Comment on "Local elastic stability for nematic liquid crystals"

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We discuss a theory recently proposed by Virga and co-workers for the analysis of the local elastic stability of nematic liquid crystals [R. Rosso, E. G. Virga, and S. Kralj, Phys. Rev. E. **70**, 011710 (2004)]. The periodic instability in a nematic sample induced by the saddle-splay elastic constant or by the coupling of an external field with the flexoelectric polarization is reconsidered. We show that in the case in which the two surfaces limiting the sample are characterized by the same easy angle the analysis previously proposed by us coincides with the one proposed by Virga *et al.*

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In a series of papers [1–6] we analyzed the stability of a nondeformed director pattern, $\mathbf{n}(\mathbf{r})=\mathbf{N}$, with respect to a periodic one. In our analysis the source of the periodic instability is the saddle-splay elastic constant or the coupling of an external field with the flexoelectric polarization. The theoretical analysis is based on the assumption that the two surfaces were characterized by the same easy angle. In this framework the nondeformed state of the director, where the nematic director is position independent, is a solution of the bulk differential equations, and satisfies the relevant boundary conditions, since it is along the easy axis. The analysis proposed in [2–6] is based on the following procedure. The nondeformed state is $\mathbf{n}(\mathbf{r})=\mathbf{N}$, and the relevant total energy for the sample under consideration is $F(\mathbf{N})$. We consider also a distorted director field $\mathbf{n}(\mathbf{r})=\mathbf{N}+\mathbf{p}(\mathbf{r})$, where $\mathbf{p}(\mathbf{r})=\varepsilon\,\mathbf{u}(\mathbf{r})$, and ε is a small quantity that is considered as an expansion parameter in a perturbational analysis. Then, we expand the total energy of the sample up to the second order in ε. Since the modulus of the nematic director is such that $\mathbf{n}\cdot\mathbf{n}=1$ it follows that $\mathbf{n}\cdot\mathbf{n}=\mathbf{N}\cdot\mathbf{N}=1$, and hence, at the first order in ε, $\mathbf{N}\cdot\mathbf{p}=0$. When $\mathbf{N}\to\mathbf{n}=\mathbf{N}+\mathbf{p}$ we get $F(\mathbf{n})=F(\mathbf{N})+\delta F(\mathbf{u})$, where $\delta F(\mathbf{u})$ is of the second order in ε [2–6]. By minimizing $F(\mathbf{n})$, i.e., $\delta F(\mathbf{u})$ with respect to $\mathbf{u}(\mathbf{r})$, we obtain the new bulk differential equations and boundary conditions of the problem. The analysis of $\delta F(\mathbf{u})\geqslant 0$ for the $\mathbf{u}(\mathbf{r})$ extremizing $\delta F(\mathbf{u})$ determines the threshold of the instability. This procedure has been recently reconsidered by Virga *et al.* [7] for the following reason. Since $\delta F(\mathbf{u})$ is of the second order in ε it is not enough to put $\mathbf{p}(\mathbf{r})=\varepsilon\,\mathbf{u}(\mathbf{r})$, but it is necessary to consider $\mathbf{p}(\mathbf{r})=\varepsilon\,\mathbf{u}(\mathbf{r})+\varepsilon^2\mathbf{v}(\mathbf{r})$, because from the condition $\mathbf{n}\cdot\mathbf{n}=1$ it follows that, at the second order in ε, $2\varepsilon\mathbf{N}\cdot\mathbf{u}+\varepsilon^2(2\mathbf{N}\cdot\mathbf{v}+\mathbf{u}\cdot\mathbf{u})=0$. Whence, $\mathbf{N}\cdot\mathbf{u}=0$, and $\mathbf{N}\cdot\mathbf{v}=-(1/2)\mathbf{u}\cdot\mathbf{u}$, at the first and second order in ε, respectively. From this observation it follows that $\mathbf{N}\cdot\mathbf{p}=-(1/2)\varepsilon^2\mathbf{u}\cdot\mathbf{u}$. As shown below, the contribution to the total energy connected to $\mathbf{N}\cdot\mathbf{p}$ has to be taken into account if the total energy is expanded up to the second order in ε. However, we will show that in the case in which the nematic sample is characterized by the same easy angle on the two surfaces, this contribution vanishes identically.

