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Energetics of screw dislocations in smectic A liquid crystals

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We derive the self-energy of a single screw dislocation in smectic A liquid crystals allowing for bend curvature in the bulk. For the core region two models are investigated: a nematic one including bend and twist curvature and an isotropic one including surface curvature energy. The former is energetically favourable. For both models the interaction force between two parallel screw dislocations is zero within the linear theory. Taking into account non-linearities perturbatively, an interaction potential is obtained, which is proportional to the logarithm of the distance of the screw dislocations.

1. Introduction and results

The study of screw dislocation defects in smectic systems is important, not only because they are numerous in a real sample and influence the macroscopic behaviour of smectics, but also since they serve as a prototype of defects for deriving macroscopic laws of motion for them.

In the present paper we treat the statics (energetics) of one or more screw dislocations, amending earlier treatments of that problem [1–6]. First we allow for bend curvature in the bulk. Although generally present in distorted smectics, bend is usually neglected against elasticity, if the distortions are small. Near the screw dislocation defect, this omission is, however, unjustified. The total bend curvature energy in the bulk is comparable to the total elastic energy due to compression or dilation of the smectic layers. Both energies are 'non-linear', i.e. they would vanish in a linearized theory. In a model, where the core of the defect is nematic (i.e. no smectic layers inside the core, but a director field), the inside director field is found to be free of singularities, continuous at the core boundary and carrying twist and bend distortions. The appropriate total inside twist and bend energies are again comparable to the outside curvature and elastic energies (§ 3). In Appendix A it is shown that the inclusion of bend and (inside the core) twist does not change the results for the magnitude of the core radius ϱ_c [4]. In § 3 a model with an isotropic core is studied. The lack of a director field inside the core relieves the system of the inside curvature energy at the expense of a curvature surface energy. The importance of this surface energy in the presence of defects has been stressed previously [3]. Comparing the energies of the two different models, we come to the conclusion that a nematic core is the most favourable. The reason is mainly that, at a temperature, where the bulk of the smectic state is in equilibrium, usually the thermodynamic energy of an isotropic core is higher than that of a nematic core. For screw dislocations with large Burgers vectors the isotropic core becomes even more unfavourable, since the thermodynamic energy increases (with the square of the Burgers vector), while the curvature energies are independent of it. The surface curvature elastic constant was thereby assumed to be smaller, but of comparable magnitude than the Frank constants (Appendix B).

In § 4 the interaction of two screw dislocations at a distance L is discussed. Within the linearized theory, both models, one with bend and splay inside the core and the other with the surface curvature at the core radius, show no interaction energy at all—a result already well-known with respect to bulk properties [1]. An attempt is made to derive the interaction due to the non-linearities in the elastic and curvature energies by means of a perturbation expansion. In the first step interaction forces are obtained by using approximate solutions of the non-linear elastic equilibrium problem in the usual Peach–Koehler formula as well as by using the linear solutions in a non-linear Peach–Koehler formula (with non-linear stresses). In the leading order of ϱ_c/L this interaction force falls off proportional to L^{-1} giving rise to a logarithmic interaction potential. This greatly resembles the interaction of straight, parallel electrical currents. Of course, this analogy with (two-dimensional) magnetostatics does not come as a surprise [1]. An array of parallel screw dislocations thus behaves (at least in the approximation used) similar to flux lines or tubes in a type II superconductor above the first critical magnetic field. For a dilute system of screw dislocations the elastic constant of an equilibrium array seems to be very small and a liquid-like behaviour more probable. The motion of the screw dislocations is then overdamped [5].

2. Bulk bend energy of a screw dislocation

In the conventional description of smectic A liquid crystals and their defects the gradient free energy contains layer elasticity and splay curvature of the director. Bend curvature is usually neglected in smectics, since for small gradients it is smaller by two orders of gradients than the leading elastic energy contribution. For large gradients, however, the bend term can become comparable to the other gradient energy terms and is no longer negligible. This is precisely what happens near the dislocation defect (or its core). In the following we will investigate the influence of the bend term to the energetics of a screw dislocation.

