

## Surface variations of the density and scalar order parameter and the elastic constants of a uniaxial nematic phase

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The elastic constants  $K_{24}$  and  $K_{13}$  of a spatially restricted nematic phase are found to essentially depend on behavior of the density  $\rho$  and orientational order parameter  $\eta$  at the surface. The cancellation of the effective constant  $K_{13}$ , recently revealed by Faetti and Riccardi [J. Phys. II **5**, 1165 (1995)], is obtained as a particular case of a constant  $\eta$  and arbitrary  $\rho$ ; whereas a spatial-dependent  $\eta$  violates this cancellation and restores a finite  $K_{13}$  term. [S1063-651X(99)51802-3]

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### I. INTRODUCTION

More than a quarter of a century ago the elastic theory of a uniaxial nematic liquid crystal had taken the final form in the series of papers [1] by Nehring and Saupe. In this theory, the nematic phase is described by the director  $\mathbf{n}(\mathbf{x})$ , which is a unit vector pointing along the average direction of the long molecular axes in the vicinity of the point  $\mathbf{x}$ . The director deformations associated with nonvanishing director derivatives  $\partial n$  are assumed to be sufficiently weak, i.e.,  $\varepsilon = l_M \partial n \ll 1$ , where  $l_M$  is the molecular length (of order of the interaction range). This approach, however, essentially presupposes that the local symmetry in the vicinity of any spatial point inside the nematic body is the *symmetry of infinite nematic medium*. By virtue of this symmetry, leading terms in the deformation free energy (FE) appear to be quadratic in  $\varepsilon$ . The studies of the recent decade have shown that incorporating spatial boundedness into the elastic approach is not trivial and does not reduce to just considering a surface tension.

First, surface was shown to induce an additional elastic term  $F_1$  linear in  $\partial n$  whose density vanishes in the bulk [2]. Then, the leading part [up to terms  $O(\varepsilon^2)$ ] of the deformation FE of a nematic liquid crystal contained in the volume  $V$  actually takes the form

$$F = \frac{1}{2} K_{\alpha\alpha} F_{\alpha\alpha} - K_{24} F_{24} + K_{13} F_{13} + F_1, \quad (1)$$

where  $\alpha = 1, 2, 3$ , and the standard infinite-medium quadratic FE terms  $F_{\alpha\beta}$  are given by [1]

$$\begin{aligned} F_{11} &= \int dV (\nabla \cdot \mathbf{n})^2, & F_{22} &= \int dV (\mathbf{n} \cdot \nabla \times \mathbf{n})^2, \\ F_{33} &= \int dV (\mathbf{n} \times \nabla \times \mathbf{n})^2; \\ F_{24} &= \int dV \nabla \cdot [(\nabla \cdot \mathbf{n}) - (\mathbf{n} \cdot \nabla) \mathbf{n}], \\ F_{13} &= \int dV \nabla \cdot [\mathbf{n} \cdot (\nabla \cdot \mathbf{n})]. \end{aligned} \quad (2)$$

The infinite-medium elastic constants  $K_{\alpha\alpha}$  and  $K_{13}$  can be calculated provided the pairwise interaction  $G(\mathbf{n}(\mathbf{x}'), \mathbf{n}(\mathbf{x}), \mathbf{x}' - \mathbf{x})$  between two infinitesimal nematic volumes centered at the points  $\mathbf{x}'$  and  $\mathbf{x}$  is known, while  $K_{24} = (K_{11} + K_{22} + 2K_{13})/4$  [1]. The form of  $F_1$  will be discussed somewhat below. The scalar  $G$  depends on the vectors  $\mathbf{n}' = \mathbf{n}(\mathbf{x}')$ ,  $\mathbf{n}$ , and  $\mathbf{r} = \mathbf{x}' - \mathbf{x}$  only through the scalar combinations  $\alpha = \mathbf{n} \cdot \mathbf{n}'$ ,  $\beta = \mathbf{r} \cdot \mathbf{n}$ ,  $\beta' = \mathbf{r} \cdot \mathbf{n}'$ , and  $r = |\mathbf{r}|$ , i.e.,  $G = G(\alpha, \beta, \beta', r)$ .