We indicate by $\mathbf{N}$ the nondistorted nematic field, and by $\mathbf{n}(\mathbf{r})=\mathbf{N}+\mathbf{p}(\mathbf{r})$ the distorted one. The total energy of the sample, of volume V limited by the surface S, is given by

$$F[\mathbf{n}(\mathbf{r})]=\int\int\int_V f(n_i,n_{i,j})dV+\int\int_S g(n_i)dS, \qquad (1)$$

where $n_{i,j}=\partial n_i/\partial x_j$ are the spatial derivatives of the components of the nematic director. In Eq. (1) $f(n_i,n_{i,j})$ is the bulk energy density, containing the elastic terms and the contribution describing the interaction of the nematic material with the external fields [8], and $g(n_i)$ the anisotropic part of the surface tension [9]. The actual nematic director field $\mathbf{n}(\mathbf{r})$ is the one minimizing $F[\mathbf{n}(\mathbf{r})]$. Standard calculations give for the bulk differential equations

$$\frac{\partial f}{\partial n_i}-\partial_j\frac{\partial f}{\partial n_{i,j}}=\lambda_v n_i, \qquad (2)$$

where $\partial_j=\partial/\partial x_j$, and for the boundary conditions

$$\frac{\partial f}{\partial n_{i,j}}\nu_i+\frac{\partial g}{\partial n_i}=\lambda_s n_i, \qquad (3)$$

where ν_i are the Cartesian components of the outer geometrical normal to the bounding surface S. In Eqs. (2) and (3) λ_v and λ_s are the Lagrange multipliers connected with the constraint $\mathbf{n}\cdot\mathbf{n}=1$ in all the volume V limited by S, and Einstein's convention has been used on the repeated subscript.

We evaluate now the variation of F when $\mathbf{N}\to\mathbf{n}=\mathbf{N}+\mathbf{p}$. For this transformation the bulk energy density becomes $f(n_i,n_{i,j})=f(N_i+p_i,p_{i,j})$. By expanding f in power series of p_i and $p_{i,j}$ up to the second order we get $f(n_i,n_{i,j})=f(N_i,0)+\delta_1 f+\delta_2 f$, where

$$\delta_1 f=\left(\frac{\partial f}{\partial n_\alpha}\right)_{\mathbf{N}}p_\alpha+\left(\frac{\partial f}{\partial n_{\alpha,\beta}}\right)_{\mathbf{N}}p_{\alpha,\beta}, \qquad (4)$$

and

$$\delta_2 f=\frac{1}{2}\left\{\frac{\partial^2 f}{\partial n_\alpha\,\partial n_\beta}p_\alpha p_\beta+2\frac{\partial^2 f}{\partial n_\alpha\,\partial n_{\gamma,\mu}}p_\alpha p_{\gamma,\mu}+\frac{\partial^2 f}{\partial n_{\alpha,\beta}\,\partial n_{\gamma,\mu}}p_{\alpha,\beta}p_{\gamma,\mu}\right\}_{\mathbf{N}}. \qquad (5)$$

By operating in a similar manner with $g(n_i)$ we get

$$g(n_i)=g(N_i)+\left(\frac{\partial g}{\partial n_\alpha}\right)_{\mathbf{N}}p_\alpha+\frac{1}{2}\left(\frac{\partial^2 g}{\partial n_\alpha\,\partial n_\beta}\right)_{\mathbf{N}}p_\alpha p_\beta. \quad (6)$$

From Eq. (2) we have

$$\left(\frac{\partial f}{\partial n_\alpha}\right)_{\mathbf{N}}=\left(\partial_\beta\frac{\partial f}{\partial n_{\alpha,\beta}}+\lambda_v n_\alpha\right)_{\mathbf{N}}. \quad (7)$$

Consequently, $\delta_1 f$ given by Eq. (4) can be rewritten as

$$\delta_1 f=\partial_\beta\left(\frac{\partial f}{\partial n_{\alpha,\beta}}p_\alpha\right)+\lambda_v N_\alpha p_\alpha. \quad (8)$$

Hence, when $\mathbf{N}\to\mathbf{n}=\mathbf{N}+\mathbf{p}$, $F(\mathbf{N})\to F(\mathbf{n})=F(\mathbf{N}+\mathbf{p})=F(\mathbf{N})+\delta F$, where $\delta F=\delta_1 F+\delta_2 F$, with

$$\delta_1 F=\int\int_S\left(\nu_\beta\frac{\partial f}{\partial n_{\alpha,\beta}}+\frac{\partial g}{\partial n_\alpha}\right)_{\mathbf{N}}p_\alpha dS, \quad (9)$$

and

$$\delta_2 F=\int\int\int_V(\delta_2 f+\lambda_v N_\alpha p_\alpha)dV+\frac{1}{2}\int\int_S\left(\frac{\partial^2 g}{\partial n_\alpha\,\partial n_\beta}\right)_{\mathbf{N}}p_\alpha p_\beta dS. \quad (10)$$

