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Coarse-graining analysis of the Berreman anchoring

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By means of a coarse-graining technique, we derive the effective anchoring energy of a nematic liquid crystal in contact with a macroscopically corrugated surface imposing a weak degenerate planar anchoring. For coarse-grained nematic director's profiles that vary only in the direction perpendicular to the average surface's plane, our results generalize those already known by including the anisotropy of the elastic constants. In the general case, on the contrary, we show that extra surface gradient terms appear that generally are not negligible. [S1063-651X(99)14908-0]

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The anchoring properties of nematic liquid crystals in contact with solid substrates generally depend on the details of the surface interactions [1]. This is the case, e.g., of the zenithal anchoring on a flat amorphous surface. Conversely, the azimuthal anchoring on a grooved amorphous substrate can be explained by purely elastic effects [1,2]. In the past, the effective azimuthal anchoring energy of a sinusoidally modulated amorphous surface was derived by computing the elastic energy per unit surface stored in a semi-infinite system, the nematic director of which is forced to lie in the plane orthogonal to the grooves' direction [1–3]. The cases of infinite [1,2] and finite [3] zenithal anchoring were considered, in the approximation of equal elastic constants. No analysis was carried out to establish to what extent such a geometric anchoring is *equivalent* to a true homogeneous weak anchoring. This point is particularly interesting since, recently, using holographic techniques, controlled undulated surfaces were realized, making possible accurate comparisons between theory and experiment [4].

In this Brief Report, by means of a coarse-graining technique, we derive exact expressions for the effective anchoring of a nematic liquid crystal in contact with a sinusoidally modulated surface imposing a weak degenerate planar anchoring. Our analysis holds for small macroscopic undulations around a planar average surface, and small deviations of the nematic director from the effective easy axis. For nematic director's profiles that vary only in the direction perpendicular to the average surface's plane, we obtain a generalization of the already known results to the case of unequal elastic constants. For general distortions, we show that surface gradient terms must be generally taken into account.

Let us consider a nematic liquid crystal in contact with an undulated surface, whose height $z=A\cos(q_0 y)$ weakly departs from the (x,y) plane ($\epsilon\equiv q_0 A\ll 1$). We suppose that the nematic director $\mathbf{n}$ is subject to a degenerate planar anchoring on the surface, with a finite anchoring strength W. For small deviations of the nematic director from the plane of the surface, we write the anchoring energy in the Rapini-Papoular form [5]

$$V=\int d\mathbf{r}_\perp \frac{1}{2} W(\mathbf{n}\cdot\boldsymbol{\nu})^2, \tag{1}$$

where $\boldsymbol{\nu}$ is the unit vector normal to the undulating surface and $\mathbf{r}_\perp$ is a generic point of the (x,y) plane. Expressing the nematic director in terms of the zenithal angle θ with respect to the (x,y) plane and of the azimuthal angle ϕ with respect to the grooves' direction x, $\mathbf{n}=(\cos\theta\cos\phi,\cos\theta\sin\phi,\sin\theta)$ (see Fig. 1), and keeping in Eq. (1) only terms up to second order in θ and ϕ, and to second order in ϵ, we arrive at the following anchoring energy

$$V=\int d\mathbf{r}_\perp \frac{1}{2} W\{\theta^2[1-\epsilon^2\sin^2(q_0 y)]+\phi^2\epsilon^2\sin^2(q_0 y) +2\theta\phi\epsilon\sin(q_0 y)\}. \tag{2}$$

This expression holds for small deviations of the surface director from the grooves' direction and for small inclinations ϵ of the undulating surface.