Second, the  $K_{24}$  and  $K_{13}$  terms in Eq. (2) are total divergences and in a restricted body can be written as surface integrals with the density linear in  $\partial n$ . In spite of this, in three dimensions the  $K_{24}$  and  $K_{13}$  terms do not reduce to a surface tension (anchoring) [3,4] and, possessing a unique ability to gain the FE for finite deformations, are an important source of pattern formation (see reviews [5,6]). For instance, it was found that both the  $K_{24}$  and  $K_{13}$  terms are responsible for the stripe domains in thin nematic films [7,8].

Third, the very possibility of having a nonzero  $K_{13}$  requires justification. The problem derives from the important result by Faetti and Riccardi [9] revealed that the sum  $F_1 - K_{24} F_{24} + K_{13} F_{13} = -\frac{1}{4}(K_{11} + K_{22}) F_{24}$ , and thus the term  $F_{13}$  is cancelled out. Recently, this cancellation was shown to be dictated by the FE symmetry [10]. In this situation, the problem of status of the  $K_{13}$  term has turned into a search for possible additional sources thereof hidden in subsurface phenomena. Presently, the only such source of nonzero  $K_{13}$  considered in the literature [10–12] is nondeformational, the so-called homogeneous part of the nematic FE giving rise to the intrinsic anchoring. However, in Ref. [3] where this source was pointed out, the derivative-dependent terms and, in particular, the term apparently similar to the  $K_{13}$  term, were shown to be much smaller than the anchoring. Thus, this source cannot provide a non-negligible value of  $K_{13}$ .

Nonetheless, the result  $K_{13} = 0$  obtained in [9,10] might be inconclusive for another reason recently considered by Pergamenschchik [4]. Indeed, it assumes an unrealistic ideal surface where the density  $\rho$  and order parameter  $\eta$  constant everywhere in the nematic body abruptly vanish. However, in the general case of a nonideal surface where  $\rho$  and  $\eta$  are spatially dependent the value of  $K_{13}$  can change [4]. Physically, substantial surface variations of  $\eta$  were suggested to be essential for anchoring related phenomena

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[13,14,4], and were reportedly observed in experiment [15]. Mathematically,  $\rho$  smoothly vanishing at the surface brings the lower boundary to the FE with a nonzero  $K_{13}$  term [4] which is missing for the ideal surface with steplike  $\rho$  [16,3]. This provides the minimization procedure that yields a stable director field for  $K_{13} \neq 0$  [4]. In this Rapid Communication we incorporate a realistic nonideal surface into the elastic theory. We report formulas for all the elastic constants in the general case when  $\rho$  and  $\eta$  are constant in the bulk and arbitrary functions of coordinates in a thin subsurface layer of a microscopic thickness  $l_S$ . It is shown that the master role in the  $K_{13}$  cancellation is played by surface variation of the order parameter: the cancellation takes place only if  $\eta$  is constant, whereas for spatial-dependent  $\eta$  a finite  $K_{13}$  restores. The constants  $K_{\alpha\alpha}$  do not depend on the surface behavior, whereas both  $K_{13}$  and  $K_{24}$  do. This justifies the theory [4] with a finite  $K_{13}$  term and means that the behavior in a microscopically thin surface layer can have an observable elastic effect in the bulk.