The starting point is, therefore, the following gradient energy:

$$\varepsilon_> = \frac{B}{2}(1 - |\hat{e}_z - \nabla u|)^2 + \frac{K_1}{2}(\operatorname{div} \hat{n})^2 + \frac{K_3}{2}(\hat{n} \times \operatorname{curl} \hat{n})^2, \tag{2.1}$$

where u is the displacement of the layer structure along the layer normal $\hat{n} = (\hat{e}_z - \nabla u)|\hat{e}_z - \nabla u|^{-1}$.

In the conventional description (i.e. without the bend term) the equilibrium solution, $\delta\varepsilon/\delta u = 0$, appropriate to the topology of a screw defect of strength m, is (in cylindrical coordinates) [1]

$$u = \hbar\theta, \tag{2.2a}$$

$$\hat{n} = \left(\hat{e}_z - \frac{\hbar}{\varrho}\hat{e}_\theta\right)\left(1 + \frac{\hbar^2}{\varrho^2}\right)^{-1/2}, \tag{2.2b}$$

where the pitch of the screw, $\hbar$, is related to the layer thickness d by $\hbar = md_0/2\pi$ ($m = \pm 1, \pm 2, \ldots$). This solution (equations (2.2)) is valid only outside the core region ($\varrho \geqslant \varrho_c$), while inside the core—in the simplest model for the core, which we wish to adopt here—the smectic order parameter is zero and there are no layers and thus, u is not defined [4].

Taking into account the bend term, it is easily recognized that the solution (equations (2.2)) is no longer an exact equilibrium solution. It is, however, an

equilibrium solution if $\varrho \gg \hbar$. We will in the following still use equations (2.2) in the whole outside region assuming that it deviates only slightly from the exact solution for $\varrho \gtrsim \varrho_c$. This procedure is justified by the observation that for calculating energies the use of approximate formulas, which are exact only for $\varrho \gg \hbar$, nevertheless lead to energy expressions, which are quite close to the exact ones, even if $\varrho_c = \hbar$ (cf. the discussion in [4] after equations (13)). For the gradient energy we then find

$$E^{>} = \pi B\,[\hbar^2 \ln \tfrac{1}{2}(1 + \hbar^2 \varrho_c^{-2}]^{1/2}) + \varrho_c^2([1 + \hbar^2 \varrho_c^{-2}]^{1/2} - 1) - \tfrac{1}{2}\hbar] + \frac{\pi}{2} K_3[\ln(1 + \hbar^2 \varrho_c^{-2}) - \hbar^2(\hbar^2 + \varrho_c^2)^{-1}], \tag{2.3a}$$

$$\approx \frac{\pi}{8} B\hbar^4 \varrho_c^{-2} + \frac{\pi}{4} K_3 \hbar^4 \varrho_c^{-4} \quad \text{for} \quad \varrho_c \gg \hbar. \tag{2.3b}$$

Since K_3 and $B\hbar^2$ are of the same order of magnitude, so are the bend and the elastic energy and the omission of the former is not justified.

3. Core energy of a screw dislocation

3.1. *Nematic case*

Up to this point we have only considered the region outside the core. Inside the core region there are no layers and no elastic energy due to their displacement. There is, however, still the director field and its distortions give rise to curvature energy. Of course, the specific form $\hat{n}$ in the outside region, equation (2.2*b*), cannot be transferred to the inside region. In that case $\hat{n}$ would be ill-defined for $\varrho = 0$ and the associated bend energy would diverge (logarithmically). There is also no topological need for such a defect in the $\hat{n}$ field and a non-singular $\hat{n}$ field can be expected. Indeed, equation (2.2*b*) was obtained under the restriction that the director is identical with the layer normal in smectic A. However, inside the core this condition on $\hat{n}$ is lifted and the equilibrium structure of the $\hat{n}$ field is determined by minimizing the Frank curvature energy (now including twist) under the conditions, that $\hat{n}$ is non-singular and fits to the outside $\hat{n}$ field at the core boundary $\varrho = \varrho_c$. In the following we will adopt $\varrho_c = \hbar$; although this result was derived in [4] neglecting bend (and twist), in Appendix A it is shown that it remains true in the present case. Thus, the boundary condition for the inside $\hat{n}$ field is

