Chapter One
Variational Calculus

1.1. Introduction

The total elastic energy of a sample of a given material is obtained by integrating the elastic energy density over the volume of the sample, taking into account the surface contributions. In the simple case in which the sample is a slab of thickness d, the total energy per unit area is given by

$$F = \int_{-d/2}^{d/2} f(\phi, \phi')\mathrm{d}z + \gamma(\phi_1) + \gamma(\phi_2)\,, \tag{1.1}$$

where ϕ characterizes the deformation, and $\phi' = d\phi/dz$ is the equivalent of the deformation tensor. In Eq. (1.1), f is the bulk elastic energy density and $\gamma(\phi_1)$, $\gamma(\phi_2)$ the surface energy density, with $\phi_1 = \phi(-d/2)$ and $\phi_2 = \phi(d/2)$. According to general principles, the stable state is the one minimizing Eq. (1.1). F which is given by Eq. (1.1) is the number associated to the function $\phi(z)$, i.e. a functional. It is a generalization of the concept of function, where to a number corresponds a number.

The technique by means of which it is possible to find the function extremizing Eq. (1.1) is analyzed in this chapter devoted to the variational calculus.

We shall consider first the standard problem, where ϕ_1 and ϕ_2 are fixed on the boundaries. This corresponds to the case in which the surface contribution are very large with respect to the bulk contribution in Eq. (1.1):

AN ELEMENTARY COURSE ON THE CONTINUUM THEORY FOR NEMATIC LIQUID CRYSTALS

$$\gamma \gg \int_{-d/2}^{d/2} f(\phi, \phi')\mathrm{d}z\,.$$

The more general case in which the two contributions are of the same order will also be analyzed. This represents the so-called *weak anchoring*, where the values of ϕ_1 and ϕ_2 depends on the bulk distortions. We shall consider then cases in which f depends also on ϕ'', obtaining the new bulk differential equations. Special attention will be dedicated to well-posed and ill-posed problems. An extension of the calculations to cases such as $f = f(\phi, \psi, \phi', \psi')$, or to cases in which $\phi = \phi(x, z)$ is also reported.

1.2. Standard Variational Problem: Strong Anchoring

Determine the function $\phi(z) \in C_1$ extremizing the functional

$$F[\phi(z)] = \int_{-d/2}^{d/2} f[\phi(z), \phi'(z); z]\mathrm{d}z\,, \tag{1.2}$$

and assuming the values

$$\phi(z = -d/2) = \Phi_1\,, \quad \phi(z = d/2) = \Phi_2\,, \tag{1.3}$$

on the boundaries. This case, in which the values of the unknown function $\phi(z)$ are fixed on the border, is the so-called *strong-anchoring* situation.

Solution

Let $\tilde{\phi}(z) \in C_1$ be the function minimizing Eq. (1.2) and satisfying the boundary conditions (1.3), and $\phi(z) \in C_1$ a function close to $\tilde{\phi}(z)$ and satisfying the same boundary conditions (1.3) (see Fig. 1).

From now on, $\phi(z)$ close to $\tilde{\phi}(z)$ means that

$$\delta\phi(z) = \phi(z) - \tilde{\phi}(z) \tag{1.4}$$

is a small quantity, i.e. $|\delta\phi(z)| \ll 1$, $\forall\, z \in [-d/2, d/2]$. Since, for hypothesis, $\tilde{\phi}(z)$ is the function minimizing Eq. (1.2), it follows that

$$F[\phi(z)] > F[\tilde{\phi}(z)]\,. \tag{1.5}$$

Let us choose $\phi(z)$ close to $\tilde{\phi}(z)$, in the following way:

$$\phi(z) = \tilde{\phi}(z) + \alpha v(z)\,, \tag{1.6}$$

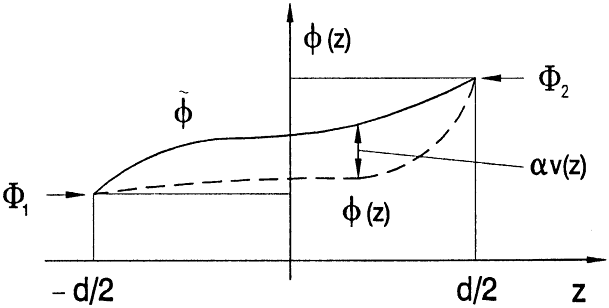

Fig. 1. $\tilde{\phi}(z)$ is the function extremizing the functional F and $\phi(z)$, a function close to it. In the strong-anchoring case under consideration $\tilde{\phi}(\pm d/2) = \phi(\pm d/2)$, i.e. the arbitrary function $v(z)$, vanishes for $z = \pm d/2$.

where $v(z) \in C_1$ is an arbitrary function and α a small parameter. By using Eq. (1.6), the functional Eq. (1.2) may be rewritten as

$$F[\phi(z)] = \int_{-d/2}^{d/2} f[\tilde{\phi}(z) + \alpha v(z), \tilde{\phi}'(z) + \alpha v'(z); z]\mathrm{d}z\,. \tag{1.7}$$

Equation (1.7) shows that $F[\phi(z)]$, considered as an ordinary function of the parameter α for hypothesis, has to reach its minimum value for $\alpha = 0$. Hence,

$$\left\{\frac{d}{d\alpha}\int_{-d/2}^{d/2} f[\tilde{\phi}(z) + \alpha v(z), \tilde{\phi}'(z) + \alpha v'(z); z]\mathrm{d}z\right\}_{\alpha=0} = 0\,. \tag{1.8}$$

By using elementary theorems on the derivation of functions defined by means of integrals, from Eq. (1.8) we obtain

$$\int_{-d/2}^{d/2}\left[\frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial \alpha} + \frac{\partial f}{\partial \phi'}\frac{\partial \phi'}{\partial \alpha}\right]_{\alpha=0}\mathrm{d}z = 0\,. \tag{1.9}$$

The quantities $\partial\phi/\partial\alpha$ and $\partial\phi'/\partial\alpha$ may be easily evaluated from Eq. (1.6), and they are found to be

$$\frac{\partial \phi(z)}{\partial \alpha} = v(z)\,, \quad \frac{\partial \phi'}{\partial \alpha} = v'(z)\,.$$

Consequently, the condition (1.9) can be rewritten in the form

$$\int_{-d/2}^{d/2}\left[\frac{\partial f}{\partial \tilde{\phi}}v(z) + \frac{\partial f}{\partial \tilde{\phi}'}v'(z)\right]\mathrm{d}z = 0\,. \tag{1.10}$$

Equation (1.10) tells us that $\tilde{\phi}(z)$ minimizes F, if the first variation of F, defined by

$$\delta_1 F = \left(\frac{\partial F}{\partial \alpha}\right)_{\alpha=0} \alpha\,,$$

vanishes $\forall\, v(z) \in C_1$. On the other hand, since

$$\frac{\partial f}{\partial \tilde{\phi}'} v'(z) = \frac{d}{dz}\left[\frac{\partial f}{\partial \tilde{\phi}'} v(z)\right] - \left[\frac{d}{dz}\frac{\partial f}{\partial \tilde{\phi}'}\right] v(z)\,,$$

Equation (1.10) may be rewritten in the following manner:

$$\int_{-d/2}^{d/2} \left[\frac{\partial f}{\partial \tilde{\phi}} - \frac{d}{dz}\frac{\partial f}{\partial \tilde{\phi}'}\right] v(z)\mathrm{d}z + \left[\frac{\partial f}{\partial \tilde{\phi}'} v(z)\right]_{-d/2}^{d/2} = 0\,. \qquad (1.11)$$

In the strong-anchoring case, the values of $\phi(z = \pm d/2)$ are fixed. This implies that not only $\tilde{\phi}(z)$, but also all the $\phi(z)$ have to satisfy the boundary conditions (1.3). If we take into account Eq. (1.6), it follows that the function $v(z)$ has to satisfy the boundary conditions

$$v(z = \pm d/2) = 0\,.$$

Consequently, Eq. (1.11) is simply written as

$$\int_{-d/2}^{d/2} \left[\frac{\partial f}{\partial \tilde{\phi}} - \frac{d}{dz}\frac{\partial f}{\partial \tilde{\phi}'}\right] v(z)\mathrm{d}z = 0\,, \quad \forall\, v(z) \in C_1\,. \qquad (1.12)$$

From Eq. (1.12), it follows that the minimizing function $\tilde{\phi}(z)$ we are looking for has to be a solution of the differential equation (Euler–Lagrange equation),

$$\frac{\partial f}{\partial \tilde{\phi}} - \frac{d}{dz}\frac{\partial f}{\partial \tilde{\phi}'} = 0\,, \quad \forall\, z \in (-d/2, d/2)\,, \qquad (1.13)$$

and to satisfy the boundary conditions (1.3). Since $F = f(\phi, \phi'; z)$, Eq. (1.13) is an ordinary differential equation of the second order, which has to be solved with the boundary conditions (1.3). In the case in which f is of the kind

$$f = f(\phi'; z)\,,$$

i.e. independent of ϕ, the quantity

$$m = \frac{\partial f}{\partial \phi'}$$

is independent of z, as it follows from Eq. (1.13). Furthermore, in the case in which f does not depend explicitly on the z coordinate, the quantity

$$p = \phi' \frac{\partial f}{\partial \phi'} - f \,, \tag{1.14}$$

is independent of z. In fact, if $f = f(\phi, \phi')$, from Eq. (1.14), it follows that

$$\begin{aligned} \frac{dp}{dz} &= \phi'' \frac{\partial f}{\partial \phi'} + \phi' \frac{d}{dz} \frac{\partial f}{\partial \phi'} - \frac{df}{dz} \\ &= \phi'' \frac{\partial f}{\partial \phi'} + \phi' \frac{d}{dz} \frac{\partial f}{\partial \phi'} - \frac{\partial f}{\partial \phi} \phi' - \frac{\partial f}{\partial \phi'} \phi'' \\ &= \phi' \left[\frac{d}{dz} \frac{\partial f}{\partial \phi'} - \frac{\partial f}{\partial \phi} \right] = 0 \,, \end{aligned}$$

because $\phi(z)$ has to satisfy Eq. (1.13).

The calculations reported above show that the function extremizing the functional Eq. (1.2) has to satisfy the Euler–Lagrange equation and the boundary conditions (1.3). In order to know if the extremizing function, solution of Eq. (1.13), minimizes or maximizes Eq. (1.2), it is necessary to evaluate the second variation of F, defined as

$$\delta_2 F = \frac{1}{2} \left(\frac{\partial^2 F}{\partial \alpha^2} \right)_{\alpha=0} \alpha^2 \,,$$

and to analyze its sign. This will be done in Sec. 1.5.

As an example, let us consider the case in which

$$f[\phi(z), \phi'(z); z] = \frac{1}{2} K(z) {\phi'}^2 + \frac{1}{2} U(z) \phi^2 \,, \tag{1.15}$$

which will be widely analyzed in the following. In the continuum theory of nematic liquid crystals (NLC), $K(z)$ is a material parameter describing the elastic properties of the medium. The second addendum describes the anisotropic interaction between the liquid crystal and an external field. Hence, the function $U(z)$ takes into account the external field and some anisotropy of the liquid crystal with respect to this field. If $K(z)$ and $U(z)$ are continuous functions in the range $-d/2 \leq z \leq d/2$, the function $\phi(z)$ extremizing Eq. (1.2), where f is given by Eq. (1.15), is a solution of the Euler–Lagrange Eq. (1.13) satisfying the boundary conditions (1.3). The bulk differential equation writes for the present case as

$$\frac{d}{dz}[K(z)\phi'(z)] - U(z)\phi(z) = 0\,. \tag{1.16}$$

The solution of Eq. (1.16) is a continuous function.

A simple analysis shows that all discontinuous functions $\hat{\phi}(z)$ are such that $F[\hat{\phi}] > F[\tilde{\phi}]$, where $\tilde{\phi}$ is the solution of Eq. (1.16) with the boundary conditions (1.3).