## II. SPATIAL-DEPENDENT DENSITY AND SCALAR ORDER PARAMETER AND THE EFFECTIVE PAIRWISE POTENTIAL

Here we incorporate surface nonideality in the form of spatial variations of  $\rho$  and  $\eta$  in the macroscopic approach neglecting biaxiality. For brevity, we denote function of a primed argument by the function with prime. Then the energy of a pairwise interaction of particles with orientational coordinates  $\omega$  and spatial coordinates  $\mathbf{x}$  has the form

$$E = \int d\mathbf{x} d\mathbf{x}' \int d\omega d\omega' f U g_2 f', \quad (3)$$

where  $f = f(\mathbf{x}, \omega)$  is the one-particle distribution function,  $U$  is the microscopic pairwise interaction potential, and  $g_2$  is the pair correlation function. The scalar  $U$  depends on the available scalar pairwise combinations of its arguments and the absolute value  $r$  of the separation vector  $\mathbf{r}$ , i.e.,  $U = U(\omega\omega', (\mathbf{r}\omega)(\mathbf{r}\omega'), r)$ . At the same time  $g_2$  can explicitly depend on the coordinates through the functions  $\rho$ ,  $\rho'$ ,  $\eta$  and  $\eta'$ , i.e.,  $g_2 = g_2(\omega\omega', (\mathbf{r}\omega)(\mathbf{r}\omega'), r, \mathbf{x}, \mathbf{x}')$ . Both  $U$  and  $g_2$  are invariant under permutations of  $\omega$  and  $\omega'$ , and  $\mathbf{x}$  and  $\mathbf{x}'$ .

In a uniaxial phase, the distribution function of a system of molecules with long axes along  $\omega$  depends on the angle between the macroscopic axis  $\mathbf{n}(\mathbf{x})$  and  $\omega$ ,  $f = f(\mathbf{n}\omega, \mathbf{x})$ . The general form of this function is an expansion series in the Legendre polynomials. As usual, restricting this expansion to the first nontrivial nematic-symmetry-allowed polynomial  $P_2$ , one has

$$f(\mathbf{n}\omega, \mathbf{x}) = \frac{\rho(\mathbf{x})}{4\pi} [1 - \eta(\mathbf{x}) + 3\eta(\mathbf{x})(\mathbf{n}\omega)^2], \quad (4)$$

which automatically satisfies the density definition  $\rho(\mathbf{x}) = \int d\omega f$ ; the order parameter  $\eta$  is normalized in such a way that the isotropic fraction vanishes and the system is maximally ordered for  $\eta = 1$ .

The deformational FE can be separated from  $E$  by using the identity  $G(\mathbf{n}, \mathbf{n}') = G(\mathbf{n}, \mathbf{n}) + \Delta G(\mathbf{n}, \mathbf{n}')$  where  $\Delta G(\mathbf{n}, \mathbf{n}')$

$= G(\mathbf{n}, \mathbf{n}') - G(\mathbf{n}, \mathbf{n})$  is the deformational part of the potential. Substituting Eq. (4) into Eq. (3) the elastic fraction  $F$  is obtained in the form

$$F\{\mathbf{n}\} = \int d\mathbf{x} d\mathbf{x}' \Delta G_{nid}, \quad (5)$$

$$\Delta G_{nid} = A_{\eta\eta} \Delta G_{\eta\eta} + A_{\eta} \Delta G_{\eta}. \quad (6)$$

Here  $A_{\eta\eta} = \rho\rho' \eta\eta'$  and  $A_{\eta} = \frac{1}{2}\rho\rho'(\eta' - \eta)$ , and the kernels entering this formula can be written as

$$G_{\eta\eta}(\alpha, \beta\beta') = \frac{9}{(4\pi)^2} \int d\omega d\omega' (\mathbf{n}\omega)^2 U g_2(\mathbf{n}\omega')^2, \quad (7)$$

$$G_{\eta}(\beta^2, \beta'^2) = \frac{3}{(4\pi)^2} \int d\omega d\omega' [(\mathbf{n}\omega)^2 + (\mathbf{n}'\omega')^2] U g_2. \quad (8)$$

The indicated arguments of the functions  $G_{\eta\eta}$  and  $G_{\eta}$  follow immediately from their scalar character and the arguments of the function  $U g_2$ , while the explicit symmetric dependence on  $\mathbf{x}$  and  $\mathbf{x}'$  is not indicated for simplicity. The form of the last term in Eq. (6) takes into account that  $\Delta G_{\eta}$  is antisymmetric in  $\mathbf{x}$  and  $\mathbf{x}'$ , i.e.,  $\Delta G_{\eta}(\mathbf{n}', \mathbf{n}, \mathbf{x}', \mathbf{x}, r) = -\Delta G_{\eta}(\mathbf{n}, \mathbf{n}', \mathbf{x}, \mathbf{x}', r)$ .

