Derivative-Dependent Surface-Energy Terms in Nematic Liquid Crystals (*)

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Summary. — The boundary energy terms dependent on the first derivative of the director are analysed theoretically. Although these terms necessarily arise from nonlocal interactions, they are generally written as purely surface terms. We show that, in this case, the stable director configurations are described by functions with discontinuous derivatives at the boundaries. All the solutions given in literature, which are found by explicitly assuming the continuity of the derivatives, must, therefore, be revised. In a more correct formulation of the problem, the ranges of the interaction forces should be taken into account and continuous solutions are then obtained, which are generally well approximated by the discontinuous ones. The approximation, instead, is not good in the case of the energy term proposed by Dubois-Violette and Parodi, where the discontinuity has the form of a Dirac function. In this case a physically meaningful solution can be found only on the basis of a more suitable expression of the boundary energy.

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1. Introduction.

The equations which determine the equilibrium configuration of the director field in a nematic cell are obtained from a variational principle, i.e. from the requirement that the total free energy $F$ is a minimum (1). $F$ is generally written as the sum of volume and surface terms. The first ones give the conditions for local equilibrium in the bulk, which are expressed by second-order differential equations in the director components $n_i$. The surface terms give the boundary conditions. In the case of strong anchoring the director configuration at the surface is practically predetermined. This means that the values of $n_i$ at the boundary surface are given. On the contrary, for weak anchoring, the boundary conditions are expressed by a relation between $n_i$ and $\partial n_i / \partial x_1$ at the sample surface (2). Discrepancies among different authors are found when the derivatives $\partial n_i / \partial x_1$ explicitly appear in a surface energy term $G$ (3-4).

By analysing the origin of these discrepancies, the authors found that none of the previously given solutions (5-10) is correct. This very drastic conclusion can be understood with the following argument. When energy terms are written as purely surface ones, local forces are assumed. This is, strictly speaking, never rigorous and is certainly not correct when $G$ depends on the normal derivative of $n_i$. The interaction forces giving rise to terms of this kind are, in fact, essentially nonlocal.

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(1) See, for example, P. G. De Gennes: The Physics of Liquid Crystals (Clarendon Press, Oxford, 1974).