In fact, let $\hat{\phi}$ be a discontinuous function of the kind shown in Fig. 2, in the limit $\epsilon \to 0$. Hence, the functional $F[\hat{\phi}]$ can be evaluated as follows:

$$F[\hat{\phi}] = \lim_{\epsilon\to 0} F[\phi] = \lim_{\epsilon\to 0}\left\{\int_{-d/2}^{z^*-\epsilon/2} f\mathrm{d}z + \int_{z^*-\epsilon/2}^{z^*+\epsilon/2} f\mathrm{d}z + \int_{z^*+\epsilon/2}^{d/2} f\mathrm{d}z\right\}. \tag{1.17}$$

For $-d/2 \le z \le z^* - \epsilon/2$ and $z^* + \epsilon/2 \le z \le d/2$, the function $\hat{\phi}$ is continuous. Let us put

$$F_p[\hat{\phi}] = \lim_{\epsilon\to 0}\left\{\int_{-d/2}^{z^*-\epsilon/2} f\mathrm{d}z + \int_{z^*+\epsilon/2}^{d/2} f\mathrm{d}z\right\}, \tag{1.18}$$

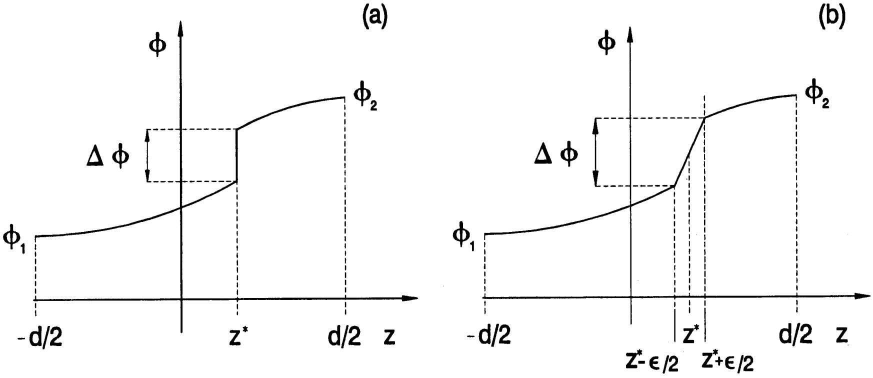

Fig. 2. (a) A function presenting a discontinuity in z^* such that $\hat{\phi}(z^*_+) - \hat{\phi}(z^*_-) = \Delta\phi$, (b) a continuous function $\phi(z)$ such that $\lim_{\epsilon\to 0}\phi(z) = \hat{\phi}$. Note that for $z^* - \epsilon/2 \le z \le z^* + \epsilon/2$, $\phi'(z) = \Delta\phi/\epsilon$.

which is a finite quantity. For all $z^* - \epsilon/2 \leq z \leq z^* + \epsilon/2$, $\phi' = \Delta\phi/\epsilon$, and hence, Eq. (1.15) reads

$$F = \frac{1}{2}K(z)\left(\frac{\Delta\phi}{\epsilon}\right)^2 + \frac{1}{2}U(z)\phi^2 .$$

It follows that

$$\lim_{\epsilon\to 0}\int_{z^*-\epsilon/2}^{z^*+\epsilon/2} f\mathrm{d}z = \lim_{\epsilon\to 0}\left(\frac{1}{2}\langle K\rangle\frac{(\Delta\phi)^2}{\epsilon}\right), \tag{1.19}$$

where

$$\langle K\rangle = \frac{1}{\epsilon}\int_{z^*-\epsilon/2}^{z^*+\epsilon/2} K(z)\mathrm{d}z$$

is the average value of $K(z)$ in the range $z^* - \epsilon/2 \leq z \leq z^* + \epsilon/2$, which is a finite quantity. By taking into account Eqs. (1.19) and (1.18), $F[\hat{\phi}]$ given by Eq. (1.17) becomes

$$F[\hat{\phi}] = F_p[\hat{\phi}] + \lim_{\epsilon\to 0}\left(\frac{\langle K\rangle}{2\epsilon}(\Delta\phi)^2\right),$$

which diverges in the considered limit. Hence,

$$F[\hat{\phi}] > F[\tilde{\phi}] ,$$

showing that the function minimizing $F[\phi]$ given by Eq. (1.2) when f is of the Eq. (1.15) kind, with $K(z)$ and $U(z)$ continuous, is a continuous function.

1.3. Standard Variational Problem: Weak Anchoring

Determine the function $\phi(z) \in C_1$ extremizing the functional

$$F[\phi(z)] = \int_{-d/2}^{d/2} f[\phi(z), \phi'(z); z]\mathrm{d}z + \gamma_1(\phi_1) + \gamma_2(\phi_2) , \tag{1.20}$$

in which again, $\phi_1 = \phi(-d/2)$ and $\phi_2 = \phi(d/2)$. The functional of the present problem contains, besides the usual part integrated over the thickness of the sample d, two other terms depending only on the values of the unknown function at the boundaries $\pm d/2$. This corresponds to the so-called *weak-anchoring* situation, in which the values of $\phi(\pm d/2)$ are not fixed.

Solution

In the present case, ϕ_1 and ϕ_2 cannot be considered fixed. If $\tilde{\phi}(z)$ is the function minimizing the functional $F[\phi(z)]$ given by Eq. (1.20), a function $\phi(z)$

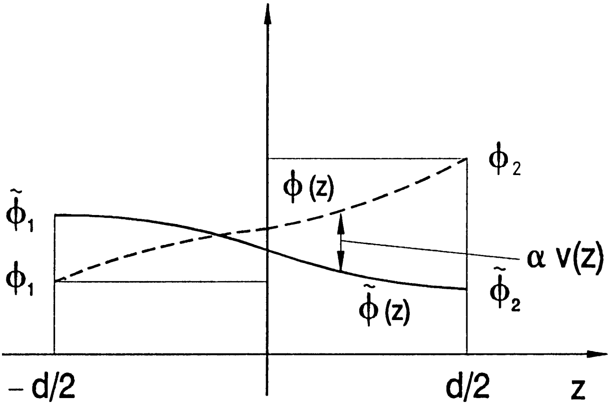

Fig. 3. $\tilde{\phi}(z)$ is the function extremizing the functional F and $\phi(z)$, a function close to it. In the weak-anchoring case, the values of the extremizing function on the boundaries are not imposed. Hence, $\tilde{\phi}(\pm d/2) \neq \phi(\pm d/2)$ and the arbitrary function $v(z)$ does not vanish for $z = \pm d/2$.

close to $\tilde{\phi}(z)$ can be of the kind shown in Fig. 3. By operating as in the Sec. 1.2, let $\tilde{\phi}(z)$ be the minimizing function, and $\phi(z) = \tilde{\phi}(z) + \alpha v(z)$, a function close to $\tilde{\phi}(z)$.

Now the values $v(\pm d/2)$ are arbitrary. By indicating with $\tilde{\phi}_1 = \tilde{\phi}(z = -d/2)$ and $\tilde{\phi}_2 = \tilde{\phi}(z = d/2)$, the values of the minimizing function $\tilde{\phi}(z)$ at the boundaries, we have

$$\gamma_1(\phi_1) = \gamma_1[\tilde{\phi}_1 + \alpha v(-d/2)] \quad \text{and} \quad \gamma_2(\phi_2) = \gamma_2[\tilde{\phi}_2 + \alpha v(d/2)]\,.$$

Consequently,

$$\begin{aligned} \frac{d\gamma_1(\phi_1)}{d\alpha} &= \frac{d\gamma_1}{d\phi_1}\frac{d\phi_1}{d\alpha} = \frac{d\gamma_1}{d\phi_1}v(-d/2)\,, \\ \frac{d\gamma_2(\phi_2)}{d\alpha} &= \frac{d\gamma_2}{d\phi_2}\frac{d\phi_2}{d\alpha} = \frac{d\gamma_2}{d\phi_2}v(d/2)\,. \end{aligned} \tag{1.21}$$

It follows that the quantity

$$\left[\frac{dF}{d\alpha}\right]_{\alpha=0} = \left\{\frac{d}{d\alpha}\int_{-d/2}^{d/2} f[\phi(z), \phi'(z); z]\mathrm{d}z + \frac{d\gamma_1(\phi_1)}{d\alpha} + \frac{d\gamma_2(\phi_2)}{d\alpha}\right\}_{\alpha=0},$$

by taking into account Eqs. (1.11) and (1.21), may be rewritten as

$$\begin{aligned}\left[\frac{dF}{d\alpha}\right]_{\alpha=0} = &\left\{\int_{-d/2}^{d/2}\left[\frac{\partial f}{\partial \phi} - \frac{d}{dz}\frac{\partial f}{\partial \phi'}\right] v(z)\mathrm{d}z\right\}_{\alpha=0}\\ &+\left\{\left[\left(\frac{\partial f}{\partial \phi'}\right)_{d/2} + \frac{d\gamma_2}{d\phi_2}\right] v(d/2)\right\}_{\alpha=0}\\ &+\left\{\left[-\left(\frac{\partial f}{\partial \phi'}\right)_{-d/2} + \frac{d\gamma_1}{d\phi_1}\right] v(-d/2)\right\}_{\alpha=0} . \end{aligned} \tag{1.22}$$

Since $\tilde{\phi}(z)$ minimizes F, we deduce that

$$\delta_1 F = \left(\frac{dF}{d\alpha}\right)_{\alpha=0} \alpha = 0\,, \quad \forall\, v(z) \in C_1\,.$$

Consequently, from Eq. (1.22), it follows that $\tilde{\phi}(z)$ is still a solution of the differential Eq. (1.13), but now it satisfies the boundary conditions

$$-\frac{\partial f}{\partial \tilde{\phi}'} + \frac{d\gamma_1}{d\phi_1} = 0\,, \quad \frac{\partial f}{\partial \tilde{\phi}'} + \frac{d\gamma_2}{d\phi_2} = 0\,, \tag{1.23}$$

for $z = -d/2$ and $z = d/2$, respectively.

In the particular case in which, for instance, $\gamma_1 = 0$, the first boundary condition appearing in Eqs. (1.23) reads

$$\frac{\partial f}{\partial \tilde{\phi}'} = 0\,, \tag{1.24}$$

for $z = -d/2$. This condition is usually called "condition of transversality." A boundary condition of this kind is present all the time if the value of the function we are looking for is completely arbitrary at the border. This border is called "free border."

Since the bulk equation is the same obtained in the strong-anchoring case, all the discussion concerning m and p remains valid in the present situation (see Eq. (1.14)).

