid crystal, which is similar to the edge dislocation in the smectic. Santangelo and Kamien [3] found an elegant method for obtaining the solution [1], which allows an increase in the number of exactly solvable nonlinear problems.

In this study, we determine isolated deformation sources for which the linear approximation is sufficient and sources for which nonlinear effects in long-range asymptotic expressions are important. The asymptotic expression appears to be determined by only nonlinearity in some cases.

The energy of small deformations of the smectic is given by the expression [4]

$$\mathscr{E} = \int \frac{A}{2}\left\{\left(\partial_z u - \frac{(\partial_\alpha u)^2}{2}\right)^2 + \lambda^2(\Delta_\perp u)^2\right\} dV, \qquad (1)$$

where u is the displacement of the layers along the smectic z axis, A is the elasticity modulus, λ is the length parameter, ∂_α is the gradient in the xy layer plane, and $\Delta_\perp = \partial_\alpha^2$.

The variational equilibrium equations have the form

$$\lambda^2\Delta_\perp^2 u - \partial_z^2 u + \partial_z(\partial_\alpha u)^2 + (\partial_z u)(\Delta_\perp u) - \frac{1}{2}\partial_\alpha[(\partial_\beta u)^2\partial_\alpha u] = \frac{F(\mathbf{r})}{A}, \qquad (2)$$

where $F(\mathbf{r})$ is the density of the external forces and the multipole forces of defects.

In the linear approximation, the asymptotic expression for the displacement around a certain point defect at distances much larger than the molecular distances ($\sim a$) and at a slope of the radius vector that is not small with respect to the layers, when $z \gg a$, has the form

$$u \propto \lambda\left(\frac{z}{\lambda}\right)^\alpha f\left(\frac{\rho^2}{\lambda z}, \frac{y}{x}\right), \qquad (3)$$

where the function f is on the order of one and $\rho = \sqrt{x^2+y^2}$. For linear defects lying in the smectic plane, $u \propto \lambda(z/\lambda)^\alpha f(x^2/\lambda z)$. For linear defects parallel to the z axis, $u \propto \lambda(\rho/\lambda)^\alpha f(y/x)$. Finally, $u \propto \lambda(x/\lambda)^\alpha$ for a planar defect (wall) perpendicular to the smectic layers.

Comparison of different terms in energy (1) for these asymptotic expressions shows that the linear approximation is valid only for $\alpha < 0$. Then, similar to in electrodynamics, the field of any defect is determined from the given source of multipole forces by differentiating the linear Green's functions:

$$G = \frac{1}{2\pi A\lambda}\left(\int_{\frac{\rho}{\sqrt{\lambda|z|}}}^{\infty} \exp\left(-\frac{v^2}{4}\right)\frac{dv}{v} + \ln\frac{\rho}{\rho_0}\right) \qquad (4)$$

for the point force distribution at $\alpha = 0$,

$$G_\perp = \frac{\sqrt{|z|}}{2\sqrt{\pi\lambda}A}\left(\frac{x}{\sqrt{\lambda|z|}}\int_0^{\frac{x}{\sqrt{\lambda|z|}}} \exp\left(-\frac{v^2}{4}\right)\frac{dv}{2} + \exp\left(-\frac{x^2}{4\lambda|z|}\right)\right) \qquad (5)$$

for the force distribution on the $x = z = 0$ line at $\alpha = 1/2$, and

$$G_\parallel = \frac{1}{8\pi A\lambda^2}\rho^2\ln\frac{\rho}{\rho_0}. \qquad (6)$$

for the force distribution on the $x = y = 0$ line at $\alpha = 2$.

Note that Green's functions (4) and (5) at $z = 0$ beyond the force application points satisfy the boundary condition on the free boundary ($\sigma_{zz} = 0$). For this reason, they are also surface Green's functions.

The exponent α corresponding to each multipole order is easily calculated from the exponent of the corresponding Green's function. The asymptotic expressions in the linear approximation are exact for the following cases.

(i) $\alpha = -1$ correspond to point defects (impurities) in the bulk, which are described by the elastic contribution to the energy density $\propto \partial_z u \delta(\mathbf{r})$ (the asymptotic expressions for such inclusions was determined in [3]). When a defect has no $z \longrightarrow -z$ symmetry, it is necessary to take into account the contribution $\kappa_0^{\alpha\beta} \partial_\alpha \partial_\beta u \delta(\mathbf{r})$ from an impurity on the basis face of the smectic; the invariant has the form $\kappa^{\alpha\beta} \partial_\alpha \partial_\beta u \delta(x) \delta(y)$.