By taking into account Eq. (3) $\delta_1 F$ can be rewritten as

$$\delta_1 F=\int\int_S\lambda_s N_\alpha p_\alpha dS. \quad (11)$$

It follows that, explicitly, δF is given by

$$\begin{aligned}\delta F=&\int\int\int_V\lambda_v N_\alpha p_\alpha dV+\int\int_S\lambda_s N_\alpha p_\alpha dS\\&+\frac{1}{2}\int\int\int_V\left(\frac{\partial^2 f}{\partial n_\alpha\,\partial n_\beta}p_\alpha p_\beta+2\frac{\partial^2 f}{\partial n_\alpha\,\partial n_{\gamma,\mu}}p_\alpha p_{\gamma,\mu}\right.\\&\left.+\frac{\partial^2 f}{\partial n_{\alpha,\beta}\,\partial n_{\gamma,\mu}}p_{\alpha,\beta}p_{\gamma,\mu}\right)_{\mathbf{N}}dV\\&+\frac{1}{2}\int\int_S\left(\frac{\partial^2 g}{\partial n_\alpha\,\partial n_\beta}\right)_{\mathbf{N}}p_\alpha p_\beta dS. \quad (12)\end{aligned}$$

In our previous analysis we put $\mathbf{n}=\mathbf{N}+\varepsilon\mathbf{u}$. From the condition $\mathbf{n}\cdot\mathbf{n}=\mathbf{N}\cdot\mathbf{N}=1$ we get $\mathbf{N}\cdot\mathbf{u}=0$. Furthermore, since $\mathbf{p}=\varepsilon\mathbf{u}$ from (12) we have

$$\begin{aligned}\delta_B F=\frac{1}{2}\Bigg\{&\int\int\int_V\left(\frac{\partial^2 f}{\partial n_\alpha\,\partial n_\beta}u_\alpha u_\beta+2\frac{\partial^2 f}{\partial n_\alpha\,\partial n_{\gamma,\mu}}u_\alpha u_{\gamma,\mu}\right.\\&\left.+\frac{\partial^2 f}{\partial n_{\alpha,\beta}\,\partial n_{\gamma,\mu}}u_{\alpha,\beta}u_{\gamma,\mu}\right)_{\mathbf{N}}dV\\&+\int\int_S\left(\frac{\partial^2 g}{\partial n_\alpha\,\partial n_\beta}\right)_{\mathbf{N}}u_\alpha u_\beta dS\Bigg\}\varepsilon^2, \quad (13)\end{aligned}$$

quadratic in ε.

As underlined by Virga *et al.* [7] the correct procedure implies to consider also the second-order variation of the director field, i.e., $\mathbf{n}=\mathbf{N}+\mathbf{p}$, with $\mathbf{p}=\varepsilon\mathbf{u}+\varepsilon^2\mathbf{v}$. In this case from the condition $\mathbf{n}\cdot\mathbf{n}=\mathbf{N}\cdot\mathbf{N}=1$ it follows that $\mathbf{N}\cdot\mathbf{u}=0$, and $\mathbf{N}\cdot\mathbf{v}=-(1/2)\mathbf{u}\cdot\mathbf{u}$, at the first and second order in ε, respectively. Consequently $\mathbf{N}\cdot\mathbf{p}=\varepsilon^2\mathbf{N}\cdot\mathbf{v}=-(1/2)\varepsilon^2\mathbf{u}\cdot\mathbf{u}$, and from (12) δF is, according to Virga *et al.* [7],

$$\delta_V F=-\frac{1}{2}\left\{\int\int\int_V\lambda_v u_\alpha u_\alpha dV+\int\int_S\lambda_s u_\alpha u_\alpha dS\right\}\varepsilon^2+\delta_B F. \quad (14)$$

Equation (14) shows that the assumption $\mathbf{v}=0$ gives a different result if δF is expanded up to the second order in ε.

In our previous papers [2–6] we have investigated the stability of the undistorted configuration in the presence of the saddle-splay elastic constant or of an external field coupled with the flexoelectric polarization. In our theoretical analyses the two surfaces have the same easy angle. Hence, $\mathbf{N}$ is a minimizer of the anisotropic part of the surface tensions on both surfaces. Consequently, $\mathbf{N}$ was such that $\lambda_v=\lambda_s=0$. In this case, as discussed above, $\delta_V F=\delta_B F$. It follows that the results reported in [2,3] are correct, provided that $\delta_B F$ is minimized over *all* admissible fields $\mathbf{u}$. Of course, in order to analyze the stability of the periodic deformation in a hybrid nematic cell, where $\lambda_s\neq 0$, it is necessary to use the procedure proposed by Virga *et al.* [7].

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