Formulas (5)–(8) connect the microscopic description to the effective pairwise potential  $\Delta G_{nid}$ , which is the starting point of the elastic theory [1]. If the functions  $\rho(\mathbf{x})$  and  $\eta(\mathbf{x})$  are constant in the volume  $V$  and abruptly vanish on its boundary, one has an ideally restricted body, and the kernel  $\Delta G_{nid}$  becomes  $G_{id} = G_{id}(\alpha, \beta, \beta', r)$ , which has been considered in the elastic theory of a nematic liquid crystal. We see that compared to the case of an ideal surface  $\eta = \text{const}$ ,  $\rho = \text{const}$ , the surface nonideality gives rise to an additional term with the density  $\frac{1}{2}\rho\rho'[\eta(\mathbf{x}') - \eta(\mathbf{x})]\Delta G_{\eta}$ , which is nonzero only if  $\eta(\mathbf{x})$  is not a constant. We will see that this term alone contributes to the effective constant  $K_{13}$ . The full physical information that Eqs. (3)–(8) might convey goes far beyond the subject of this paper. Here we will consider only the consequences of these formulas to the elastic theory of a nematic phase (note, however, that these can be applied to any uniaxial phase, e.g., for SmA) assuming  $\rho(\mathbf{x})$  and  $\eta(\mathbf{x})$  to be given functions which is justified far from the phase transitions.

## III. ELASTIC CONSTANTS OF A NEMATIC LIQUID CRYSTAL WITH NONIDEAL SURFACE

Both  $A_{\eta\eta}$  and  $A_{\eta}$  entering  $\Delta G_{nid}$  (6) are assumed to differ from their constant bulk value only close to the surface where both  $\mathbf{x}$  and  $\mathbf{x}'$  are separated from the surface by a distance less than  $l_S \sim \text{few } l_M$ . Obviously, the bulk value  $A_{\eta\eta, b} = \rho_b^2 \eta_b^2$ , where  $\rho_b$  and  $\eta_b$  are the bulk density and order parameter; while  $A_{\eta, b} = 0$ . The functions  $A_{\eta\eta}$  and  $A_{\eta}$  represent a general nonideal surface.

Let us first show that the only elastic term affected by the nonideality in the leading order is  $F_1$ , whereas the changes of all other terms can be neglected. Indeed, any quadratic term has density  $\sim K/d^2$ , where  $d$  is of order of the system size. Then any bulk quadratic term  $K_{\alpha\beta} F_{\alpha\beta}$  is of order

$d(Kd^{-2})=K/d$  whereas its change in the surface layer can be estimated as  $l_M(Kd^{-2})=\varepsilon K/d \ll K/d$ . Similarly, any surface-induced quadratic term with the density nonvanishing only in the intermediate layer is of the negligible order  $\varepsilon K/d$  [that is why these terms introduced in [17] are absent in FE (1)]. The only exclusion is the surface term  $F_1 \sim K/d$  whose surface density  $K/(dl_M)$  is very high: its change  $\sim l_M K/(dl_M)=K/d$  which is of the same order as the value of the bulk terms and thus must be considered. This implies that spatial dependence of the functions  $A_{\eta\eta}$  and  $A_\eta$  in the surface layer must be taken into account only in  $F_1$ , which thus is the sum  $F_1=F_{1,\eta\eta}+F_{1,\eta}$  of the terms corresponding to  $A_{\eta\eta}\Delta G_{\eta\eta}$  and  $A_\eta\Delta G_\eta$ . In particular, the term  $A_\eta\Delta G_\eta$  contributes solely to the subsurface term  $F_{1,\eta}$  since  $A_\eta$  vanishes in the bulk; whereas in the bulk terms,  $A_{\eta\eta}$  can be replaced by its bulk value.