It is possible to derive the boundary conditions (1.23) in an alternative way. To do this, we just have to remember that in our case, $f = f(\phi, \phi'; z)$. Therefore, the differential equation (1.13) is an ordinary differential equation of the second order, whose general solution contains two integration constants

c_1 and c_2. Let us choose as integration constants, the values of the function at $z=-d/2$, $\phi_1=\phi(-d/2)$, and at $z=d/2$, $\phi_2=\phi(d/2)$. Hence, the general solution of Eq. (1.13) is of the kind

$$\phi=\phi(\phi_1,\phi_2;z)\,. \tag{1.25}$$

Substitution of Eq. (1.25) into Eq. (1.20) yields F as an *ordinary* function of ϕ_1 and ϕ_2 of the type

$$F[\phi_1,\phi_2]=\int_{-d/2}^{d/2} f[\phi(\phi_1,\phi_2;z),\phi'(\phi_1,\phi_2;z);z]\mathrm{d}z+\gamma_1(\phi_1)+\gamma_2(\phi_2)\,. \tag{1.26}$$

The parameters ϕ_1 and ϕ_2 may be deduced by looking for the minimum of $F(\phi_1,\phi_2)$. Thus, the actual values of ϕ_1 and ϕ_2, which we call $\tilde{\phi}_1$ and $\tilde{\phi}_2$, are given by

$$\frac{\partial F(\phi_1,\phi_2)}{\partial\phi_1}=\frac{\partial F(\phi_1,\phi_2)}{\partial\phi_2}=0\,. \tag{1.27}$$

The solutions of (1.27), $\tilde{\phi}_1$ and $\tilde{\phi}_2$, minimize $F(\phi_1,\phi_2)$ if

$$\left(\frac{\partial^2 F}{\partial{\phi_{1,2}}^2}\right)_{\phi_1=\tilde{\phi}_1,\phi_2=\tilde{\phi}_2}>0\,, \tag{1.28}$$

and

$$\mathcal{H}(\tilde{\phi}_1,\tilde{\phi}_2)=\left[\frac{\partial^2 F}{\partial{\phi_1}^2}\frac{\partial^2 F}{\partial{\phi_2}^2}-\left(\frac{\partial^2 F}{\partial\phi_1\partial\phi_2}\right)^2\right]_{\phi_1=\tilde{\phi}_1,\phi_2=\tilde{\phi}_2}>0\,. \tag{1.29}$$

Let us evaluate $\partial F/\partial\phi_1$, taking into account that ϕ_1 and ϕ_2 are independent quantities, and hence, $\partial\phi_1/\partial\phi_2=\partial\phi_2/\partial\phi_1=0$. Through Eq. (1.26), we obtain

$$\frac{\partial F}{\partial\phi_1}=\frac{\partial}{\partial\phi_1}\int_{-d/2}^{d/2} f[\phi(\phi_1,\phi_2;z),\phi'(\phi_1,\phi_2;z);z]\mathrm{d}z+\frac{d\gamma_1}{d\phi_1}\,. \tag{1.30}$$

Simple calculations give

$$\begin{aligned}\frac{\partial}{\partial\phi_1}\int_{-d/2}^{d/2} f(\phi,\phi';z)\mathrm{d}z&=\int_{-d/2}^{d/2}\frac{\partial f(\phi,\phi';z)}{\partial\phi_1}\mathrm{d}z\\&=\int_{-d/2}^{d/2}\left(\frac{\partial f}{\partial\phi}\frac{\partial\phi}{\partial\phi_1}+\frac{\partial f}{\partial\phi'}\frac{\partial\phi'}{\partial\phi_1}\right)\mathrm{d}z\,.\end{aligned} \tag{1.31}$$

By taking into account that

$$\frac{\partial f}{\partial \phi'}\frac{\partial \phi'}{\partial \phi_1} = \frac{\partial f}{\partial \phi'}\frac{d}{dz}\left(\frac{\partial \phi}{\partial \phi_1}\right) = \frac{d}{dz}\left[\frac{\partial f}{\partial \phi'}\frac{\partial \phi}{\partial \phi_1}\right] - \left[\frac{d}{dz}\frac{\partial f}{\partial \phi'}\right]\frac{\partial \phi}{\partial \phi_1}\,,$$

Eq. (1.31) may be rewritten as

$$\frac{\partial}{\partial \phi_1}\int_{-d/2}^{d/2} f(\phi,\phi';z)\mathrm{d}z = \int_{-d/2}^{d/2}\frac{\partial \phi}{\partial \phi_1}\left[\frac{\partial f}{\partial \phi} - \frac{d}{dz}\frac{\partial f}{\partial \phi'}\right]\mathrm{d}z + \left[\frac{\partial f}{\partial \phi'}\frac{\partial \phi}{\partial \phi_1}\right]_{-d/2}^{d/2}$$
$$= -\left(\frac{\partial f}{\partial \phi'}\right)_{-d/2}\,,$$

because $\phi(z)$ is a solution of Eq. (1.13). Consequently, Eq. (1.30) is equivalent to

$$\frac{\partial F}{\partial \phi_1} = -\left(\frac{\partial f}{\partial \phi'}\right)_{-d/2} + \frac{d\gamma_1}{d\phi_1}\,. \tag{1.32}$$

A similar calculation gives

$$\frac{\partial}{\partial \phi_2}\int_{-d/2}^{d/2} f(\phi,\phi';z)\mathrm{d}z = \left(\frac{\partial f}{\partial \phi'}\right)_{d/2}\,,$$

and hence,

$$\frac{\partial F}{\partial \phi_2} = \left(\frac{\partial f}{\partial \phi'}\right)_{d/2} + \frac{d\gamma_2}{d\phi_2}\,. \tag{1.33}$$

Substitution of Eqs. (1.32) and (1.33) into Eq. (1.27) yields

$$\frac{\partial F}{\partial \phi_1} = -\left(\frac{\partial f}{\partial \phi'}\right)_{-d/2} + \frac{d\gamma_1}{d\phi_1} = 0\,, \quad \frac{\partial F}{\partial \phi_2} = \left(\frac{\partial f}{\partial \phi'}\right)_{d/2} + \frac{d\gamma_2}{d\phi_2} = 0\,. \tag{1.34}$$

The boundary conditions (1.34) coincide with the boundary conditions (1.23) obtained above in another manner. The alternative way described now may be very useful to analyze the stability of the solution of the Euler–Lagrange equation (see Eqs. (1.28) and (1.29)).

1.4. Mechanical Interpretation of the First Variation of a Functional

Analyze the first variation of the functional

$$F[\phi(z)] = \int_{-d/2}^{d/2} f[\phi(z),\phi'(z);z]\mathrm{d}z\,, \tag{1.35}$$

in the strong-anchoring situation, in terms of virtual works. Generalize the obtained result to the weak-anchoring situation.

Solution

As in the preceding sections, let $\tilde{\phi}(z)$ be the function minimizing Eq. (1.35) and $\phi(z) = \tilde{\phi}(z) + \alpha v(z)$, a function close to $\tilde{\phi}(z)$. As we have shown in Sec. 1.2, the first variation of F is given by

$$\delta_1 F = \left(\frac{dF}{d\alpha}\right)_0 \alpha = \int_{-d/2}^{d/2} \Psi(\phi, \phi'; z)\delta\phi(z)\mathrm{d}z\,,$$

where

$$\Psi(\phi, \phi'; z) = \frac{\partial f}{\partial \phi} - \frac{d}{dz}\left(\frac{\partial f}{\partial \phi'}\right),$$

and

$$\delta\phi(z) = \phi(z) - \tilde{\phi}(z) = \alpha v(z)\,.$$

Let us imagine now that F is the free energy (per unit surface) of a physical system characterized by the dynamical variable $\phi(z)$. In this situation, $\delta_1 F$ coincides with the work done on the system to evolve from $\tilde{\phi}(z)$ to $\phi(z)$. It follows that $\Psi(\phi, \phi'; z)$ is the bulk density of force. The condition $\delta_1 F = 0, \forall\, \delta\phi(z) \in C_1$, gives

$$\Psi(\tilde{\phi}, \tilde{\phi}'; z) = \frac{\partial f}{\partial \tilde{\phi}} - \frac{d}{dz}\left(\frac{\partial f}{\partial \tilde{\phi}'}\right) = 0\,, \quad \forall\, z \in (-d/2, d/2)\,. \tag{1.36}$$

Equation (1.36) may be interpreted in the following manner: the stable state is characterized by zero bulk density force (this is the D'Alembert's principle).

In the situation of weak-anchoring, the functional is of the kind

$$F[\phi(z)] = \int_{-d/2}^{d/2} f[\phi(z), \phi'(z); z]\mathrm{d}z + \gamma_1(\phi_1) + \gamma_2(\phi_2)\,,$$

whose first variation is, as shown previously,

$$\delta_1 F = \left(\frac{dF}{d\alpha}\right)_0 \alpha = \int_{-d/2}^{d/2} \Psi(\phi, \phi'; z)\delta\phi(z)\mathrm{d}z + (t_2 + m_2)\delta\phi_2 + (t_1 - m_1)\delta\phi_1\,,$$

where

$$t_1 = \frac{d\gamma_1}{d\phi_1}\,, \quad m_1 = \left(\frac{\partial f}{\partial \phi'}\right)_{-d/2}\,, \quad \delta\phi_1 = \alpha v(-d/2)\,,$$

$$t_2 = \frac{d\gamma_2}{d\phi_2}\,, \quad m_2 = \left(\frac{\partial f}{\partial \phi'}\right)_{d/2}\,, \quad \delta\phi_2 = \alpha v(d/2)\,.$$

The quantities t_1 and t_2 may be interpreted as the forces transmitted by the surfaces to the system, whereas m_1 and m_2 as the forces transmitted by the system to the surfaces. In a situation of equilibrium

$$\Psi(\tilde{\phi}, \tilde{\phi}'; z) = 0\,, \quad \forall\, z \in (-d/2, d/2)\,,$$

states that the bulk density of force has to vanish, as we have seen before. Furthermore,

$$t_2 + m_2 = 0 \quad \text{and} \quad t_1 - m_1 = 0\,, \tag{1.37}$$

whose physical meaning is simple: the forces transmitted from the system to the surfaces have to be balanced by the forces originating from the surfaces.

We want to finish this section by considering the particular case in which $f = f[\phi'(z); z]$. As discussed in Sec. 1.2, in this situation, the quantity $m = \partial f/\partial \phi'$ is independent of z. Consequently,

$$m = m_1 = \left(\frac{\partial f}{\partial \phi'}\right)_{-d/2} = \left(\frac{\partial f}{\partial \phi'}\right)_{d/2} = m_2\,,$$

and the "boundary conditions" (1.37) write

$$t_2 + m = 0 \quad \text{and} \quad t_1 - m = 0\,,$$

giving

$$t_1 + t_2 = 0\,.$$

It follows that: if $f = f[\phi'(z); z]$, the force transmitted across the sample is constant, and the force originated by one surface is balanced by the other surface.

1.5. Second Variation and Jacobi Equation

In the strong-anchoring situation, analyze the second variation of the functional

$$F[\phi(z)] = \int_{-d/2}^{d/2} f[\phi(z), \phi'(z); z]\mathrm{d}z\,, \tag{1.38}$$

in order to decide in what case the solution of the Euler–Lagrange equation corresponds to a minimum or to a maximum of $F[\phi(z)]$.

Solution

Let $\tilde{\phi}(z)$ be the function minimizing Eq. (1.38) and $\phi(z) = \tilde{\phi}(z) + \alpha v(z)$, a function close to $\tilde{\phi}(z)$. As we have shown before,

$$\frac{dF}{d\alpha} = \int_{-d/2}^{d/2} \left[\frac{\partial f}{\partial \phi} v(z) + \frac{\partial f}{\partial \phi'} v'(z) \right] \mathrm{d}z \,. \tag{1.39}$$

From Eq. (1.39), a simple calculation gives

$$\frac{d^2F}{d\alpha^2} = \int_{-d/2}^{d/2} \left[\frac{\partial^2 f}{d\phi^2} v^2(z) + 2\frac{\partial^2 f}{\partial\phi\partial\phi'} v(z)v'(z) + \frac{\partial^2 f}{\partial\phi'^2} v'^2(z) \right] \mathrm{d}z \,. \tag{1.40}$$

In the limit $\alpha \to 0$, $F(\alpha)$ may be approximated by

$$F(\alpha) = F(0) + \left(\frac{dF}{d\alpha}\right)_0 \alpha + \frac{1}{2}\left(\frac{d^2F}{d\alpha^2}\right)_0 \alpha^2 + \dots \,.$$

The quantities

$$\delta_1 F = \left(\frac{dF}{d\alpha}\right)_0 \alpha \quad \text{and} \quad \delta_2 F = \frac{1}{2}\left(\frac{d^2F}{d\alpha^2}\right)_0 \alpha^2 \,,$$

are called first and second variation of F, respectively. The Euler–Lagrange equation, discussed in Secs. 1.2 and 1.3, has been obtained by imposing $\delta_1 F = 0$, $\forall\, v(z) \in C_1$, which implies that $(dF/d\alpha)_0 = 0$. If $\phi(z)$ is a solution of the Euler–Lagrange equation, it extremizes $F[\phi(z)]$. In order to know if the extremum is a minimum or a maximum, it is necessary to analyze the sign of $\delta_2 F$, i.e. of $(d^2F/d\alpha^2)_0$. As well known if $(d^2F/d\alpha^2)_0 > 0$, $\tilde{\phi}$ minimizes $F[\phi]$, and if $(d^2F/d\alpha^2)_0 < 0$, $\tilde{\phi}$ maximizes $F[\phi]$.