(ii) $\alpha = -1/2$ correspond to point sources of the force moment in the bulk, the invariant is $\partial_x u \delta(\mathbf{r})$, and the invariant on the surface is $\partial_x u \delta(x) \delta(y)$. Linear inclusions lying in the smectic layers, in the bulk, the invariant has the form $\partial_z u \delta(x) \delta(z)$. When the $z \longrightarrow -z$ symmetry is violated, the additional invariant $\partial_x^2 u \delta(x) \delta(z)$ appears; on the surface, the invariant has the form $\partial_x^2 u \delta(x)$.

Dislocations correspond to the boundary value $\alpha = 0$. The exponent is determined from the condition that the resulting set of the Burgers vector is independent of the contour around the dislocation core. The exponent is also equal to zero for the following cases:

(i) bulk and surface point force sources (Green's functions);

(ii) force moment distributions on lines in the smectic layers;

(iii) one-dimensional inclusion parallel to the z axis with the violated $z \longrightarrow -z$ symmetry, where the invariant is $\Delta_\perp u \delta(x) \delta(y)$;

(iv) steps on the basis face of the smectic.

For a pure screw dislocation, the situation is degenerate: the solution of the linear problem (see [4]) is also exact for the nonlinear equation.

A specific class of problems with $\alpha > 0$ consists of the following

(i) $\alpha = 1/2$. The force distribution on a line in the basal plane, in the bulk, and on the surface.

(ii) $\alpha = 1$. The force moment distribution along the line normal to the basal plane, where the invariant has the form $\partial_x^2 u \delta(x) \delta(y)$.

(iii) $\alpha = 2$. The force distribution along the line normal to the basal plane.

(iv) $\alpha = 3$. The problem of shear stresses in smectic that depend on one coordinate x (in this case, the general solution in the linear approximation reduces to a third-order polynomial).

A number of nonlinear problems for which we perform the complete analysis are discussed below.

1. First, we consider the one-dimensional case, which clarifies the essence of the asymptotic nonlinearity effect. Let the smectic be in a container with vertical walls with the coordinates $x = 0$ and $x = L$. In the simplest one-dimensional case, where the strain is a function of only the x coordinate, the equilibrium equation has the form

$$\frac{3}{2}(u')^2 u'' - \lambda^2 u'''' = 0, \tag{7}$$

where the prime means differentiation with respect to the x coordinate. The first integral is given by the expression

$$\frac{1}{2}(u')^3 - \lambda^2 u''' = -\frac{F}{A}, \tag{8}$$

where F is the tangential force with which the left wall acts on the smectic (in this case, the right wall must act with the force $-F$ in equilibrium). The second integral is

$$\frac{1}{8}(u')^4 - \frac{1}{2}\lambda^2 (u'')^2 = -\frac{F}{A}u' + C, \tag{9}$$

from which

$$\int_{u'}^{0} \frac{dt}{\sqrt{t^4 + 8Ft/A - 8C}} = \frac{x - x_0}{2\lambda}. \tag{10}$$

The integration constants are determined from the boundary conditions. The natural conditions obtained as a result of variation reduce to the two relations on each of the walls. For example, the first condition is Eq. (8) with $x = 0$ [variation with respect to $u(0)$]. The second condition is a result of variation with respect to $u'|_{x=0}$ and has the form

$$A\lambda^2 u'' = \frac{\delta\sigma}{\delta u'},$$

where σ is the energy of the smectic–wall interface. Instead of this condition, it is possible to assume that the orientation of smectic layers on the wall is fixed. Let us assume that the layers are oriented normally to the wall; in this case, $x_0 = 0$. For the case $L \longrightarrow \infty$, the homogeneous displacement is implemented far from the wall:

$$u' = -\left(\frac{2F}{A}\right)^{1/3}. \tag{11}$$

Taking into account this asymptotic expression, we determine the constant $C = -3 \times 2^{-5/3}(F/A)^{4/3}$ from the second integral given by Eq. (9). Performing integration in Eq. (10), we arrive at the expression

$$u' = \left(\frac{2F}{A}\right)^{1/3}\frac{4-3\sqrt{2}\sinh(x/\tilde{\lambda})-4\cosh(x/\tilde{\lambda})}{2+3\sqrt{2}\sinh(x/\tilde{\lambda})+4\cosh(x/\tilde{\lambda})}, \quad (12)$$

which describes the transition of the orientation of the layers in the wall region $x \sim \tilde{\lambda} = 2^{1/6}3^{-1/2}(A/|F|)^{1/3}\lambda$ from the boundary value $u' = 0$ to homogeneous displacement in the bulk (see Fig. 1). Near the wall, under the condition $x \ll \tilde{\lambda}$, solution (12) is transformed to the solution of the linear problem

$$u \approx -\mathrm{sgn}(F)\frac{3^{1/2}}{2^{4/3}}\left(\frac{F}{A}\right)^{2/3}\frac{x^2}{\lambda}+\frac{F}{6A\lambda^2}x^3.$$

These results are applicable only for a small force F, when small-angle approximation (1) is valid.