Further, it is known that in order to obtain the elastic FE in a local form the pairwise potential is expanded in a power series of the components  $\Delta n_i(\mathbf{x}',\mathbf{x})=n'_i-n_i$  of the director rotation vector up to the second order. In our case this expansion takes the form

$$F \simeq L + Q$$

$$= \int_V d\mathbf{x} d\mathbf{x}' \left( \frac{\partial \Delta G_{nid}}{\partial n'_i} \Delta n_i + \frac{1}{2} \frac{\partial^2 \Delta G_{nid}}{\partial n'_i \partial n'_j} \Delta n_i \Delta n_j \right), \quad (9)$$

where the derivatives are taken at  $\mathbf{n}'=\mathbf{n}$ , and  $L$  and  $Q$  stand for the terms linear and quadratic in  $\Delta n$ , respectively. Then, combining the above said with the known infinite-medium results [1] yields the quadratic term

$$Q = \frac{A_{\eta\eta,b}}{2} \left[ K_{\alpha\alpha}^{(0)} F_{\alpha\alpha} - \frac{1}{2} (K_{11}^{(0)} + K_{22}^{(0)}) F_{24} \right], \quad (10)$$

and the linear term  $L=L_{\eta\eta}+L_\eta$ , where the contributions of  $A_{\eta\eta}\Delta G_{\eta\eta}$  and  $A_\eta\Delta G_\eta$  have the form

$$L_{\eta\eta} = F_{1,\eta\eta} + A_{\eta\eta,b} K_{13} (-F_{11} + F_{33} + F_{13}), \quad (11)$$

$$L_\eta = F_{1,\eta}. \quad (12)$$

The bare  $K_{\alpha\alpha}^{(0)}$  and  $K_{13}$  are the standard Nehring-Saupe elastic constants for the potential  $G_{\eta\eta}$  taken for the bulk values of  $\eta$  and  $\rho$  (on which  $G_{\eta\eta}$  can depend through the pair correlation function  $g_2$ ). The renormalized  $K_{\alpha\alpha}$  entering FE (1) obtained from the above formulas in the standard form [1]

$$K_{11} = K_{11}^{(0)} - 2K_{13}, \quad K_{33} = K_{33}^{(0)} + 2K_{13}, \quad (13)$$

$$K_{22} = K_{22}^{(0)}.$$

To calculate  $F_{1,\eta\eta}$  we consider the antisymmetric part  $\Delta G_{\eta\eta,-}$  of the kernel  $\Delta G_{\eta\eta}$ , which is of the form  $\Delta G_{\eta\eta,-} = \frac{1}{2} [G_{\eta\eta}(\alpha=1, \beta'^2) - G_{\eta\eta}(\alpha=1, \beta^2)]$ . A simple direct calculation shows that, since  $\mathbf{n}^2=1$  and thus  $\Delta\alpha = \mathbf{n} \cdot \Delta\mathbf{n}$  is negligible, one has

$$\left( \frac{\partial \Delta G_{\eta\eta}}{\partial n'_i} \right)_{\mathbf{n}'=\mathbf{n}} \Delta n_i = \left( \frac{\partial \Delta G_{\eta\eta,-}}{\partial n'_i} \right)_{\mathbf{n}'=\mathbf{n}} \Delta n_i. \quad (14)$$

As a result, the kernel  $\Delta G_{\eta\eta}$  and its antisymmetric part  $\Delta G_{\eta\eta,-}$  produce the same linear term (11) and hence the same  $K_{13}$  and  $F_1$ . This will be employed below in Eq. (16).