$$\hat{n}(\varrho = \varrho_c) = 2^{-1/2}(\hat{e}_z - \hat{e}_\theta). \tag{3.1}$$

From the form, equation (2.2*b*), for the outside field and the boundary condition, equation (3.1), it is very tempting to try for the inside field

$$\hat{n}^{<} = \left(\hat{e}_z - \frac{\varrho}{\hbar}\hat{e}_\theta\right)\left(1 + \frac{\varrho^2}{\hbar^2}\right)^{-1/2}. \tag{3.2}$$

It is non-singular, fits the boundary condition (2.10) and has the additional good features that it contains no splay ($\operatorname{div}\hat{n} = 0$ like the outside field) and that bend ($\hat{n} \times \operatorname{curl}\hat{n}$) is also continuous at the core boundary. Only twist ($\hat{n}\operatorname{curl}\hat{n} \neq 0$) makes a finite jump at $\varrho = \varrho_c$, since it is zero outside the core†. However, it is not an exact

† If the curvature energy includes second order gradients of $\hat{n}$, then the first order gradients would have to be continuous at the boundary, and this jump of the twist would be smeared out.

equilibrium solution with $\delta\varepsilon_< / \delta n_i = 0$. Only for $\varrho \ll \hbar$ equation (3.2) minimizes $\varepsilon_<$. This is quite analogous to the outside solution, which is only exact for $\varrho \gg \hbar$. Again we expect that the use of equation (3.2) instead of the correct solution changes the calculated energies only by numerical factors of order unity. For the twist and bend energy inside the core one finds ($\varrho_c = \hbar$)

$$E_2^< = \pi K_2, \tag{3.3a}$$

$$E_3^< = \frac{\pi}{2} K_3(\ln 2 - \tfrac{1}{2}) \tag{3.3b}$$

the latter is identical to the bend curvature energy outside the core (equation (2.3 *a*)) for $\varrho_c = \hbar$. In addition to the curvature energy the core also contains a thermodynamic energy, since it is in a nematic state, which has a higher free energy than the smectic state. Otherwise, at the given temperature, the smectic state would not occur as the ground state in unconstrained bulk conditions. This energy can be written as

$$E_{\text{core}} = \pi \varrho_c^2 \frac{a^2}{4c}, \tag{3.4}$$

where a and c are the two first coefficients of a Ginzburg–Landau expansion for the smectic order parameter. This form of E_{core} is suitable, even if there is no bulk smectic A–nematic phase transition.

3.2. *Isotropic core*

In order to avoid the singularity of the layer structure at the centre of the screw dislocation (and the resulting divergence of the elastic energy) a nematic core was employed in the preceding section. However, instead of assuming a nematic core one can also think of an isotropic core, i.e. not only the smectic order but also the nematic order parameter is zero inside the core and neither layers nor a director is present. In such a model, there is no elastic and no curvature energy attached to the core region. The thermodynamic energy of such a core contains (in addition to equation (3.4)) the Ginzburg–Landau free energy of the nematic order parameter

$$E_{\text{core}} = \pi \varrho_c^2 \left(\frac{a^2}{4c} + \frac{\bar{a}^2}{4\bar{c}} \right), \tag{3.5}$$

where $\bar{a}$, $\bar{c}$ are the first two Ginzburg–Landau coefficients with respect to the nematic order parameter.