Let us consider the case of strong anchoring, where $v(-d/2) = v(d/2) = 0$. In this situation, the quantity

$$\begin{aligned}\int_{-d/2}^{d/2} [h'(z)v^2(z) + 2h(z)v(z)v'(z)]\mathrm{d}z &= \int_{-d/2}^{d/2} \frac{d}{dz}[h(z)v^2(z)]\mathrm{d}z \\ &= h(d/2)v^2(d/2) - h(-d/2)v^2(-d/2) \,,\end{aligned}$$

is identically zero for every function $h(z)$, because the function $v(z)$ vanishes for $z = \pm d/2$. It follows that $d^2F/d\alpha^2$, given by Eq. (1.40) can be written as

$$\begin{aligned}\frac{d^2F}{d\alpha^2} &= \int_{-d/2}^{d/2}\left[\frac{\partial^2 f}{\partial\phi^2}v^2 + 2\frac{\partial^2 f}{\partial\phi\partial\phi'}vv' + \frac{\partial^2 f}{\partial{\phi'}^2}{v'}^2\right]\mathrm{d}z\\ &= \int_{-d/2}^{d/2}\left[\left(\frac{\partial^2 f}{\partial\phi^2} + h'\right)v^2 + 2\left(\frac{\partial^2 f}{\partial\phi\partial\phi'} + h\right)vv' + \frac{\partial^2 f}{\partial{\phi'}^2}{v'}^2\right]\mathrm{d}z\\ &= \int_{-d/2}^{d/2}\frac{\partial^2 f}{\partial{\phi'}^2}\left[{v'}^2 + 2\left(\frac{\partial^2 f}{\partial\phi\partial\phi'} + h\right)\left(\frac{\partial^2 f}{\partial{\phi'}^2}\right)^{-1}vv'\right.\\ &\qquad\left. + \left(\frac{\partial^2 f}{\partial\phi^2} + h'\right)\left(\frac{\partial^2 f}{\partial{\phi'}^2}\right)^{-1}v^2\right]\mathrm{d}z\,.\end{aligned}$$

The relation obtained, shows that, in the event in which the differential equation

$$\frac{\partial^2 f}{\partial\phi^2} + h' = \left[\frac{\partial^2 f}{\partial\phi\partial\phi'} + h\right]^2\left(\frac{\partial^2 f}{\partial{\phi'}^2}\right)^{-1}, \tag{1.41}$$

has a solution, it is possible to rewrite $d^2F/d\alpha^2$ in the form

$$\frac{d^2F}{d\alpha^2} = \int_{-d/2}^{d/2}\frac{\partial^2 f}{\partial{\phi'}^2}\left[v' + \left(\frac{\partial^2 f}{\partial\phi\partial\phi'} + h\right)\left(\frac{\partial^2 f}{\partial{\phi'}^2}\right)^{-1}v\right]^2\mathrm{d}z\,, \tag{1.42}$$

by means of which it is easy to deduce information about the sign of $(d^2F/d\alpha^2)_0$. Of course, Eq. (1.42) holds only in the case in which Eq. (1.41) can be solved. Furthermore, in Eq. (1.41), the arbitrary function $v(z)$ is absent. Equation (1.41) may be rewritten as

$$\frac{\partial^2 f}{\partial{\phi'}^2}\left(\frac{\partial^2 f}{\partial\phi^2} + h'\right) = \left[\frac{\partial^2 f}{\partial\phi\partial\phi'} + h\right]^2. \tag{1.43}$$

Equation (1.43) is called Jacobi's equation. When Eq. (1.43) admits solutions, the sign of $(d^2F/d\alpha^2)_0$, given by

$$\left(\frac{d^2F}{d\alpha^2}\right)_0 = \int_{-d/2}^{d/2}\left\{\frac{\partial^2 f}{\partial{\phi'}^2}\left[v' + \left(\frac{\partial^2 f}{\partial\phi\partial\phi'} + h\right)\left(\frac{\partial^2 f}{\partial{\phi'}^2}\right)^{-1}v\right]^2\right\}_{\phi=\tilde\phi}\mathrm{d}z\,, \tag{1.44}$$

coincides with the sign of

$$\left[\frac{\partial^2 f}{\partial \phi'^2}\right]_{\phi=\tilde{\phi}}.$$

In this case, the analysis of the stability of the solution of the Euler–Lagrange equation is simple.

As an application, let us consider the case in which

$$f(\phi,\phi';z)=\frac{1}{2}K\phi'^2+\frac{1}{2}A\phi^2\,, \tag{1.45}$$

where K and A are two positive constants. As we shall see in the chapters devoted to the NLC, Eq. (1.45) represents the energy density of an NLC submitted to an external field, in the limit of small deformations. In this context, K is an elastic property of the medium, and A depends on the applied field and on the dielectric (or diamagnetic) anisotropy of the liquid crystal. Let us suppose the anchoring is strong, and call $\Phi_1=\phi(-d/2)$ and $\Phi_2=\phi(d/2)$. In this situation, the Euler–Lagrange equation relevant to this problem is

$$-K\tilde{\phi}''+A\tilde{\phi}=0\,,$$

whose solution is

$$\tilde{\phi}(z)=c_1\exp(z/l)+c_2\exp(-z/l)\,, \tag{1.46}$$

where $l^2=K/A$, and c_1 and c_2 are two integration constants. They are given by the boundary conditions

$$c_1\exp(-d/2l)+c_2\exp(d/2l)=\Phi_1\,,$$

$$c_1\exp(d/2l)+c_2\exp(-d/2l)=\Phi_2\,.$$

A simple calculation gives

$$c_1=\frac{\Phi_1\exp(-d/2l)-\Phi_2\exp(d/2l)}{\exp(-d/l)-\exp(d/l)}\,,\quad c_2=\frac{\Phi_2\exp(-d/2l)-\Phi_1\exp(d/2l)}{\exp(-d/l)-\exp(d/l)}\,.$$

Substitution of c_1 and c_2 into Eq. (1.46) yields

$$\tilde{\phi}(z)=\frac{-\Phi_1\sinh\left[(z-d/2)/l\right]+\Phi_2\sinh\left[(z+d/2)/l\right]}{\sinh(d/l)}\,. \tag{1.47}$$

In order to know if Eq. (1.47) minimizes the functional F, given by Eq. (1.38), we can use Jacobi's equation. By taking into account that

$$\frac{\partial^2 f}{\partial\phi'^2}=K\,,\quad \frac{\partial^2 f}{\partial\phi^2}=A\,,\quad \text{and}\quad \frac{\partial^2 f}{\partial\phi'\partial\phi}=0\,,$$

Eq. (1.43) can be rewritten as

$$K(A+h') = h^2\,,$$

whose solution is

$$h(z) = \sqrt{KA}\,\frac{1+\exp\left[2z/l+c\right]}{1-\exp\left[2z/l+c\right]}\,. \tag{1.48}$$

In Eq. (1.48), c is an integration constant, not important in our analysis. Since the Jacobi's equation admits solutions, Eq. (1.42) holds. Furthermore, since in the present case,

$$\left(\frac{\partial^2 f}{\partial \phi'^2}\right)_{\phi=\tilde{\phi}} = K > 0\,,$$

by means of Eq. (1.44), we deduce that

$$\left(\frac{d^2 F}{d\alpha^2}\right)_0 > 0\,.$$

Consequently, Eq. (1.47) minimizes the functional (1.38), in which $f(\phi,\phi';z)$ is given by Eq. (1.45).

In the event in which the anchoring is weak, it is possible to generalize the above procedure. However, in general, it is simpler to study the ordinary function $F(\phi_1,\phi_2)$, as shown in Sec. 1.3. In fact, we have shown that it is enough to analyze the sign of $\partial^2 F/\partial {\phi_1}^2$ and

$$\mathcal{H}(\tilde{\phi}_1,\tilde{\phi}_2) = \left[\frac{\partial^2 F}{\partial {\phi_1}^2}\frac{\partial^2 F}{\partial {\phi_2}^2} - \left(\frac{\partial^2 F}{\partial \phi_1 \partial \phi_2}\right)^2\right]\,,$$

for $\phi_1 = \tilde{\phi}_1$ and $\phi_2 = \tilde{\phi}_2$.

1.6. Well-Posed Problem: Different Approaches, Same Solution

Determine the function $\phi(z)$ extremizing the functional

$$F[\phi(z)] = \int_0^d \frac{1}{2}K{\phi'}^2(z)\mathrm{d}z + \frac{1}{2}W(\varphi-\Phi)^2\,, \tag{1.49}$$

where $K > 0$, $W > 0$, Φ is a constant and $\varphi = \phi(d)$. Suppose that the anchoring on the $z=0$ surface is strong and such that $\phi(0)=0$. Verify that the different ways to solve the problem give the same extremizing function $\phi(z)$. Furthermore, evaluate $\delta_1 F$ and $\delta_2 F$.

Solution

(a) *Direct way*

According to this method, $\tilde{\phi}(z)$ extremizing Eq. (1.49) is a solution of the Euler–Lagrange equation

$$\frac{\partial f}{\partial \phi} - \frac{d}{dz}\frac{\partial f}{\partial \phi'} = 0\,, \quad \forall\, z \in [0, d]\,, \tag{1.50}$$

satisfying the boundary conditions

$$-\frac{\partial f}{\partial \phi'} + \frac{d\gamma_1}{d\phi_1} = 0 \quad \text{and} \quad \frac{\partial f}{\partial \phi'} + \frac{d\gamma_2}{d\phi_2} = 0\,, \tag{1.51}$$

for $z = 0$ and $z = d$, respectively, as we have shown in the first part of Sec. 1.3. In the present case, the first boundary condition (1.51) is substituted by

$$\phi(0) = 0\,, \tag{1.52}$$

as it follows from the strong-anchoring hypothesis at $z = 0$. Since $f(\phi, \phi') = (1/2)\, K\phi'^2$, the main equations of the problem we are analyzing become

$$\tilde{\phi}''(z) = 0\,, \quad z \in [0, d]\,, \tag{1.53}$$

and

$$K\tilde{\phi}'(d) + W(\varphi - \Phi) = 0\,, \quad z = d\,, \tag{1.54}$$

and Eq. (1.52). The solution of Eq. (1.53) is

$$\tilde{\phi}(z) = (\varphi - \beta)\frac{z}{d} + \beta\,,$$

where the integration constant β is zero, as it follows from Eq. (1.52). By inserting

$$\tilde{\phi}(z) = \varphi\frac{z}{d}\,, \tag{1.55}$$

into Eq. (1.54), we obtain

$$\frac{K}{d}\varphi + W(\varphi - \Phi) = 0\,,$$

which determines the other integration constant $\varphi = \tilde{\phi}(d)$. A simple calculation gives

$$\varphi = \frac{W}{W + K/d}\Phi\,. \tag{1.56}$$

The function extremizing Eq. (1.49) and satisfying the boundary condition $\phi(0) = 0$ is then Eq. (1.55), in which φ is given by Eq. (1.56).

(b) *Method of the integration constants*

According to this way, it is necessary to solve the Euler–Lagrange equation, in which two integration constants are present (in our case, only one). After that, we have to substitute into Eq. (1.49) the general solution obtained. In this way, F will be an ordinary function of the integration constants. They will be determined by looking for the minimum of F. The solution of Eq. (1.53), vanishing for $z = 0$, is given by Eq. (1.55), in which appears the integration constant φ. Substitution of Eq. (1.55) into Eq. (1.49) yields

$$F(\varphi) = \frac{1}{2}K\frac{\varphi^2}{d} + \frac{1}{2}W(\varphi - \Phi)^2 \,. \tag{1.57}$$

From Eq. (1.57), simple calculations give

$$\frac{dF}{d\varphi} = \frac{K}{d}\varphi + W(\varphi - \Phi) \quad \text{and} \quad \frac{d^2F}{d\varphi^2} = \frac{K}{d} + W \,. \tag{1.58}$$

When we impose $dF/d\varphi = 0$, Eqs. (1.58) give again Eq. (1.56). Furthermore, since $d^2F/d\varphi^2 > 0$, the obtained solution minimizes $F(\phi)$. The two methods are, then, completely equivalent.