2. Further, let us consider the axially symmetric problem homogeneous along the z axis. In this case, the equilibrium equation reduces to the form

$$\left\{\lambda^2\left(\rho u''' + u'' - \frac{u'}{\rho}\right) - \frac{\rho}{2}(u')^3\right\}' = 0, \quad (13)$$

where the prime means differentiation with respect to the radius ρ. The first integral has the form

$$\lambda^2\left(\rho u''' + u'' - \frac{u'}{\rho}\right) - \frac{\rho}{2}(u')^3 = \frac{F}{2\pi A}, \quad (14)$$

where the integration constant on the right-hand side of the equation is nonzero if the defect under consideration acts on the smectic with the force F (per unit length) directed along the z symmetry axis. In this case, it is easily seen that the curvature effect can be neglected far from the defect and the asymptotic expression for the displacement is obtained from Eq. (14) in the form

$$u = -\frac{3}{2}\left(\frac{F}{\pi A}\right)^{1/3}\rho^{2/3}. \quad (15)$$

When the force F is small, there is a macroscopic region where the linear approximation is valid. Indeed, nonlinearity can be disregarded in the limit of small ρ values (but $\rho \gg \lambda$) and the solution reduces to Eq. (6). Asymptotic expressions (15) and (6) are matched at $\rho \sim \rho_0 \sim \lambda(A\lambda/|F|)^{1/2}$.

3. According to Eq. (14) with $F = 0$, the function $\psi = \rho u'/\lambda$ of the new variable $t = \ln(\gamma\rho/\lambda)$ satisfies the equation

$$2\ddot{\psi} - 4\dot{\psi} - \psi^3 = 0.$$

The second derivative can be neglected in the limit $t \longrightarrow \infty$. In this case, $\psi = \pm\sqrt{2/t}$ and the displacement field is given by the expression

$$u = \pm 2\sqrt{2}\lambda\left(\ln\frac{\gamma\rho}{\lambda}\right)^{1/2}. \quad (16)$$

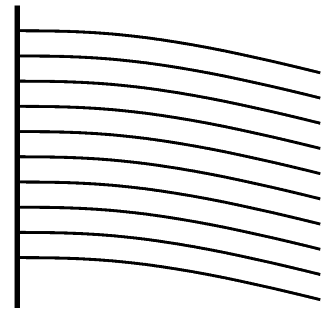

Fig. 1. Wall transition region for the case of shear deformation of a smectic.

If the parameter γ is large so that $\ln\gamma \gg 1$, solution (16) in the region $\lambda \ll \rho \ll \lambda\gamma$ has the form

$$u \approx \pm 2\sqrt{2\ln\gamma}\lambda \pm \lambda\sqrt{\frac{2}{\ln\gamma}}\ln\frac{\rho}{\lambda}. \quad (17)$$

This field is characteristic of the defect that has no $z \longrightarrow -z$ mirror symmetry when $\kappa\Delta_\perp u\delta(x)\delta(y)$ is an invariant. Defects transforming to each other under the $z \longrightarrow -z$ mirror reflection are characterized by the parameters κ differing only in sign. In the linear approximation in the amplitude κ, the following deformation field appears around such a defect:

$$u = \frac{\kappa}{8\pi A\lambda^2}\Delta_\perp\left(\rho^2\ln\frac{\rho}{\rho_0}\right) = \frac{\kappa}{2\pi A\lambda^2}\ln\frac{e\rho}{\rho_0}. \quad (18)$$

The linear asymptotic expression is transformed to the nonlinear one at $\rho \sim \gamma\lambda$. The comparison of Eqs. (17) and (18) determines the relation $\ln\gamma = 8\pi^2A^2\lambda^6\kappa^{-2}$ between the parameter γ with the microscopic characteristic κ of the defect. It is interesting that the linear approximation parameter $\rho_0 = e\gamma^{-2}\lambda$ is also reached in this case.

In the absence of the force F, the one-dimensional defect that is oriented along the z axis and has the $z \longrightarrow -z$ mirror surface (which is assumed above in Section 2) does not initiate the deformation of the smectic. In this case, the situation is the same as for defects (impurities) in a usual liquid.