In Fourier space, the total free-energy F of the system, which is the sum of the anchoring energy (2) and of the bulk Frank elastic free-energy [6]

$$F_{\mathrm{e}}=\frac{1}{2}\int d\mathbf{r}[K_1(\nabla\cdot\mathbf{n})^2+K_2(\mathbf{n}\cdot\nabla\times\mathbf{n})^2+K_3(\mathbf{n}\times\nabla\times\mathbf{n})^2], \tag{3}$$

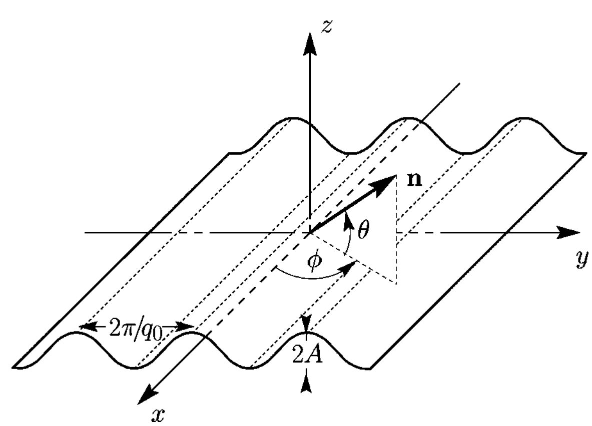

FIG. 1. Geometry of the corrugated surface.

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can be written as

$$F=\frac{1}{2}\int\frac{d\mathbf{k}\,d\mathbf{q}}{(2\pi)^6}\boldsymbol{\psi}^{\rm t}(\mathbf{k})\mathbf{G}^{-1}(-\mathbf{k},-\mathbf{q})\boldsymbol{\psi}(\mathbf{q}), \tag{4}$$

with

$$\boldsymbol{\psi}(\mathbf{k})=\int d\mathbf{r}\begin{pmatrix}\theta(\mathbf{r})\\ \phi(\mathbf{r})\end{pmatrix}e^{-i\mathbf{k}\cdot\mathbf{r}}, \tag{5}$$

and

$$\mathbf{G}^{-1}(\mathbf{k},\mathbf{q})=(2\pi)^3\mathbf{A}(\mathbf{k})\delta(\mathbf{k}+\mathbf{q})+2(2\pi)^2\sum_{n=-2}^{2}\mathbf{W}_n\delta(\mathbf{k}_\perp+\mathbf{q}_\perp+n\mathbf{q}_0). \tag{6}$$

Here $\delta(\mathbf{k})$ is the three-dimensional Dirac delta-function; $\delta(\mathbf{k}_\perp)$ is the two-dimensional Dirac delta-function in the (x,y) plane; $\mathbf{q}_0=(0,q_0,0)$ is the wave vector of the undulating surface; the matrix

$$\mathbf{A}(\mathbf{k})=\begin{pmatrix}K_3k_x^2+K_2k_y^2+K_1k_z^2 & (K_1-K_2)k_yk_z\\ (K_1-K_2)k_yk_z & K_3k_x^2+K_1k_y^2+K_2k_z^2\end{pmatrix}, \tag{7}$$

corresponds to the elastic term (3) developed to second order in θ and ϕ; and, finally, the matrices

$$\mathbf{W}_0=\begin{pmatrix}W\left(1-\frac{\epsilon^2}{2}\right) & 0\\ 0 & \frac{W\epsilon^2}{2}\end{pmatrix}, \tag{8}$$

$$\mathbf{W}_{-1}=-\mathbf{W}_1=\begin{pmatrix}0 & \frac{iW\epsilon}{2}\\ \frac{iW\epsilon}{2} & 0\end{pmatrix}, \tag{9}$$

$$\mathbf{W}_{-2}=\mathbf{W}_2=\begin{pmatrix}\frac{W\epsilon^2}{4} & 0\\ 0 & -\frac{W\epsilon^2}{4}\end{pmatrix}, \tag{10}$$

correspond to the surface term (2). For the Fourier transform of the profile to be precisely defined, we actually consider a sample consisting of two identical semi-infinite cells extending in the $z>0$ and $z<0$ half-spaces, and bounded by two identical surfaces located at $z=0^+$ and $z=0^-$, respectively: the factor of 2 in front of the summation in the right-hand side of Eq. (6) takes into account this doubling of the system [7]. Note that the correlation function

$$\mathbf{G}(\mathbf{k},\mathbf{q})=\beta\langle\boldsymbol{\psi}(\mathbf{k})\boldsymbol{\psi}^{\rm t}(\mathbf{q})\rangle, \tag{11}$$

where $\langle\cdots\rangle$ indicates thermal average and $\beta=1/k_{\rm B}T$ is the reciprocal temperature, coincides with the inverse of the Hamiltonian (6), in the sense

$$\int\frac{d\mathbf{q}}{(2\pi)^3}\mathbf{G}(\mathbf{k},\mathbf{q})\mathbf{G}^{-1}(-\mathbf{q},\boldsymbol{\ell})=(2\pi)^3\delta(\mathbf{k}+\boldsymbol{\ell})\mathbf{I}, \tag{12}$$

where $\mathbf{I}$ is the 2×2 identity matrix.