This core model introduces a free surface for the nematic order. It is well known, that with such surfaces, a surface curvature energy density [7]

$$\varepsilon_s = K_s \operatorname{div}(\hat{n} \operatorname{div} \hat{n} - (\hat{n} \cdot \nabla)\hat{n}) \tag{3.6}$$

is attached. In Appendix B it is shown, that K_s has to be negative and $|K_s|$ to be smaller than both K_1 and K_2. Since there is no general reason, however, for K_s to be small, we will assume in the following, that $|K_s| \lesssim K_1$ or K_2. For the director field, equation (2.11 *a*), the surface energy (per length) at $\varrho = \varrho_c$ is

$$E_s = 2\pi |K_s| \frac{\hbar^2}{\hbar^2 + \varrho_c^2}. \tag{3.7}$$

For $\varrho_c \gg \hbar$ equation (3.7) coincides with the appropriate result of [7], which was obtained by using a gradient expansion of ε_s valid only for $\varrho_c \gg \hbar$. The core radius ϱ_c of this model is again of the order $\hbar$ (Appendix A).

The question is then, which one of the two models of screw dislocations (model I with nematic core, and model II with isotropic core) has the lower free energy and is, therefore, the real one? Since the bulk energies are identical in both cases, they drop out of this comparison. The difference comes from the curvature core energies in I, equation (3.3), and the surface energy, equation (3.7), and the excess thermodynamic energy of II, equation (3.5), compared to I, equation (3.4)†. For $\varrho_c = \hbar$, model I has lower energy if

$$\pi K_2 + \frac{\pi}{2} K_3 (\ln 2 - \tfrac{1}{2}) < \pi |K_s| + \pi \varrho_c^2 \frac{\bar{a}^2}{4\bar{c}}. \tag{3.8}$$

To decide this clause, it is necessary to compare K_3 with $\bar{a}^2/4\bar{c}$. The latter is the free energy density of the isotropic state minus that of the nematic state. If the curvature energy of distortions of the director (with wavenumber q), say $q^2 K_3$, were of comparable magnitude as $\bar{a}^2/4\bar{c}$, these distortions would destroy the nematic state. This does, however, not happen as long as the distortions are on a macroscopic length scale. Only on a molecular scale, $q = q_0 = 2\pi/d_0$, can we expect

$$q_0^2 K_3 \approx \frac{\bar{a}^2}{4\bar{c}}. \tag{3.9}$$

Using this estimate and $|K_s| \lesssim K_2$, the inequality (3.8) reduces to

$$\tfrac{1}{2} \ln (2 - \tfrac{1}{2}) < m^2, \tag{3.10}$$

which seems to be fulfilled for screw dislocations of any strength, but certainly for those with large m. The latter fact can easily be understood. Since the core radius increases with m, the thermodynamic energy, which is proportional to the area, also increases. For the curvature energies, however, this geometrical increase is compensated by the decrease of the energy density, which occurs because the same amount of bend or twist (fixed by the boundary conditions) can then be distributed on a larger length scale. Thus, model II becomes more unfavourable, if m increases. Although equation (3.10) is true even for $m = 1$, one should keep in mind, that rather crude estimates were necessary to arrive at this result; so it is very likely but not absolutely sure, that even for $m = 1$ model I is the energetically favourite model.

4. Interaction of screw dislocations

4.1. *Linear*

We will discuss the interaction energy of two separated screw dislocations first within the linearized theory, i.e. when the Euler–Lagrange equations, which determine the displacement field, are linear. We can then employ the superposition principle to find a solution. For two screw dislocations, one of strength $\hbar_1$ along the z axis and one of strength $\hbar_2$ at $x = L$, $y = 0$, the displacement is

$$u = \hbar_1 \tan^{-1} \frac{y}{x} + \hbar_2 \tan^{-1} \frac{y}{x - L} \equiv u_1 + u_2, \tag{4.1}$$