4. Let us consider the edge-dislocation field [1]

$$u = 2\lambda\,\mathrm{sgn}(z)\ln\left(1 + \frac{\exp(b/(4\lambda))-1}{2\sqrt{\pi}}\int_{-\infty}^{\frac{x}{\sqrt{\lambda|z|}}}\exp\left(-\frac{t^2}{4}\right)dt\right), \quad (19)$$

where b is the Burgers vector of the dislocation (the "extra" layer is inserted at $z = 0$, $x > 0$). Note that the natural boundary conditions for the free boundary, $\sigma_{zz} = 0$, are satisfied everywhere excluding the microscopic vicinity of the dislocation core ($x = 0$). Thus, solution (19) considered, e.g., only for $z < 0$, specifies the field of a

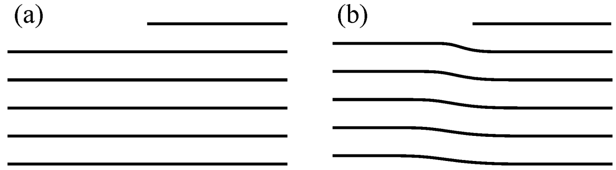

Fig. 2. Step on the smectic surface (a) without deformations and (b) with the inclusion of deformations.

certain surface linear defect. This field appears due to the action of the moment of forces applied to the surface along the defect line. Indeed, the moment of forces with which the upper part of the liquid crystal acts on the lower part through the surface $z = -h \neq 0$ is given by the expression

$$M = \int_{-\infty}^{\infty} \sigma_{zz} x dx = A\lambda(u_{+\infty} - u_{-\infty}), \qquad (20)$$

where $u_{+\infty} - u_{-\infty} - b/2$ is the asymptotic (far from the dislocation core) relative displacement of the layers.

It is clear that the finite moment of forces given by Eq. (20) is impossible in equilibrium. The situation is even worse for crystals: the integral for the moment of the forces is divergent in this case. To date, we have not seen the solution to this problem. However, it is obvious that the use of solution (19) allows the construction of the displacement field induced by the distribution of the force moment M along the line lying in the $z = 0$ plane in bulk or on the surface of the smectic. The solution can be directly used on the surface by changing the parameter b to $2M/A\lambda$. For the bulk case, it is necessary to change b to $2M/A\lambda$ and to transform the upper part of the solution ($z > 0$) as $u(x, z) \longrightarrow u(-x, z) - b/2$.

As in usual crystals [5], the elementary step on the basal plane of the smectic is characterized by the force moment equal to the product of the surface tension force and the height of the elementary step. The step height in the crystals is equal to the interplanar spacing, whereas the step height in the smectics decreases.

Note that the surface tension of the basic face of the smectic must coincide with its surface energy as in the usual liquid. Two components of the surface tension tensor exist on the other surface. The tensor component along the outcrop lines of the smectic layers coincides with the surface energy of a given orientation of the surface. The tensor component perpendicular to this line is an independent quantity as in usual crystals [5].

Since the surface energy is positive, the step height owing to deformations induced by the moment of the surface tension forces decreases and thereby reduces the moment. It is important that, in contrast to the case of usual crystals, where the displacement field decreases according to a power law with the distance from the step [5], the difference between the heights of the surface to the right and left of the step line at large distances becomes smaller than the interplanar distance (see Fig. 2), because the initial dislocation solution given by Eq. (19) in the limit $z \longrightarrow 0$ behaves as $u \longrightarrow 0$ for $x < 0$ and as $u \longrightarrow \mathrm{sgn}(z)b/2$ for $x > 0$. For this reason, the force moment must be determined self-consistently: on the one hand, $M = \sigma(b - u_{+\infty} + u_{-\infty})$ by definition and, on the other hand, $M = A\lambda(u_{+\infty} - u_{-\infty})$ according to Eq. (20). As a result, the resulting step height is expressed as

$$b - u_{+\infty} + u_{-\infty} = b\frac{A\lambda}{A\lambda + \sigma}$$

and the moment has the form $M = \sigma b A\lambda/(A\lambda + \sigma)$. Thus, the displacement field near the elementary step on the smectic surface is given by formula (19), where the quantity $b/2$ should be changed to the relative displacement $u_{+\infty} - u_{-\infty} = b\sigma/(A\lambda + \sigma)$.

The problem of deformations induced by forces localized or distributed along the lines in bulk and on the surface (nonlinear Green's functions), as well as the problem of the moment of forces distributed along the vertical line, appears to be more complex, and we have not yet found their solution.

We are grateful to E.I. Kats for stimulating discussion. V.M. is grateful to Forschungszentrum Jülich for hospitality. This study was supported by the Deutsche Forschungsgemeinschaft (grant no. MU1170/6-1).

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Translated by R. Tyapaev