To obtain the effective anchoring energy of the equivalent flat surface, we coarse-grain [8] the system on a wave vector Λ smaller than the undulation wave vector q_0, by decomposing the director's field $\boldsymbol{\psi}$ according to

$$\boldsymbol{\psi}=\boldsymbol{\psi}^<+\boldsymbol{\psi}^>, \tag{13}$$

where

$$\boldsymbol{\psi}^<=\begin{pmatrix}\theta^<\\ \phi^<\end{pmatrix} \tag{14}$$

contains the Fourier components with wave vector $|\mathbf{k}|\leqslant\Lambda$ and

$$\boldsymbol{\psi}^>=\begin{pmatrix}\theta^>\\ \phi^>\end{pmatrix} \tag{15}$$

contains the Fourier components with wave vector $|\mathbf{k}|>\Lambda$. As it is shown in [7], the free-energy $F^<[\boldsymbol{\psi}^<]$ of the coarse-grained system, which yields the total free-energy of a given slowly varying profile $\boldsymbol{\psi}^<$, taking into account the contributions coming from the high-wave-vector components, remains a harmonic function of $\boldsymbol{\psi}^<$,

$$F^<=\frac{1}{2}\int\frac{d\mathbf{k}\,d\mathbf{q}}{(2\pi)^6}\boldsymbol{\psi}^{<\rm t}(\mathbf{k})\mathbf{G}^{<-1}(-\mathbf{k},-\mathbf{q})\boldsymbol{\psi}^<(\mathbf{q}), \tag{16}$$

whose Hamiltonian $\mathbf{G}^{<-1}(\mathbf{k},\mathbf{q})$ is the inverse of the truncated correlation function

$$\mathbf{G}^<(\mathbf{k},\mathbf{q})=\mathbf{G}(\mathbf{k},\mathbf{q})h_\Lambda(\mathbf{k})h_\Lambda(\mathbf{q}), \tag{17}$$

$h_\Lambda(\mathbf{k})$ being the step function

$$h_\Lambda(\mathbf{k})=\begin{cases}1 & \text{if } |\mathbf{k}|\leqslant\Lambda,\\ 0 & \text{if } |\mathbf{k}|>\Lambda.\end{cases} \tag{18}$$

In other terms, as one might expect, Eq. (17) expresses the fact that the coarse-grained system has a correlation function that coincides with the original correlation function for wave vectors lower than the cut-off Λ, and is zero for wave vectors higher than the cut-off. This is so because the starting Hamiltonian is harmonic, which implies that the coarse-graining yields a temperature-independent renormalization of the Hamiltonian. By direct substitution, one can verify that the coarse-grained Hamiltonian $\mathbf{G}^{<-1}(\mathbf{k},\mathbf{q})$ can be more easily computed [7] from

$$\mathbf{G}^{<-1}(\mathbf{k},\mathbf{q})=\mathbf{G}^{-1}(\mathbf{k},\mathbf{q})-\int\frac{d\boldsymbol{\ell}\,d\mathbf{m}}{(2\pi)^6}\mathbf{G}^{-1}(\mathbf{k},\boldsymbol{\ell})\hat{\mathbf{G}}(-\boldsymbol{\ell},-\mathbf{m})\times\mathbf{G}^{-1}(\mathbf{m},\mathbf{q}), \tag{19}$$

where the operator $\hat{\mathbf{G}}(\mathbf{k},\mathbf{q})$ is the inverse of $\mathbf{G}^{-1}(\mathbf{k},\mathbf{q})$ in the high-wave-vector subspace, i.e., it is zero for $|\mathbf{k}|\leqslant\Lambda$ or $|\mathbf{q}|\leqslant\Lambda$, and otherwise satisfies the relation

$$\int \frac{d\mathbf{q}}{(2\pi)^3}\hat{\mathbf{G}}(\mathbf{k},\mathbf{q})\mathbf{G}^{-1}(-\mathbf{q},\boldsymbol{\ell})=(2\pi)^3\delta(\mathbf{k}+\boldsymbol{\ell})\mathbf{I}. \tag{20}$$