† There is no surface (or interface) energy in model I, since for $\varrho = \hbar$ the inside $\hat{n}$-field (3.2) and the outside field (2.2) give both the same value for $(\hat{n} \cdot \nabla)\hat{n}$.

with the appropriate $\hat{n}$ field in linear order

$$\hat{n} = \hat{e}_z - \frac{\hbar_1}{\varrho}\hat{e}_\theta - \frac{\hbar_2}{\varrho_L^2}(\varrho\hat{e}_\theta - L\hat{e}_y), \tag{4.2}$$

where $\varrho_L^2 = \varrho^2 - 2\varrho L\cos\Theta + L^2$. Equation (4.1) and (4.2) are valid only in the bulk, i.e. outside the cores of both the dislocations. It is easy to realize, that solutions (4.1) and (4.2) do not give rise to any energy (quadratic in $\hbar_1$ or $\hbar_2$). The elastic energy and the bend energy are zero in a linearized theory anyway and splay does not occur, since $\Delta_\perp u = 0$ or $\operatorname{div}\hat{n} = 0$ as in the case of a single screw dislocation. This lack of an (interaction) energy reflects the well-known fact that there is no force between screw dislocations within the linearized theory [1] (disregarding core effects). We will now show that this negative result holds even if core effects are included. We will first treat model I (nematic core).

Inside the core the $\hat{n}$ field is found by minimizing the Frank free energy, which requires in linear order

$$\nabla\operatorname{div}\hat{n} = 0, \quad \Delta\hat{n} = 0, \quad \nabla_z^2\hat{n} = 0. \tag{4.3}$$

An exact solution of equation (4.3), which contains no singularities and which fits the boundary conditions at $\varrho = \varrho_c$ set by equation (4.2) reads

$$\hat{n}^< = \hat{e}_z - \frac{\hbar_1}{\varrho_c^2}\varrho\hat{e}_\theta - \hbar_2\frac{\varrho\hat{e}_\theta - L\hat{e}_y}{\varrho^2 - 2\varrho L\cos\theta + L^2}. \tag{4.4}$$

Equation (4.4) constitutes the $\hat{n}$ field inside the core of the first screw dislocation ($\hbar_1$, along the z axis) under the influence of the second screw dislocation ($\hbar_2$, at the distance L). This field is splay-free ($\operatorname{div}\hat{n} = 0$) and, in linear order, also bend-free ($\hat{n}^< \times \operatorname{curl}\hat{n}^< = 0$) (like the outside field) but shows twist ($\hat{n}^< \cdot \operatorname{curl}\hat{n}^< \neq 0$). However, the twist curvature energy density is not influenced by the second screw dislocation and reads

$$\varepsilon_2 = \tfrac{1}{2}K_2(\hat{n}^< \cdot \operatorname{curl}\hat{n}^<)^2 = 2K_2\frac{\hbar_1^2}{\varrho_c^4}, \tag{4.5}$$

which is the result for one single crew dislocation†. There is no interaction energy and, thus, no interaction force related to the core structure. Hence, in linear approximation, screw dislocations with nematic core do not interact. The same is true for model II dislocations. The surface energy, equation (3.6), at the surface $\varrho = \varrho_c$ obtained by using the displacement field, equation (4.1), contains only a vanishing interaction part $\sim b_1 b_2$ (apart from contributions $\sim b_1^2$, $\sim b_2^2$ which do not vanish) and does not lead to an interaction force. This result coincides with a recent result in [6] (where a Peach–Koehler formula is used), if corrected for an algebraic error. Hence, for the model II screw dislocation there is no interaction within the linearized theory.