Now we consider the identity

$$F_- = \int d\mathbf{x} d\mathbf{x}' A_{\eta\eta} \Delta G_{\eta\eta,-} \equiv 0, \quad (15)$$

which follows from the fact that the integrand is antisymmetric with respect to permutation of  $\mathbf{x}$  and  $\mathbf{x}'$ . It implies that the elastic energy  $F_-$  of the kernel  $A_{\eta\eta}\Delta G_{\eta\eta,-}$  is zero. The correspondent formulas for this case can be obtained from Eqs. (9)–(13) by replacing  $F$  with  $F_-$ ,  $\Delta G_{nid}$  with  $A_{\eta\eta}\Delta G_{\eta\eta,-}$ , and the constants  $K_{\alpha\beta}$  with  $K_{\alpha\beta,-}$ . In the context of Eqs. (13) and (14), equating to zero the positive definite splay, twist, and bend terms in thus obtained elastic expansion of  $F_-$  yields  $K_{11,-}^{(0)} = -K_{33,-}^{(0)} = 2K_{13,-} = 2K_{13}$ ,  $K_{22,-}^{(0)} = 0$ . This shows that all the constants calculated for  $A_{\eta\eta}\Delta G_{\eta\eta,-}$  can be expressed in terms of a single constant  $K_{13}$  calculated for the original kernel  $A_{\eta\eta}\Delta G_{\eta\eta}$ . In particular, the coefficient  $K_{11,-}^{(0)} + K_{22,-}^{(0)}$  of the term  $F_{24}$  is equal to  $2K_{13}$ . Now equating to zero the sum of the remaining terms in the elastic expansion of  $F_-$ , one obtains the relation

$$F_{1,\eta\eta} = -K_{13} A_{\eta\eta,b} \left( F_{13} + \frac{1}{2} F_{24} \right). \quad (16)$$

Equation (16) implies that the term  $F_{13}$  is absent in  $L_{\eta\eta}$  (11). This means that if the *order parameter*  $\eta$  is constant and  $F_{1,\eta} \propto \eta' - \eta = 0$ , the *nonideal surface* with whatever  $\rho(\mathbf{x})$  does not violate the  $K_{13}$  cancellation obtained in [9] for an ideal surface.

Now we address the last remaining term  $F_{1,\eta}$  (12). This is the total FE contribution of the second term in  $\Delta G_{nid}$ , which is finite, since both  $A_\eta$  and  $\Delta G_\eta$  are antisymmetric. Inasmuch as the form of the surface-induced term does not depend on a specific nonideality that can change only its coefficient, one can write

$$F_{1,\eta} = \int_V d\mathbf{x} d\mathbf{x}' A_\eta \Delta G_\eta = -\gamma F_{1,\eta\eta}. \quad (17)$$

Here  $\gamma = -F_{1,\eta}/F_{1,\eta\eta}$  is the coefficient that characterizes restoration of a finite  $K_{13}$  by given nonideality:  $\gamma=0$  if  $A_\eta=0$ . Since the expression for  $F_{1,\eta\eta}$  is known [17],  $\gamma$  is determined by Eq. (17) (the formula is given below). From Eqs. (16) and (17), the general form of  $F_1$  can be written as

$$F_1 + A_{\eta\eta,b} K_{13} F_{13} = A_{\eta\eta,b} K_{13} \left( \gamma F_{13} - \frac{1-\gamma}{2} F_{24} \right). \quad (18)$$

The  $K_{13}$  cancellation [9] obtains from this formula only in the particular case  $\gamma=0$ . This means that *the effective  $K_{13}$  is nonzero if the order parameter in the intermediate layer is spatially dependent and  $A_\eta \propto \eta' - \eta \neq 0$ .*