(c) *Evaluation of the first and second variation of F*

In order to evaluate $\delta_1 F$ and $\delta_2 F$, let us consider the function

$$\phi(z) = \tilde{\phi}(z) + \frac{1}{2}\alpha z^2 \,, \tag{1.59}$$

where $\tilde{\phi}(z)$ is given by Eq. (1.55) in which φ has the value as in Eq. (1.56). By substituting Eq. (1.59) into Eq. (1.49), routine calculations give

$$F(\alpha) = \frac{K}{2}\left(\frac{\varphi^2}{d} + \frac{1}{3}\alpha^2 d^3 + \alpha\, d\,\varphi\right) + \frac{W}{2}\left(\varphi + \frac{1}{2}\alpha\, d^2 - \Phi\right)^2 ,$$

from which we obtain

$$\frac{dF}{d\alpha} = \frac{K}{2}\left(\frac{2}{3}\alpha\, d^3 + \varphi d\right) + \frac{W}{2}\left(\varphi + \frac{1}{2}\alpha\, d^2 - \Phi\right) d^2 \,, \tag{1.60}$$

and

$$\frac{d^2F}{d\alpha^2} = \frac{1}{3}d^4\left(\frac{K}{d} + \frac{3}{4}W\right) > 0 \,.$$

Furthermore, from Eq. (1.60) we have that

$$\left(\frac{dF}{d\alpha}\right)_0 = \frac{1}{2}\left(\frac{K}{d}+W\right)d^2\left(\varphi-\frac{W}{W+K/d}\Phi\right),$$

which is identically zero in the case in which φ is given by Eq. (1.56). Consequently, $\delta_1 F$ and $\delta_2 F$ are found to be

$$\delta_1 F = \left(\frac{\partial F}{d\alpha}\right)_0 \alpha = 0\,,$$

$$\delta_2 F = \frac{1}{2}\left(\frac{d^2F}{d\alpha^2}\right)_0 \alpha^2 = \frac{1}{6}d^4\left(\frac{K}{d}+\frac{3}{4}W\right)\alpha^2 > 0\,.$$

The circumstance $\delta_2 F > 0$ tells us that the function $\tilde{\phi}(z)$ minimizes $F[\phi]$. We can then conclude that in the case in which the problem is well-posed, the different ways give the same minimizing function $\tilde{\phi}(z)$. This function is such that $\delta_1 F = 0$. We remember that a problem is well-posed when the number of boundary conditions is equal to the number of integration constants to be determined.

1.7. Functionals Containing $\phi''(z)$: Strong Anchoring

Find the extremizing function $\phi(z)$ of the functional

$$F[\phi(z)] = \int_{-d/2}^{d/2} f[\phi(z),\phi'(z),\phi''(z)]\mathrm{d}z, \tag{1.61}$$

where $\phi' = d\phi(z)/dz$ and $\phi'' = d^2\phi(z)/dz^2$, in the hypothesis of strong anchoring in which $\phi(-d/2) = \Phi_1$ and $\phi(d/2) = \Phi_2$.

Solution

Functionals of the type (1.61) play an important role in some elastic problems, in which the spatial variation of some physical parameter is very large near the surface limiting the sample. In those cases, a description of the Landau–Ginzburg kind for the elastic energy density is not enough. It is usually necessary to introduce in the nonuniform part of the energy density, not only the term proportional to ϕ'^2, but also a term proportional to ϕ''^2. In order to find the function $\tilde{\phi}(z)$ minimizing functional (1.61), we can operate in the usual manner. Let $\phi(z)$ be a function close to $\tilde{\phi}(z)$ of the kind $\phi(z) = \tilde{\phi}(z) + \alpha v(z)$, where $v(\pm d/2) = 0$ for the strong-anchoring hypothesis. Then, simple calculations give

$$\frac{dF}{d\alpha} = \int_{-d/2}^{d/2} \left[\frac{\partial f}{\partial \phi} v + \frac{\partial f}{\partial \phi'} v' + \frac{\partial f}{\partial \phi''} v'' \right] \mathrm{d}z. \tag{1.62}$$

By taking into account that

$$\frac{\partial f}{\partial \phi'} v' = \frac{d}{dz} \left(\frac{\partial f}{\partial \phi'} v \right) - v \frac{d}{dz} \frac{\partial f}{\partial \phi'} ,$$

$$\frac{\partial f}{\partial \phi''} v'' = \frac{d}{dz} \left(v' \frac{\partial f}{\partial \phi''} - v \frac{d}{dz} \frac{\partial f}{\partial \phi''} \right) + v \frac{d^2}{dz^2} \frac{\partial f}{\partial \phi''} ,$$

expression (1.62) may be rewritten as

$$\begin{aligned} \frac{dF}{d\alpha} = & \int_{-d/2}^{d/2} \left(\frac{\partial f}{\partial \phi} - \frac{d}{dz} \frac{\partial f}{\partial \phi'} + \frac{d^2}{dz^2} \frac{\partial f}{\partial \phi''} \right) v \mathrm{d}z \\ & + \left[\left(\frac{\partial f}{\partial \phi'} - \frac{d}{dz} \frac{\partial f}{\partial \phi''} \right) v + \frac{\partial f}{\partial \phi''} v' \right]_{-d/2}^{d/2} . \end{aligned} \tag{1.63}$$

Since we are considering the case of strong anchoring, $v(\pm d/2) = 0$, whereas, $v'(\pm d/2)$ are arbitrary quantities. Consequently, the condition $(dF/d\alpha)_0 = 0, \forall\, v(z) \in C_2$ gives

$$\frac{\partial f}{\partial \phi} - \frac{d}{dz} \frac{\partial f}{\partial \phi'} + \frac{d^2}{dz^2} \frac{\partial f}{\partial \phi''} = 0 , \qquad \forall\, z \in (-d/2, d/2) , \tag{1.64}$$

and the boundary conditions

$$\begin{gathered} \phi(-d/2) = \Phi_1 , \qquad \phi(d/2) = \Phi_2 , \\ \left(\frac{\partial f}{\partial \phi''} \right)_{-d/2} = 0 , \qquad \left(\frac{\partial f}{\partial \phi\prime\prime} \right)_{d/2} = 0 . \end{gathered} \tag{1.65}$$

Equation (1.64) shows that in the event in which $f = f(\phi', \phi'', z)$, the quantity

$$\mu = -\frac{\partial f}{\partial \phi'} + \frac{d}{dz} \frac{\partial f}{\partial \phi''} ,$$

is independent of z. This is a generalization of the quantity m introduced in Sec. 1.2.

In the case in which not only the values of $\phi(z)$ are fixed for $z = \pm d/2$, but also its derivatives $\phi'(z)$, Eq. (1.64) has to be solved with the boundary conditions

$$\phi(-d/2) = \Phi_1,\ \phi'(-d/2) = \Phi_1', \quad \text{and} \quad \phi(d/2) = \Phi_2, \quad \phi'(d/2) = \Phi_2',$$

instead of using (1.65).

It is also possible to obtain a generalization of the quantity p introduced in the same Sec. 1.2. With this aim in mind, let us consider the general case in which

$$f = f[z, \phi(z), \phi'(z), \phi''(z)]$$

and evaluate df/dz. Simple calculations give

$$\frac{df}{dz} = \frac{\partial f}{\partial z} + \frac{\partial f}{\partial \phi}\phi' + \frac{\partial f}{\partial \phi'}\phi'' + \frac{\partial f}{\partial \phi''}\phi'''. \tag{1.66}$$

From the Euler–Lagrange equation (see Eq. (1.64)), one obtains

$$\phi'\frac{\partial f}{\partial \phi} = \phi'\frac{d}{dz}\left[\left(\frac{\partial f}{\partial \phi'}\right) - \frac{d}{dz}\left(\frac{\partial f}{\partial \phi''}\right)\right]. \tag{1.67}$$

By substituting Eq. (1.67) into Eq. (1.66), we find

$$\frac{df}{dz} = \frac{\partial f}{\partial z} + \phi'\frac{d}{dz}\left[\left(\frac{\partial f}{\partial \phi'}\right) - \frac{d}{dz}\left(\frac{\partial f}{\partial \phi''}\right)\right] + \phi''\frac{\partial f}{\partial \phi'} + \phi'''\frac{\partial f}{\partial \phi''}. \tag{1.68}$$

Now, if we take into account that

$$\begin{aligned}
&\frac{d}{dz}\left\{\phi'\left[\left(\frac{\partial f}{\partial \phi'}\right) - \frac{d}{dz}\left(\frac{\partial f}{\partial \phi''}\right)\right] + \phi''\frac{\partial f}{\partial \phi''}\right\} \\
&\quad = \phi''\left[\left(\frac{\partial f}{\partial \phi'}\right) - \frac{d}{dz}\left(\frac{\partial f}{\partial \phi''}\right)\right] + \phi'\frac{d}{dz}\left[\left(\frac{\partial f}{\partial \phi'}\right) - \frac{d}{dz}\left(\frac{\partial f}{\partial \phi''}\right)\right] \\
&\qquad + \phi'''\frac{\partial f}{\partial \phi''} + \phi''\frac{d}{dz}\left(\frac{\partial f}{\partial \phi''}\right) \\
&\quad = \phi'\frac{d}{dz}\left[\left(\frac{\partial f}{\partial \phi'}\right) - \frac{d}{dz}\left(\frac{\partial f}{\partial \phi''}\right)\right] + \phi''\frac{\partial f}{\partial \phi'} + \phi'''\frac{\partial f}{\partial \phi''},
\end{aligned}$$

it is possible to rewrite Eq. (1.68) in the form

$$\frac{d}{dz}\left\{f - \phi'\left[\left(\frac{\partial f}{\partial \phi'}\right) - \frac{d}{dz}\left(\frac{\partial f}{\partial \phi''}\right)\right] + \phi''\frac{\partial f}{\partial \phi''}\right\} = \frac{\partial f}{\partial z}. \tag{1.69}$$

From Eq. (1.69), we derive that in the case in which f does not depend explicitly on z, the quantity

$$\pi = -f + \phi' \left[\left(\frac{\partial f}{\partial \phi'} \right) - \frac{d}{dz} \left(\frac{\partial f}{\partial \phi''} \right) \right] - \phi'' \frac{\partial f}{\partial \phi''} \,, \tag{1.70}$$

is constant with respect to z, i.e. $d\pi/dz = 0$. A simple analysis shows that π reduces to p when f is independent of ϕ''. This result is in agreement with the one obtained in Sec. 1.2.

If f is of the kind

$$f(\phi, \phi', \phi'') = \frac{1}{2} K {\phi'}^2 + \frac{1}{2} K^* {\phi''}^2 \,,$$

with K and K^* position independent, the quantity π introduced above reads

$$\begin{aligned} -\pi &= \frac{1}{2} K {\phi'}^2 + \frac{1}{2} K^* {\phi''}^2 - \phi' \left[K\phi' - K^* \phi''' \right] - K^* {\phi''}^2 \\ &= -\frac{1}{2} K {\phi'}^2 - \frac{1}{2} K^* {\phi''}^2 + K^* \phi' \phi''' \,, \end{aligned}$$

i.e. in the form

$$\pi = \frac{1}{2} K {\phi'}^2 + \frac{1}{2} K^* {\phi''}^2 - K^* \phi' \phi''' \,.$$

For this special case also μ is constant. It is given by

$$\mu = -K\phi' + K^* \phi''' \,.$$

1.8. Functionals Containing $\phi''(z)$: Weak Anchoring

Determine the function $\phi(z)$ extremizing the functional

$$F[\phi(z)] = \int_{-d/2}^{d/2} f[\phi(z), \phi'(z), \phi''(z)] \mathrm{d}z + \gamma_1(\phi_1, \phi_1') + \gamma_2(\phi_2, \phi_2') \,, \tag{1.71}$$

where $\phi_1 = \phi(-d/2)$, $\phi_2 = \phi(d/2)$, $\phi_1' = \phi'(z = -d/2)$, and $\phi_2' = \phi'(z = d/2)$.