4.2. *Non-linear*

There is, of course, an interaction between screw dislocations if the linearization is avoided. To derive that energy, one has to know, however, the exact displacement field (and $\hat{n}$ field inside the core), which minimizes equation (2.1) under the topological

† Equation (4.5) leads to a total twist curvature energy, which is off by a factor of 2 compared to equation (3.3 *a*), because of the linearization employed in § 3.1.

constraints of two screw dislocations. Clearly, equation (4.1) is not such a solution, and until now, no analytic solution has been found. Nevertheless, it is possible to obtain a glimpse of the interaction by using a perturbation expansion. With an ansatz, $u = u_1 + u_2 + u_W$, where u_1 and u_2 are the linear solutions, equation (4.1), and splitting up the Euler–Lagrange equation appropriate to equation (2.1) into linear and non-linear parts, one obtains in a first order perturbation an equation for u_W of the form $\mathfrak{L}_{lin} u_W + \mathfrak{L}_{non\text{-}lin}(u_1 + u_2) = 0$. A solution of this equation for $L \gg \varrho$ is (only Δu_W is needed in the following)

$$\Delta u_W = \frac{\hbar_1^2 \hbar_2}{K_1 L} (B\varrho^{-1} \ln \varrho + K_3 \varrho^{-3}) \sin \theta \tag{4.6}$$

This u_W constitutes the perturbation of the simply superimposed solution $u_1 + u_2$ due to non-linearities in the vicinity of the first screw line ($L \gg \varrho \gtrsim \varrho_{c_1}$). Such a perturbation expansion cannot be expected to converge for $L \approx \varrho_c$; but for $L \gg \varrho_c$, where the linearized theory is not too bad, one can hope that it is an asymptotic expansion, whose first terms approximate the exact result. Using Equation (4.6) in the usual Peach-Koehler formula (with linear stresses) [1] one obtains in leading order of ϱ_c/L

$$F_x^{(1)} = (B\varrho_{c_1}^2 + K_3) \frac{\hbar_1^3 \hbar_2}{\varrho_{c_1}^4} \frac{1}{L} + (\text{sub } 1 \Leftrightarrow \text{sub } 2) \tag{4.7}$$

the force per unit length on the first screw dislocation due to the presence of the second one at the distance L apart ($\varrho_{c_i} \approx b_i$).

There is a second contribution to the interaction force in first order. Using the linear solution, equation (4.1), in a non-linear Peach–Koehler formula, i.e. one with non-linear stresses (cf. equation (12) of [5]) one finds (in the lowest order of ϱ_c/L) the result, equation (4.7), once again. The core energies do not contribute to the interaction force in order L^{-1}. The forces, equation (4.7), can be expressed by an interaction potential

$$U = 2\alpha \ln L, \tag{4.8}$$

with $\alpha = B\hbar_1 \hbar_2 + K_3(\hbar_1/\hbar_2 + \hbar_2/\hbar_1)$ for $\varrho_{c1} = |\hbar_1|$, $\varrho_{c2} = |\hbar_2|$. This result reminds use of two-dimensional electrodynamics, and indeed the analogy is closest with magnetostatics in the presence of constant line currents. The current strength corresponds to the dislocation strength, the magnetic field to ∇u and equation (4.7) to Ampère's law (at least the B part of it). Of course, this analogy breaks down in the next step of perturbation expansion.

The interaction, equation (4.8), is long-ranged, which clearly shows that there is no characteristic length at which the linearization procedure is a good one (i.e. at which the interaction vanishes). The result, equation (4.8), is valid for $L \gg \varrho_c$ only, and for $L \gtrsim \varrho_c$ higher order terms (e.g. ϱ_c/L etc.) come into play. These higher order terms can, at least in principle, destroy the monotony of the interaction potential. In that case, there can be a potential wall for screw dislocation of opposite handedness, preventing their annihilation, or there can be a potential minimum for screw dislocation with equal handedness, giving rise to bound pairs. Such phenomena can be provided by terms like $b_1^2 b_z^2 L^{-2}$ (in the force, equation (4.7)), which do not change sign with the handedness of the screw dislocations. However, for $L \gg \varrho_c$ such a behaviour is ruled out by equation (4.8). If the screw dislocations are very near to each other ($L \sim 2\varrho_c$), the whole perturbation scheme is likely to break down and the really

non-linear nature of the interaction shows up. Since the distortions due to the different screw dislocations are no longer additive, the interaction does depend on the number and the position of *all* screw dislocation. Hence, the interaction forces become non-local and n body forces. This is however beyond the scope of the present investigation.