Given the Hamiltonian (6), we look for $\hat{\mathbf{G}}(\mathbf{k},\mathbf{q})$ satisfying relation (20) in the form (for $|\mathbf{k}|>\Lambda$ and $|\mathbf{q}|>\Lambda$)

$$\hat{\mathbf{G}}(\mathbf{k},\mathbf{q})=(2\pi)^3\mathbf{A}'(\mathbf{k})\delta(\mathbf{k}+\mathbf{q}) + 2(2\pi)^2\sum_n \mathbf{W}'_n(\mathbf{k})\mathbf{W}''_n(\mathbf{q})\delta(\mathbf{k}_\perp+\mathbf{q}_\perp+n\mathbf{q}_0). \tag{21}$$

By direct substitution, we obtain the relations

$$\mathbf{A}'(\mathbf{k})=\mathbf{W}'_n(\mathbf{k})=\mathbf{A}^{-1}(\mathbf{k}), \tag{22}$$

$$\mathbf{W}''_n(\mathbf{q})+2\sum_m \mathbf{W}_{n-m}\mathbf{A}^{-1}_{>}(-\mathbf{q}_\perp-m\mathbf{q}_0)\mathbf{W}''_m(\mathbf{q}) = -\mathbf{W}_n\mathbf{A}^{-1}(-\mathbf{q}), \tag{23}$$

where $\mathbf{A}^{-1}(\mathbf{k})$ is the inverse of the matrix (7), and

$$\mathbf{A}^{-1}_{>}(\mathbf{q}_\perp)=\int_{|\mathbf{q}|>\Lambda}\frac{dq_z}{2\pi}\mathbf{A}^{-1}(\mathbf{q}_\perp,q_z) \tag{24}$$

is the 2D Fourier transform of $\mathbf{A}^{-1}(\mathbf{r}_\perp,z=0)$ truncated in the high-wave-vector shell. Consequently, according to Eq. (19), the coarse-grained Hamiltonian is

$$\mathbf{G}^{<-1}(\mathbf{k},\mathbf{q}) =(2\pi)^3\mathbf{A}(\mathbf{k})\delta(\mathbf{k}+\mathbf{q}) +2(2\pi)^2\left[\mathbf{W}_0+2\sum_n \mathbf{W}''_{n>}(-\mathbf{k}_\perp-n\mathbf{q}_0)\mathbf{W}_{-n}\right] \times\delta(\mathbf{k}_\perp+\mathbf{q}_\perp), \tag{25}$$

where, similar to Eq. (24), we have defined

$$\mathbf{W}''_{n>}(\mathbf{q}_\perp)=\int_{|\mathbf{q}|>\Lambda}\frac{dq_z}{2\pi}\mathbf{W}''_n(\mathbf{q}_\perp,q_z), \tag{26}$$

and the $\mathbf{W}''_n(\mathbf{q})$ are implicitly defined by the set of linear equations (23). Therefore, the bulk elasticity is not affected, while the coarse-grained anchoring energy can be written in Fourier space as

$$V^{<}=\frac{1}{2}\int\frac{d\mathbf{k}_\perp}{(2\pi)^2}\boldsymbol{\psi}^{<\mathrm{t}}(\mathbf{k}_\perp)\overline{\mathbf{W}}(-\mathbf{k}_\perp)\boldsymbol{\psi}^{<}(-\mathbf{k}_\perp), \tag{27}$$

in which $\boldsymbol{\psi}^{<}(\mathbf{k}_\perp)$ is the 2D Fourier transform of the long-wavelength surface director's profile $\boldsymbol{\psi}^{<}(\mathbf{r}_\perp,z=0)$ and