Solution

This section is a generalization of Sec. 1.3 devoted to the weak anchoring. Let $\tilde{\phi}(z)$ be the function minimizing Eq. (1.71) and $\phi(z) = \tilde{\phi}(z) + \alpha v(z)$, a function close to $\tilde{\phi}(z)$. Hence,

$$\frac{d\gamma_1}{d\alpha} = \frac{\partial \gamma_1}{\partial \phi_1}\frac{\partial \phi_1}{\partial \alpha} + \frac{\partial \gamma_1}{\partial \phi_1'}\frac{\partial \phi_1'}{\partial \alpha}$$
$$= \frac{\partial \gamma_1}{\partial \phi_1} v\left(-\frac{d}{2}\right) + \frac{\partial \gamma_1}{\partial \phi_1'} v'\left(-\frac{d}{2}\right) .$$

A similar relation is valid for $d\gamma_2/d\alpha$. Consequently, by using Eq. (1.63) we obtain

$$\frac{dF}{d\alpha} = \int_{-d/2}^{d/2}\left(\frac{\partial f}{\partial \phi} - \frac{d}{dz}\frac{\partial f}{\partial \phi'} + \frac{d^2}{dz^2}\frac{\partial f}{\partial \phi''}\right) v \mathrm{d}z$$
$$+ \left[\left(\frac{\partial f}{\partial \phi'} - \frac{d}{dz}\frac{\partial f}{\partial \phi''}\right) v + \frac{\partial f}{\partial \phi''} v'\right]_{-d/2}^{d/2}$$
$$+ \frac{\partial \gamma_1}{\partial \phi_1} v\left(-\frac{d}{2}\right) + \frac{\partial \gamma_1}{\partial \phi_1'} v'\left(-\frac{d}{2}\right) + \frac{\partial \gamma_2}{\partial \phi_2} v\left(\frac{d}{2}\right) + \frac{\partial \gamma_2}{\partial \phi_2'} v'\left(\frac{d}{2}\right) .$$

The condition $(dF/d\alpha)_0 = 0, \forall\, v(z) \in C_2$ then gives

$$\frac{\partial f}{\partial \phi} - \frac{d}{dz}\frac{\partial f}{\partial \phi'} + \frac{d^2}{dz^2}\frac{\partial f}{\partial \phi''} = 0\,, \qquad \forall\, z \in (-d/2, d/2)\,, \tag{1.72}$$

with

$$-\left(\frac{\partial f}{\partial \phi'} - \frac{d}{dz}\frac{\partial f}{\partial \phi''}\right) + \frac{\partial \gamma_1}{\partial \phi_1} = 0\,,$$
$$-\frac{\partial f}{\partial \phi''} + \frac{\partial \gamma_1}{\partial \phi_1'} = 0\,, \qquad z = -d/2\,, \tag{1.73}$$

and

$$\left(\frac{\partial f}{\partial \phi'} - \frac{d}{dz}\frac{\partial f}{\partial \phi''}\right) + \frac{\partial \gamma_2}{\partial \phi_2} = 0\,,$$
$$\frac{\partial f}{\partial \phi''} + \frac{\partial \gamma_2}{\partial \phi_2'} = 0\,, \qquad z = d/2\,. \tag{1.74}$$

The boundary conditions (1.73) and (1.74) are obtained by taking into account that $v(\pm d/2)$ are independent of $v'(\pm d/2)$, as it is easy to verify by considering the following example. If

$$v(z) = \Omega \sin[(2z/d)^2 - 1]\,,$$

where Ω is a constant, we have

$$v(-d/2) = v(d/2) = 0\,,$$

and

$$v'(-d/2) = -\frac{4}{d}\Omega\,, \qquad v'(d/2) = \frac{4}{d}\Omega\,.$$

This means that a relation of the kind $v'(-d/2) = \lambda v(-d/2)$ does not exist.

The boundary conditions (1.73) and (1.74) may be also obtained by following the way discussed in Sec. 1.3. According to this way, the functional F is considered as an ordinary function of the integration constants of the solution of the Euler–Lagrange equation. Let us indicate by $\phi(\phi_1, \phi_2, p_1, p_2; z)$ the general solution of Eq. (1.72), where $\phi_{1,2} = \phi(\mp d/2)$ and $p_{1,2} = \phi'(z = \mp d/2)$ are the new integration constants. By substituting $\phi(\phi_1, \phi_2, p_1, p_2; z)$ into Eq. (1.71), F will be an ordinary function of ϕ_1, ϕ_2, p_1 and p_2, namely

$$F(\phi_1, \phi_2, p_1, p_2) = \int_{-d/2}^{d/2} f[\phi(\phi_1, \phi_2, z), \phi'(\phi_1, \phi_2, z), \phi''(\phi_1, \phi_2, z); z)]\mathrm{d}z \\ + \gamma_1(\phi_1, p_1) + \gamma_2(\phi_2, p_2)\,. \tag{1.75}$$

The actual values of $\phi_{1,2}$ and $p_{1,2}$ are determined by looking for the minimum of Eq. (1.75). Hence, the integration constants are obtained by solving the systems of equations

$$\frac{\partial F}{\partial \phi_1} = \frac{\partial F}{\partial \phi_2} = \frac{\partial F}{\partial p_1} = \frac{\partial F}{\partial p_2} = 0\,,$$

where ϕ_1, ϕ_2, p_1 and p_2 are linearly independent, i.e.

$$\frac{\partial \phi_1}{\partial \phi_2} = \frac{\partial \phi_1}{\partial p_1} = \frac{\partial \phi_1}{\partial p_2} = 0\,,$$

and similar. From Eq. (1.75), we obtain

$$\frac{\partial F}{\partial \phi_1} = \frac{\partial}{\partial \phi_1}\int_{-d/2}^{d/2} f(\phi, \phi', \phi''; z)\mathrm{d}z + \frac{\partial \gamma_1}{\partial \phi_1}\,. \tag{1.76}$$

The first addendum of Eq. (1.76) may be rewritten as

$$\frac{\partial}{\partial \phi_1}\int_{-d/2}^{d/2} f(\phi, \phi', \phi''; z)\mathrm{d}z = \int_{-d/2}^{d/2} \frac{\partial f}{\partial \phi_1}\mathrm{d}z \\ = \int_{-d/2}^{d/2}\left(\frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial \phi_1} + \frac{\partial f}{\partial \phi'}\frac{\partial \phi'}{\partial \phi_1} + \frac{\partial f}{\partial \phi''}\frac{\partial \phi''}{\partial \phi_1}\right)\mathrm{d}z\,.$$

Simple calculations give

$$\frac{\partial f}{\partial \phi'}\frac{\partial \phi'}{\partial \phi_1} = \frac{d}{dz}\left(\frac{\partial f}{\partial \phi'}\frac{\partial \phi}{\partial \phi_1}\right) - \frac{\partial \phi}{\partial \phi_1}\frac{d}{dz}\left(\frac{\partial f}{\partial \phi'}\right),$$

$$\frac{\partial f}{\partial \phi''}\frac{\partial \phi''}{\partial \phi_1} = \frac{d}{dz}\left[\frac{\partial f}{\partial \phi''}\frac{\partial \phi'}{\partial \phi_1} - \frac{\partial \phi}{\partial \phi_1}\frac{d}{dz}\left(\frac{\partial f}{\partial \phi''}\right)\right] + \frac{\partial \phi}{\partial \phi_1}\frac{d^2}{dz^2}\left(\frac{\partial f}{\partial \phi''}\right).$$

Consequently, we have

$$\begin{aligned}\frac{\partial}{\partial \phi_1}\int_{-d/2}^{d/2} & f(\phi, \phi', \phi''; z)\mathrm{d}z \\ &= \int_{-d/2}^{d/2}\left[\frac{\partial f}{\partial \phi} - \frac{d}{dz}\left(\frac{\partial f}{\partial \phi'}\right) + \frac{d^2}{dz^2}\left(\frac{\partial f}{\partial \phi''}\right)\right]\frac{\partial \phi}{\partial \phi_1}\mathrm{d}z \\ &\quad + \left\{\left[\frac{\partial f}{\partial \phi'} - \frac{d}{dz}\left(\frac{\partial f}{\partial \phi''}\right)\right]\frac{\partial \phi}{\partial \phi_1} + \frac{\partial \phi'}{\partial \phi_1}\frac{\partial f}{\partial \phi''}\right\}_{-d/2}^{d/2}. \end{aligned} \tag{1.77}$$

Since ϕ is, for hypothesis, the solution of Eq. (1.72) and the integration constants are linearly independent, Eq. (1.77) is equivalent to

$$\frac{\partial}{\partial \phi_1}\int_{-d/2}^{d/2} f(\phi, \phi', \phi''; z)\mathrm{d}z = -\left(\frac{\partial f}{\partial \phi'} - \frac{d}{dz}\frac{\partial f}{\partial \phi''}\right)_{-d/2},$$

and Eq. (1.76) becomes

$$\frac{\partial F}{\partial \phi_1} = -\left(\frac{\partial f}{\partial \phi'} - \frac{d}{dz}\frac{\partial f}{\partial \phi''}\right)_{-d/2} + \frac{\partial \gamma_1}{\partial \phi_1}.$$

If we impose the condition $\partial F/\partial \phi_1 = 0$, we obtain the first of the boundary conditions (1.73). To proceed, let us consider now $\partial F/\partial p_1$. It is given by

$$\frac{\partial F}{\partial p_1} = \frac{\partial}{\partial p_1}\int_{-d/2}^{d/2} f(\phi, \phi', \phi''; z)\mathrm{d}z + \frac{\partial \gamma_1}{\partial p_1},$$

where the first addendum is equivalent to

$$\frac{\partial}{\partial p_1}\int_{-d/2}^{d/2} f(\phi, \phi', \phi''; z)\mathrm{d}z = -\left(\frac{\partial f}{\partial \phi''}\right)_{-d/2},$$

as it is easy to show with calculations similar to the previous one. Consequently,

$$\frac{\partial F}{\partial p_1} = -\left(\frac{\partial f}{\partial \phi''}\right)_{-d/2} + \frac{\partial \gamma_1}{\partial p_1}\,.$$

Now if we put $\partial F/\partial p_1 = 0$, we obtain the second of the boundary conditions (1.73). In a similar manner, it is possible to obtain the boundary conditions (1.74).

Let us consider the simple case in which

$$f = f[\phi'(z), \phi''(z); z]\,.$$

In this situation, as we have shown in Sec. 1.7, the quantity

$$\mu = -\frac{\partial f}{\partial \phi'} + \frac{d}{dz}\left(\frac{\partial f}{\partial \phi''}\right), \tag{1.78}$$

is independent of z. Hence, instead to solve Eq. (1.72), it is possible to solve Eq. (1.78) with respect to $\phi(z)$. The integration constants are then deduced by the boundary conditions (1.73) and (1.74), which in the present case reduce to

$$\mu_1 + \frac{\partial \gamma_1}{\partial \phi_1} = 0\,, \quad -\frac{\partial f}{\partial \phi''} + \frac{\partial \gamma_1}{\partial p_1} = 0\,, \tag{1.79}$$

at $z = -d/2$, and

$$-\mu_2 + \frac{\partial \gamma_2}{\partial \phi_2} = 0\,, \qquad \frac{\partial f}{\partial \phi''} + \frac{\partial \gamma_2}{\partial p_2} = 0\,, \tag{1.80}$$

at $z = d/2$. In Eqs. (1.79) and (1.80), $\mu_1 = \mu(z = -d/2)$ and $\mu_2 = \mu(z = d/2)$. Since in the case we are examining μ is constant across the sample, $\mu_1 = \mu_2$. Hence, from the boundary conditions (1.79) and (1.80), we obtain

$$\frac{\partial \gamma_1}{\partial \phi_1} + \frac{\partial \gamma_2}{\partial \phi_2} = 0\,,$$

stating that the action of the surface at $z = -d/2$ over the medium is balanced by the surface at $z = d/2$.