For a dilute system of screw dislocations ($L \gg \varrho_c$) small displacements Δ from a given equilibrium position give rise to restoring forces of the order of $(\partial^2 U/\partial L^2)\Delta$. The elastic constant of such an equilibrium configuration is, therefore, $\propto L^{-2}$, which is much smaller than the elastic constant of the smectic layers themselves. Probably, thermal fluctuations destroy such a weak 'lattice' of screw dislocations leaving them in a liquid state. For more condensed systems (L smaller) this may be completely different. Moving as 'liquid' particles, the screw dislocations experience inertial forces (with an inertial mass somewhat larger than their physical mass [5]), friction forces proportional to their velocity [5] and the interaction forces. Since friction is large, strongly overdamped motions can be expected.

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Appendix A
Core radius

(*a*) *Nematic core*

In [4] the core radius was determined by minimizing the sum of the outside and inside energies of a screw dislocation without bend and twist. In this Appendix we will show that the same procedure with bend and twist included does not change the result $\varrho_c \approx \hbar$.

The bend energy for the outside region and bend and splay for the inside region (equation (3.3) without putting $\varrho_c = \hbar$) are together the total curvature energy of the screw dislocation

$$E_{\text{curv}} = \pi K_3 \left(\ln \left(1 + \frac{\hbar^2}{\varrho_c^2} \right) - \frac{\hbar^2}{\hbar^2 + \varrho_c^2} \right) + 2\pi K_2 \frac{\hbar^2}{\hbar^2 + \varrho_c^2} . \tag{A 1}$$

For $\hbar \approx \varrho_c$, which is the expected result, and for $K_2 \approx K_3/4$, $Bb^2 \approx K_3$ the total curvature energy is approximately equal to the elastic energy E_{el}. Instead of minimizing the sum $E_{\text{el}} + E_{\text{core}}$ as in [4], we now have to minimize $2E_{\text{el}} + E_{\text{core}}$. The core radius obtained, is by an (irrelevant) factor of $2^{1/4}$ larger than the old one, which shows, that the curvature energies do not change the estimate for the core radius.

(*b*) *Isotropic core*

In this case the additional energies not considered in [4] are the surface energy, equation (3.7), the bend energy in the outside region and the excess thermodynamic energy for the core being isotropic rather than nematic (cf. equation (3.5) $\Delta E_{\text{core}} = \pi \varrho_c^2 \bar{a}^2/4\bar{c}$. Minimizing the sum of these three new energy contributions alone leads to $\varrho_c \approx \hbar$, which shows that these energies cannot change the estimate for ϱ_c. For this, it is assumed that the actual temperature is far from the bulk phase transition temperature, so that $\bar{a}^2/4\bar{c} \approx K_3 \hbar^{-2}$.

Appendix B

Surface free energy

The Frank free energy density for director flutuations including the surface term [7] can be written in the following equivalent forms

$$\varepsilon = \frac{K_1}{2}(\operatorname{div}\hat{n})^2 + \frac{K_2}{2}(\hat{n}\cdot\operatorname{curl}\hat{n})^2 + \frac{K_3}{2}(\hat{n}\times\operatorname{curl}\hat{n})^2$$

$$+ \mathbf{K}_s[(\operatorname{div}\hat{n})^2 - (\nabla\hat{n}):(\widetilde{\nabla\hat{n}})], \tag{B 1}$$

$$= (\tfrac{1}{2}K_1 + K_s)(\nabla_i n_i)(\nabla_j n_j) + \tfrac{1}{2}K_2(\nabla_i n_j)(\nabla_i n_j)$$

$$-(\tfrac{1}{2}K_2 + K_s)(\nabla_i n_j)(\nabla_j n_i) + \tfrac{1}{2}(K_3 - K_2)(n_i\nabla_j n_k)(n_j\nabla_j n_k). \tag{B 2}$$