$$\overline{\mathbf{W}}(\mathbf{k}_\perp)=\mathbf{W}_0+2\sum_n \mathbf{W}''_{n>}(-\mathbf{k}_\perp-n\mathbf{q}_0)\mathbf{W}_{-n} \tag{28}$$

is the effective, wave-vector-dependent, coarse-grained anchoring strength. The wave-vector dependence of $\overline{\mathbf{W}}$ gives rise to a nonlocal anchoring energy in the direct space. Expanding $\overline{\mathbf{W}}(\mathbf{k}_\perp)$ in power series of $\mathbf{k}_\perp$ around $\mathbf{k}_\perp=\mathbf{0}$, one obtains a surface gradient expansion of the coarse-grained anchoring energy. The lowest-order approximation $\overline{\mathbf{W}}(\mathbf{k}_\perp)\simeq\overline{\mathbf{W}}(\mathbf{0})$ yields the homogeneous part

$$V^{<}_{\mathrm{h}}=\int d\mathbf{r}_\perp\frac{1}{2}(W_\theta\theta^{<2}+W_\phi\phi^{<2}), \tag{29}$$

with

$$W_\theta=\frac{\pi\Lambda K_1 W}{\pi\Lambda K_1+2W}+O(\epsilon^2), \tag{30}$$

$$W_\phi=\frac{K_1K_2q_0W}{2K_1K_2q_0+(K_1+K_2)W}\epsilon^2+O(\epsilon^4). \tag{31}$$

The renormalization of the zenithal anchoring (30) is discussed in [7]. It is best understood by noting that the zenithal extrapolation length $\ell_\theta=K_1/W_\theta$ is augmented, with respect to the bare extrapolation length $\ell=K_1/W$, by the size $2/\pi\Lambda$ over which the nematic director has been averaged by the coarse-graining procedure. In other terms, the apparent increase of the extrapolation length is caused by the elastic energy stored in a surface layer of thickness $\approx\Lambda^{-1}$. The effective azimuthal anchoring (31), which is purely due to the corrugation of the surface, reproduces, in the limit of equal elastic constants, the result of Faetti [3]. No Λ-dependence appears in Eq. (31), since the renormalization due to the cut-off is of order ϵ^4. Note also that the azimuthal and the zenithal anchoring are decoupled. In the limit of infinite anchoring strength, $W\to\infty$, the effective anchoring remain finite and of purely elastic origin

$$W_{\theta\infty}=\frac{1}{2}\pi\Lambda K_1+O(\epsilon^2), \tag{32}$$

$$W_{\phi\infty}=\frac{K_1K_2}{K_1+K_2}q_0\epsilon^2+O(\epsilon^4). \tag{33}$$

A second-order expansion of Eq. (28) in $\mathbf{k}_\perp$ around $\mathbf{k}_\perp=\mathbf{0}$ yields the surface gradient contribution

$$V^{<}_{\mathrm{g}}=\int d\mathbf{r}_\perp\frac{1}{2}\left[W_{\theta x}\left(\frac{\partial\theta^{<}}{\partial x}\right)^2+W_{\theta y}\left(\frac{\partial\theta^{<}}{\partial y}\right)^2+W_{\phi x}\left(\frac{\partial\phi^{<}}{\partial x}\right)^2 +W_{\phi y}\left(\frac{\partial\phi^{<}}{\partial y}\right)^2\right], \tag{34}$$

with

$$W_{\theta x}=\frac{2\pi K_3W^2}{3\Lambda(\pi\Lambda K_1+2W)^2}+O(\epsilon^2), \tag{35}$$

$$W_{\theta y}=\frac{2\pi K_1(2K_2-K_1)W^2}{3K_2\Lambda(\pi\Lambda K_1+2W)^2}+O(\epsilon^2), \tag{36}$$

$$W_{\phi x}=\frac{K_3(K_2^2+3K_1^2)W^2}{4q_0[2K_1K_2q_0+(K_1+K_2)W]^2}\epsilon^2+O(\epsilon^4), \tag{37}$$

$$W_{\phi y}=-\frac{2K_1^2K_2^2(K_1+K_2)W^2}{[2K_1K_2q_0+(K_1+K_2)W]^3}\epsilon^2+O(\epsilon^4). \tag{38}$$