1.9. Functional with Discontinuous Extremizing Function

Show that the extremizing function $\phi(z)$ of the functional

$$F[\phi(z)] = \int_{-d/2}^{d/2} f[\phi(z), \phi'(z); z]\mathrm{d}z + \gamma_1(\phi_1, \phi_1') + \gamma_2(\phi_2, \phi_2')\,, \tag{1.81}$$

is, in general, a discontinuous function.

Solution

In this case, the bulk equation is

$$\frac{\partial f}{\partial \phi} - \frac{d}{dz}\frac{\partial f}{\partial \phi'} = 0\,, \qquad \forall\, z \in (-d/2, d/2)\,,$$

as it follows from Eq. (1.72). Its general solution is of the kind

$$\phi = \phi(c_1, c_2, ; z)\,,$$

where c_1 and c_2 are two integration constants. The boundary conditions are

$$-\frac{\partial f}{\partial \phi'} + \frac{\partial \gamma_1}{\partial \phi_1} = 0\,, \qquad \frac{\partial \gamma_1}{\partial \phi_1'} = 0\,, \tag{1.82}$$

at $z = -d/2$, and

$$\frac{\partial f}{\partial \phi'} + \frac{\partial \gamma_2}{\partial \phi_2} = 0\,, \quad \frac{\partial \gamma_2}{\partial \phi_2'} = 0\,, \tag{1.83}$$

at $z = d/2$, as it follows from boundary conditions (1.73) and (1.74). Hence, the integration constants c_1 and c_2 have to satisfy four conditions. This is in general, impossible. Consequently, the function $\phi(z)$ extremizing Eq. (1.81) is usually a discontinuous function.

This case deserves a deep analysis, since it is rather important in the theory of elasticity of NLC, in connection with the so-called K_{13} problem. Let us suppose that in Eq. (1.81), $f(\phi, \phi')$ and $\gamma(\phi, \phi')$ are of the kind

$$f(\phi, \phi') = \frac{1}{2}K{\phi'}^2 + H(\phi) \quad \text{and} \quad \gamma(\phi, \phi') = \tilde{K}\phi\phi'\,,$$

where $H(\phi)$ is connected to the interaction of the NLC with an external field, K is the usual elastic constant and $\tilde{K}$ is a surface-like elastic constant (usually indicated by K_{13}). Let us suppose, furthermore, strong anchoring on $z = \pm d/2$, i.e.

$$\phi(-d/2) = 0\,, \qquad \phi(d/2) = \Phi\,. \tag{1.84}$$

In this particular case, the functional (1.81) reads

$$F[\phi] = \int_{-d/2}^{d/2} \left[\frac{1}{2}K{\phi'}^2 + H(\phi)\right] \mathrm{d}z + \tilde{K}\Phi\phi'(d/2)\,.$$

The relevant Euler–Lagrange equation is

$$K\phi'' - \frac{dH}{d\phi} = 0\,, \tag{1.85}$$

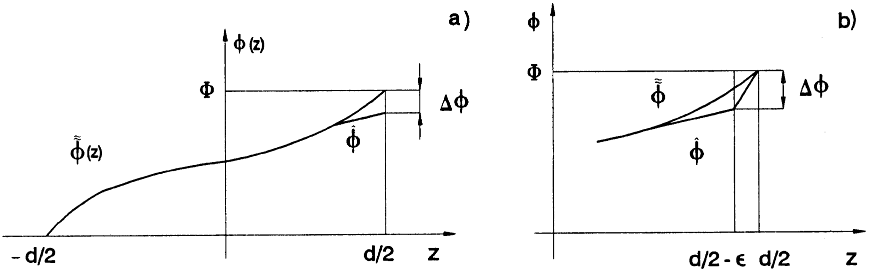

Fig. 4. Solution of the Euler–Lagrange equation connected to the functional $F[\phi]$ and the discontinuous function $\hat{\phi}$. The discontinuous function $\hat{\phi}$ is a solution of the Euler–Lagrange equation in the bulk, but presents a surface discontinuity at the border $\Delta\phi$ of (a). The discontinuous function $\hat{\phi}$ is obtained as the limit for $\epsilon \to 0$ of the continuous function shown in (b).

whose solution, satisfying boundary conditions (1.84) can be easily determined. In all this analysis, $\tilde{K}$ does not play any role, since it is absent from Eq. (1.85) and from the boundary conditions (1.84).

Let us indicate by $\tilde{\phi}(z)$, the solution of Eq. (1.85) with Eq. (1.84). We want to show that a discontinuous function $\hat{\phi}$, coinciding in the bulk with a solution of the Euler–Lagrange equation, $\tilde{\tilde{\phi}}$, is such that

$$F[\hat{\phi}] < F[\tilde{\phi}]\,.$$

To do this, let us consider the situation shown in Fig. 4, where $\epsilon \to 0$ and $\Delta\phi$ is the surface discontinuity.

In the bulk, i.e. $\forall\, z \in (-d/2, d/2-\epsilon)$, $\hat{\phi}(z) = \tilde{\tilde{\phi}}(z)$, whereas in the surface layer $z \in (d/2-\epsilon, d/2)$, $\phi' \simeq \Delta\phi/\epsilon$ and $\phi \simeq \Phi$. It follows that $F[\hat{\phi}]$ is given by the following limit

$$\begin{aligned}
&\lim_{\epsilon\to 0}\left\{\int_{-d/2}^{d/2-\epsilon}\left[\frac{1}{2}K\phi'^2 + H(\phi)\right]\mathrm{d}z + \int_{d/2-\epsilon}^{d/2}\left[\frac{1}{2}K\phi'^2 + H(\phi)\right]\mathrm{d}z + \tilde{K}\Phi\frac{\Delta\phi}{\epsilon}\right\}\\
&\quad = \lim_{\epsilon\to 0}\left\{\int_{-d/2}^{d/2-\epsilon}\left[\frac{1}{2}K\phi'^2 + H(\phi)\right]\mathrm{d}z + \frac{1}{2}K\frac{(\Delta\phi)^2}{\epsilon} + H(\Phi)\epsilon + \tilde{K}\Phi\frac{\Delta\phi}{\epsilon}\right\}\\
&\quad = \lim_{\epsilon\to 0}\left\{\int_{-d/2}^{d/2-\epsilon}\left[\frac{1}{2}K\phi'^2 + H(\phi)\right]\mathrm{d}z + \frac{1}{2}K\frac{(\Delta\phi)}{\epsilon}(\Delta\phi + 2\frac{\tilde{K}}{K})\Phi\right\}\,.
\end{aligned}$$

The relation obtained shows that

$$F[\hat{\phi}] = F[\tilde{\tilde{\phi}}] + \lim_{\epsilon \to 0} F_D \,,$$

where the divergent part F_D is given by

$$F_D = \frac{K}{2\epsilon}(\Delta\phi)^2 + \frac{\tilde{K}}{\epsilon}\Phi\Delta\phi \,.$$

F_D reaches its minimum value for

$$\Delta\phi = -\frac{\tilde{K}}{K}\Phi \,,$$

whose value is

$$F_D(\min) = F_D\left(\Delta\phi = -\frac{\tilde{K}}{K}\Phi\right) = -\frac{\tilde{K}^2}{2K\epsilon}\Phi^2 < 0 \,.$$

In the limit $\epsilon \to 0$, $F_D \to -\infty$, and also $F[\hat{\phi}]$ whereas $F[\tilde{\phi}]$ is a finite quantity. Hence $F[\hat{\phi}] < F[\tilde{\phi}]$, and the function minimizing functional (1.81) presents a surface discontinuity.

1.10. Ill-Posed Problem: Different Approaches, Different Solutions

Determine the function $\phi(z)$ extremizing the functional

$$F[\phi(z)] = \int_0^d \frac{1}{2}K{\phi'}^2(z)\mathrm{d}z + \frac{1}{2}W(\varphi - \Phi)^2 + \tilde{K}\varphi\phi'(d) \,, \tag{1.86}$$

by supposing that for $z = 0$ the anchoring is strong, and $\phi(0) = 0$. In Eq. (1.86), $K > 0$, $W > 0$, Φ is a constant and $\varphi = \phi(d)$. Solve the problem in the direct way and by means of the alternative manner, in which F is considered as an ordinary function of the integration constants. Furthermore, evaluate the first and second variation of F.

Solution

This problem is similar to the one presented in Sec. 1.6.

(a) *Direct way*

The Euler–Lagrange equation connected with the bulk part of $F[\phi(z)]$ given by Eq. (1.86) is $\tilde{\phi}''(z) = 0$, whose solution is

$$\tilde{\phi}(z) = \frac{\varphi - \beta}{d}z + \beta \,,$$

where φ and β are two integration constants. They have to satisfy the boundary conditions

$$\begin{aligned} \tilde{\phi}(0) &= 0\,, \\ K\tilde{\phi}'(d) + W(\varphi - \Phi) + \tilde{K}\tilde{\phi}'(d) &= 0\,, \\ \tilde{K}\varphi &= 0\,, \end{aligned}$$

due to the strong-anchoring case at $z = 0$, and to the fact that $v(d)$ and $v'(d)$ are independent quantities (see Eqs. (1.83)). These are three boundary conditions, two integration constants. The problem cannot be solved. The solution minimizing Eq. (1.86) does not belong to the C_1-class.

(b) *Method of the integration constant*

The function $\tilde{\phi}(z) = (\varphi/d)z$ satisfies the boundary condition $\tilde{\phi}(0) = 0$, due to the strong-anchoring condition. By substituting it into Eq. (1.86), one has

$$F(\varphi) = \frac{K + 2\tilde{K}}{2d}\varphi^2 + \frac{W}{2}(\varphi - \Phi)^2\,. \tag{1.87}$$

This means that F is an ordinary function of the integration constant φ. From Eq. (1.87), we obtain

$$\begin{aligned} \frac{dF}{d\varphi} &= \frac{K + 2\tilde{K}}{d}\varphi + W(\varphi - \Phi)\,, \\ \frac{d^2F}{d\varphi^2} &= \frac{K + 2\tilde{K}}{d} + W\,. \end{aligned}$$

By putting $dF(\varphi)/d\varphi = 0$, we derive

$$\varphi = \frac{W}{W + (K + 2\tilde{K})/d}\Phi\,. \tag{1.88}$$

Equation (1.88) in the case $\tilde{K} = 0$ reduces to Eq. (1.56). Furthermore, $d^2F/d\varphi^2 > 0$.

(c) *Evaluation of the first and second variation of F*

Let us consider the following function $\phi(z)$ near to $\tilde{\phi}(z)$:

$$\phi(z) = \tilde{\phi}(z) + \frac{1}{2}\alpha z^2\,. \tag{1.89}$$

By substituting Eq. (1.89) into Eq. (1.86), one obtains

$$F(\alpha) = F(0) + \frac{d^2}{2}\left[\frac{K+3\tilde{K}}{d}\varphi + W(\varphi-\Phi)\right]\alpha + \frac{d^2}{6}\left[\frac{K+3\tilde{K}}{d} + \frac{3}{4}W\right]\alpha^2\,, \tag{1.90}$$

where

$$F(0) = \frac{K+2\tilde{K}}{2d}\varphi^2 + \frac{W}{2}(\varphi-\Phi)^2\,,$$

coincides with $F(\varphi)$ given by Eq. (1.87). From Eq. (1.90), we derive

$$\left(\frac{dF(\alpha)}{d\alpha}\right)_{\alpha=0} = \frac{d^2}{2}\left[\frac{K+3\tilde{K}}{d}\varphi + W(\varphi-\Phi)\right]\,,$$

which is different from zero if φ is given by Eq. (1.88). It follows that the function $\tilde{\phi} = (\varphi/d)z$, with φ given by Eq. (1.88), does not minimize the functional (1.86). It is, among the solutions of the Euler–Lagrange equation, the one minimizing $F[\phi]$. But other functions, which are not solutions of the Euler–Lagrange equation, ϕ_n, are such that $F[\phi_n] < F[\phi]$.