Thermodynamic (i.e. static) stability requires that ε is a non-negative quadratic form of small deviations from the true equilibrium solution $\hat{n}^0 = \text{const}$. For an infinite system equation (B 1) immediately shows, that $K_1 \geqslant 0$, $K_2 \geqslant 0$, $K_3 \geqslant 0$ are the well-known necessary and sufficient stability conditions. In a finite system the surface term does not drop out. In the special case that the fluctuations of $\hat{n}$, δn, can be written as $\delta\mathbf{n} = -\nabla_\perp u$ ($\nabla_\perp$ is the gradient perpendicular to $\hat{n}^0 \equiv \hat{e}_z$) which is the relevant case for slightly distorted smectics), equations (B 1) and (B 2) reduce to

$$\varepsilon = \frac{K_1}{2}\left[\left(\frac{\partial^2 u}{\partial x^2}\right)^2 + \left(\frac{\partial^2 u}{\partial y^2}\right)^2\right] + (K_1 + 2K_s)\frac{\partial^2 u}{\partial x^2}\frac{\partial^2 u}{\partial y^2} - 2K_s\left(\frac{\partial^2 u}{\partial x\partial y}\right)^2. \tag{B 3}$$

This is a non-negative quadratic form, if (in addition to $K_1 \geqslant 0$)

$$K_s \leqslant 0, \quad |K_s| \leqslant K_1. \tag{B 4}$$

In the general case, $\hat{n} = (\delta n_x, \delta n_y, 1 - (1/2)[\delta n_x^2 + \delta n_y^2])$, the part of ε, which is bilinear in gradients of δn_x and δn_y, turns out to be non-negative, if (in addition to the stability conditions above) there is also

$$|K_s| \leqslant K_2. \tag{B 5}$$

For thermotropic, rod-like, low molecular weight molecules, equation (B 5) is usually the stronger condition than $|K_s| \leqslant K_1$.

In addition to the surface term $K_s\operatorname{div}[\hat{n}\operatorname{div}\hat{n} - (\hat{n}\cdot\nabla)\hat{n}]$ used in equation (B 1), one could think of another surface term [7] $K_{s2}\operatorname{div}[\hat{n}\operatorname{div}\hat{n} + (\hat{n}\cdot\nabla)\hat{n}]$. Although the latter does not change the equilibrium condition, it leads to a first order term $2K_{s2}n_i\nabla_i\nabla_j n_j$ in the energy density which is not compatible with thermodynamic stability. Hence, $K_{s2} \equiv 0$. An illustrative example for this feature is a fluctuation of the form $\delta n = \alpha x z\hat{e}_x$ about the equilibrium solution $\hat{n}^0 = \hat{e}_z$. The free energy would then be $K_{s2}\alpha + \bar{K}\alpha^2$, which is not positive semi-definite, except for $K_{s2} \equiv 0$.

In [7] the surface curvature constant K_s was related to K_1 and K_2 via a simplified molecular picture. In our notation this relation reads

$$-K_s = \tfrac{1}{2}(K_1 - K_2), \tag{B 6}$$

which is consistent with the stability requirements, if $K_1 < 3K_2$. For the usual smectic systems this inequality seems to be fulfilled and the underlying molecular picture to be appropriate. Since typically $K_1 \approx 2K_2$, equation (B 6) predicts $-K_s \approx K_2/2 \approx K_1/4$ which shows that although $|K_s|$ has to be smaller than K_1 or K_2, it is still of comparable magnitude.

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