Note that Eq. (38) is always negative, thus lowering the energy cost for oscillations of the azimuthal angle perpendicularly to the grooves' direction; as we shall see, however, this destabilizing term is negligible in all practical situations. Since Λ^{-1} is the shortest length-scale over which the coarse-grained surface director can vary, the ratios

$$r_{\alpha i}=\frac{W_{\alpha i}\Lambda^2}{W_\alpha}, \tag{39}$$

with $\alpha=\theta,\phi$ and $i=x,y$, determine whether or not the gradient contributions can always be neglected. Given that the bulk elastic constant are of comparable magnitude, we set $K_1=K_2=K_3\equiv K$. Then, from the previous expressions,

$$r_{\theta x}=r_{\theta y}=\frac{1}{3}\left(1+\frac{\pi}{2}\frac{\Lambda}{q_0}\ell q_0\right)^{-1}, \tag{40}$$

$$r_{\phi x}=\frac{1}{2}\left(\frac{\Lambda}{q_0}\right)^2\frac{1}{1+\ell q_0}, \tag{41}$$

$$r_{\phi y}=-\left(\frac{\Lambda}{q_0}\right)^2\frac{\ell q_0}{(1+\ell q_0)^2}. \tag{42}$$

With the same approximation, the effective homogeneous azimuthal anchoring energy (31) becomes $W_\phi=1/2Kq_0\epsilon^2(1+\ell q_0)^{-1}$. Therefore, to have a non-negligible effective azimuthal anchoring, the bare extrapolation length ℓ must not be large with respect to the period of the undulating surface, $\ell q_0\lesssim 1$. Considering this case, since $\Lambda<q_0$, according to Eq. (40) it is always necessary to take into account the gradient terms in the effective zenithal anchoring. On the contrary, provided that $\Lambda\ll q_0$, according to Eqs. (41) and (42) the gradient terms in the effective azimuthal anchoring can be neglected altogether; they play a role only when $\Lambda\approx q_0$, and only in the direction of the grooves if $\ell q_0\ll 1$. When the gradient terms are not negligible, the full renormalized surface energy (27) must be used. The latter has a simple expression only in the case of equal elastic constants, for which Eq. (28) becomes

$$\overline{\mathbf{W}}(\mathbf{k}_\perp)=\begin{pmatrix} W_\theta(\mathbf{k}_\perp) & 0 \\ 0 & W_\phi(\mathbf{k}_\perp)\end{pmatrix}, \tag{43}$$

with

$$W_\theta(\mathbf{k}_\perp)=W\left[1+2W\frac{\tan^{-1}(|\mathbf{k}_\perp|/\Lambda)}{\pi K|\mathbf{k}_\perp|}\right]^{-1}+O(\epsilon^2), \tag{44}$$

$$W_\phi(\mathbf{k}_\perp)=\frac{W}{4}\left[\left(1+\frac{W}{K|\mathbf{q}_0-\mathbf{k}_\perp|}\right)^{-1}+\left(1+\frac{W}{K|\mathbf{q}_0+\mathbf{k}_\perp|}\right)^{-1}\right]\epsilon^2+O(\epsilon^4). \tag{45}$$

To conclude, using a coarse-graining technique, we have derived a general expression for the effective anchoring of a nematic liquid crystal in contact with an undulated surface. Our results, that are useful for the correct interpretation of the experimental data on controlled undulated surfaces [4], show that the geometric azimuthal anchoring is equivalent to a homogeneous weak anchoring only for surface distortions which occur on a scale large with respect to the period of the undulations.

Finally, we note that our model is based on the bulk Frank macroscopic elastic free-energy, and therefore can be applied only to undulated surfaces with period $\lambda=2\pi/q_0$ large with respect to the characteristic size ξ_s over which the nematic scalar order-parameter S varies close to the surface. When $\lambda<\xi_s$, a decrease of S is expected in the vicinity of the surface [9]; this effect could be taken into account by explicitly including S in the starting free energy [10]. Moreover, since the surface energy is actually spread over a thin interfacial layer of thickness δ ($\simeq 10$ nm for dispersion forces), the validity of our analysis also requires $\lambda\gg\delta$.

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