Now we can write down formulas for the deformation FE of a nematic body with a nonideal surface for given  $\rho$  and  $\eta$ . Substituting Eqs. (10)–(12), and (18) into the deformation FE  $F=L+Q$  yields

$$F = \frac{1}{2} K_{\alpha\alpha}^* F_{\alpha\alpha} - K_{24}^* F_{24} + K_{13}^* F_{13}, \quad (19)$$

where  $K_{\alpha\beta}^*$  are the effective elastic constants of a nonideally restricted body. These constants are connected to the Nehring-Saupe infinite-medium constants  $K_{\alpha\beta, \eta\eta}$  corresponding to the kernel  $G_{\eta\eta}$  (7) (above the symbol  $\eta\eta$  in the subscripts of the elastic constants was omitted for brevity) and the bulk values of the density and scalar order parameter as

$$K_{\alpha\alpha}^* = \rho_b^2 \eta_b^2 K_{\alpha\alpha, \eta\eta}, \quad \alpha = 1, 2, 3;$$

$$K_{13}^* = \gamma \rho_b^2 \eta_b K_{13, \eta\eta}, \quad (20)$$

$$K_{24}^* = \frac{1}{4} (K_{11}^* + K_{22}^* - 2K_{13}^*).$$

Direct calculation using the definition of the term  $F_1$  (see, e.g., [17]) results in the following formula for  $\gamma$ :

$$K_{13}^* n_3 = \gamma \rho_b^2 \eta_b K_{13, \eta\eta} n_3$$

$$= \frac{1}{2} \int_0^{l_s} dz \int_{-z}^{\infty} dr_3 r_3^2 \int_{-\infty}^{\infty} dr_1 dr_2 \rho(z) \rho(z+r_3)$$

$$\times [\eta(z+r_3) - \eta(z)] \left( r_3 \frac{\partial G_\eta}{\partial \beta} - n_3 r_2^2 \frac{\partial G_\eta}{\partial \beta^2} \right).$$

(21)

The integration is performed in the reference frame where the outer normal to the surface given by  $z=0$  is  $\nu=(0,0,-1)$ , and director on the surface  $\mathbf{n}(z=0)=(n_1, 0, n_3)$ . A finite  $K_{13}^*$  is obtained only if the scalar order parameter varies in the surface layer: only then the quantity  $\eta(z+r_3) - \eta(z)$

does not vanish and  $\gamma \neq 0$ . Thus, both  $K_{13}^*$  and  $K_{24}^*$  depend on the surface behavior of  $\rho$  and  $\eta$  through  $\gamma$ ; whereas  $K_{\alpha\alpha}^*$  remain surface independent and take their infinite-medium values. If  $\eta(\mathbf{x})$  is sufficiently smooth, a simple estimate gives  $K_{13}^* \sim (\eta_b - \eta_{z=0}) \rho_b^2 K_{13,b}$ , i.e., the effective value is proportional to the drop of the order parameter over the intermediate layer. A similar contribution to  $K_{13}$  (up to a factor) can be obtained in the Landau–de Gennes theory [18]. However, the relation (18) cannot be obtained in this pure phenomenological approach. Moreover, in contrast to this theory which to the leading order  $\eta^2$  predicts the ratio  $K_{11}^*/K_{33}^*=1$ , our result (20) is that the ratio remains arbitrary as in the Nehring-Saupe theory. In another recent paper [19], the terms linear in  $\eta$  were not considered in the Landau–de Gennes FE.

The final goal of the elastic theory is to find the equilibrium director field. The boundary condition, which determines the director along with the Euler-Lagrange equations, depends on the surface behavior of  $\eta$  and  $\rho$  solely through the effective values of the elastic constants [4]. This makes possible the elastic description of a nematic body with a nonideal surface. The elastic constants obtained above give a necessary connection of this elastic theory with the microscopic properties and details of the surface behavior. In particular, our result justifies a finite effective constant  $K_{13}$ . The above estimate shows that the maximum value of  $K_{13}^*$  is  $\rho_b^2 \eta_b K_{13, \eta}$  where  $K_{13, \eta}$  is the standard constant corresponding to the kernel  $G_\eta$ .

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