In order to find the solution of the proposed problem, let us consider the functional

$$F^* = \int_0^d \left[\frac{1}{2}K\phi'^2 + \frac{1}{2}K^*\phi''^2\right]\mathrm{d}z + \frac{1}{2}W(\varphi-\Phi)^2 + \tilde{K}\phi\phi'\,. \tag{1.91}$$

One observes that F^* reduces to F given by Eq. (1.86) when $K^* \to 0$. We can easily find the function minimizing F^*. It depends on K^*. The function minimizing Eq. (1.86) is then found by performing the limit $K^* \to 0$ of the function minimizing Eq. (1.91). As discussed in Sec. 1.8, the Euler–Lagrange equation of the functional (1.91) is

$$K^*\phi'''' - K\phi'' = 0\,. \tag{1.92}$$

The quantity $K^*/K = b^2$ is the square of a length. At the end of the calculation we will perform the limit $b \to 0$. The solution of Eq. (1.92) is

$$\phi(z) = A\sinh(z/b) + B\cosh(z/b) + Cz/b + D\,, \tag{1.93}$$

where the integration constants A, B, C and D are determined by means of the boundary conditions (1.73) and (1.74). Since for $z = 0$, $\phi(0) = 0$ due to the strong anchoring, the boundary conditions for the present case read

$$\phi(0) = 0 \qquad \text{and} \qquad \phi''(0) = 0\,, \tag{1.94}$$

at $z = 0$, and

$$(1+R)\phi'(d) - b^2\phi'''(d) + \frac{1}{L}(\varphi - \Phi) = 0 \quad \text{and} \quad b^2\phi''(d) + R\phi(d) = 0\,, \tag{1.95}$$

at $z = d$, where $R = -\tilde{K}/K$ and $L = K/W$. Substitution of Eq. (1.93) into Eqs. (1.94) and (1.95) yields

$$B = D = 0\,, \qquad A = -\frac{R}{1+R}\frac{d/b}{\sinh(d/b)}C\,,$$

and

$$C = \frac{1+R}{(1+R)^2 + d/L - R^2 d/b\coth(d/b)}\frac{b}{L}\Phi\,,$$

where $\coth(d/b) \approx 1$, since the case that is interesting in our analysis is the one in which $d/b \to \infty$. It follows that $\phi(z)$ given by Eq. (1.93) reads

$$\phi(z) = \left[-\frac{R}{1+R}d\frac{\sinh(z/b)}{\sinh(d/b)} + z\right]\frac{C}{b}\,. \tag{1.96}$$

As underlined above, $d/b \gg 1$, and hence $\sinh(z/b)/\sinh(d/2b)$ is practically zero in the "bulk", i.e. in the range $0 \le z < d - b$. In this range, $\phi(z)$ is well approximated by

$$\phi^*(z) = C\frac{z}{b},$$

whose extrapolation value at $z = d$ is

$$\phi^*(d) = C\frac{d}{b}\,.$$

On the contrary, the true surface value given by Eq. (1.96) is

$$\varphi = \phi(d) = \frac{1}{1+R}C\frac{d}{b}\,.$$

It follows that the "subsurface discontinuity" is

$$\phi(d) - \phi^*(d) = -R\phi(d)\,.$$

The solution is the one shown in Fig. 5.

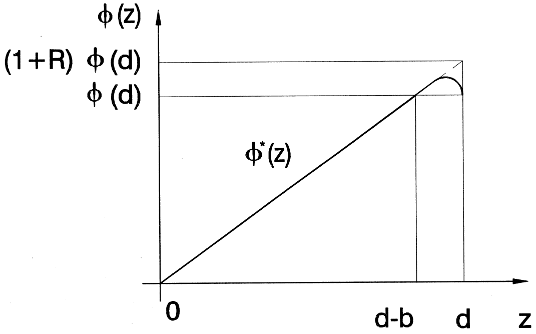

Fig. 5. Discontinuous and continuous (ϕ^*) functions minimizing the functional F. The continuous solution has been obtained by considering the generalized functional F^*, where a term in ϕ''^2 has been introduced.

We stress that in the limit $b \to 0$ (or $K^* \to 0$), the function minimizing Eq. (1.81) coincides with $\phi^*(z)$ (which is a solution of the Euler–Lagrange equation connected to Eq. (1.86)), $\forall\, z \in [0, d)$ and presents a surface discontinuity $\Delta\phi = -R\phi(d)$. This discontinuity coincides with the one evaluated in Sec. 1.9. However, in the limit $b \to 0$, the function minimizing Eq. (1.86) abandons the set of the functions of C_1-class in $(0, d)$.

1.11. Functionals Depending on Two Functions $\phi(z)$ and $\psi(z)$

Determine the functions $\phi(z)$ and $\psi(z) \in C_1$ minimizing the functional

$$F[\phi(z), \psi(z)] = \int_{-d/2}^{d/2} f[\phi(z), \phi'(z), \psi(z), \psi'(z); z]\mathrm{d}z\,, \tag{1.97}$$

in the strong-anchoring case in which

$$\phi(-d/2) = \Phi_1, \qquad \phi(d/2) = \Phi_2\,, \qquad \psi(-d/2) = \Psi_1\,, \qquad \psi(d/2) = \Psi_2\,. \tag{1.98}$$

Generalize the analysis to the weak-anchoring case.

Solution

To find the differential equations satisfied by $\phi(z)$ and $\psi(z)$ we just have to generalize the procedure used in Sec. 1.2, in which $F = F[\phi]$ only. Let $\tilde{\phi}(z)$ and $\tilde{\psi}(z)$ be the functions minimizing $F[\phi, \psi]$ given by Eq. (1.97), and

$$\phi(z) = \tilde{\phi}(z) + \alpha v(z)\,, \qquad \psi(z) = \tilde{\psi}(z) + \beta u(z)\,, \tag{1.99}$$

two functions close to $\tilde{\phi}(z)$ and $\tilde{\psi}(z)$. In Eq. (1.99), α and β are two small parameters and $v(z)$ and $u(z)$, two arbitrary functions belonging to the C_1-class. The boundary conditions (1.98) imply that

$$v(\pm d/2) = u(\pm d/2) = 0. \tag{1.100}$$

Since $\tilde{\phi}(z)$ and $\tilde{\psi}(z)$ minimize $F[\phi, \psi]$, we have that $F[\phi, \psi] > F[\tilde{\phi}, \tilde{\psi}]$, or in terms of α and β, as it follows from Eq. (1.99),

$$F(\alpha, \beta) > F(0,0)\,.$$

This implies that

$$\left(\frac{\partial F}{\partial \alpha}\right)_{0,0} = \left(\frac{\partial F}{\partial \beta}\right)_{0,0} = 0\,, \tag{1.101}$$

for all $v(z)$ and $u(z)$ of the C_1-class. Routine calculations give

$$\begin{aligned}
\frac{\partial F}{\partial \alpha} &= \int_{-d/2}^{d/2} \frac{\partial f}{\partial \alpha} \mathrm{d}z = \int_{-d/2}^{d/2} \left[\frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial \alpha} + \frac{\partial f}{\partial \phi'}\frac{\partial \phi'}{\partial \alpha}\right] \mathrm{d}z \\
&= \int_{-d/2}^{d/2} \left[\frac{\partial f}{\partial \phi} v(z) + \frac{\partial f}{\partial \phi'} v'(z)\right] \mathrm{d}z \\
&= \int_{-d/2}^{d/2} \left[\frac{\partial f}{\partial \phi} - \frac{d}{dz}\frac{\partial f}{\partial \phi'}\right] v(z)\mathrm{d}z + \left[\frac{\partial f}{\partial \phi'} v(z)\right]_{-d/2}^{d/2}\,.
\end{aligned}$$

By imposing Eq. (1.101) and taking into account Eq. (1.100), one derives that the functions extremizing Eq. (1.97) are solutions of the differential equations

$$\frac{\partial f}{\partial \phi} - \frac{d}{dz}\frac{\partial f}{\partial \phi'} = 0 \quad \text{and} \quad \frac{\partial f}{\partial \psi} - \frac{d}{dz}\frac{\partial f}{\partial \psi'} = 0\,, \tag{1.102}$$

for $-d/2 \leq z \leq d/2$. In the strong-anchoring case, the solution of Eq. (1.102) have to satisfy the boundary conditions (1.98).

From Eq. (1.102), we derive that if f is independent of ϕ or ψ, the quantity $\partial f/\partial \phi'$ or $\partial f/\partial \psi'$ is z independent. Furthermore, if f does not depend explicitly on z, there exists another first integral which corresponds to the quantity p introduced in Eq. (1.14). In fact, the quantity

$$p = \phi' \frac{\partial f}{\partial \phi'} + \psi' \frac{\partial f}{\partial \psi'} - f\,, \tag{1.103}$$

is such that

$$\frac{dp}{dz} = \phi' \left[-\frac{\partial f}{\partial \phi} + \frac{d}{dz}\frac{\partial f}{\partial \phi'} \right] + \psi' \left[-\frac{\partial f}{\partial \psi} + \frac{d}{dz}\frac{\partial f}{\partial \psi'} \right] + \frac{\partial f}{\partial z} = \frac{\partial f}{\partial z}\,,$$

since $\phi(z)$ and $\psi(z)$ are solutions of Eq. (1.102). Hence, if f does not depend explicitly on z, $dp/dz = 0$, i.e. p is constant across the sample.

In the case of weak anchoring $F[\phi(z), \psi(z)]$ is of the kind

$$\begin{aligned} F[\phi(z), \psi(z)] = &\int_{-d/2}^{d/2} f[\phi(z), \phi'(z), \psi(z), \psi'(z); z] \mathrm{d}z \\ &+ \gamma_1(\phi_1, \psi_1) + \gamma_2(\phi_2, \psi_2)\,, \end{aligned} \tag{1.104}$$

where $\phi_1 = \phi(-d/2)$, $\phi_2 = \phi(d/2)$, $\psi_1 = \psi(-d/2)$ and $\psi_2 = \psi(d/2)$.

Let us suppose again that $\tilde{\phi}(z)$ and $\tilde{\psi}(z)$ are the functions extremizing $F[\phi(z), \psi(z)]$, of the kind Eq. (1.99). Since

$$\gamma_1(\phi_1, \psi_1) = \gamma_1 \left[\tilde{\phi}_1 + \alpha v(-d/2), \tilde{\psi}_1 + \beta u(-d/2) \right]\,,$$

one obtains

$$\frac{\partial \gamma_1}{\partial \alpha} = \frac{\partial \gamma_1}{\partial \phi_1}\frac{\partial \phi_1}{\partial \alpha} = \frac{\partial \gamma_1}{\partial \phi_1} v(-d/2)\,.$$

Similar expressions are obtained for $\partial\gamma_1/\partial\beta$, $\partial\gamma_2/\partial\alpha$ and $\partial\gamma_2/\partial\beta$. It follows that from Eq. (1.104), $\delta_1 F = (\partial F/\partial\alpha)_{0,0}\alpha + (\partial F/\partial\beta)_{0,0}\beta$ is found to be

$$\begin{aligned} \delta F = &\int_{-d/2}^{d/2} \left[\alpha \left(\frac{\partial f}{\partial \phi} - \frac{d}{dz}\frac{\partial f}{\partial \phi'} \right) v(z) + \beta \left(\frac{\partial f}{\partial \psi} - \frac{d}{dz}\frac{\partial f}{\partial \psi'} \right) u(z) \right] \mathrm{d}z \\ &+ \alpha \left\{ \left[\frac{\partial f}{\partial \phi'} + \frac{\partial \gamma_2}{\partial \phi_2} \right]_{d/2} v(d/2) + \left[-\frac{\partial f}{\partial \phi'} + \frac{\partial \gamma_1}{\partial \phi_1} \right]_{-d/2} v(-d/2) \right\} \\ &+ \beta \left\{ \left[\frac{\partial f}{\partial \psi'} + \frac{\partial \gamma_2}{\partial \psi_2} \right]_{d/2} u(d/2) + \left[-\frac{\partial f}{\partial \psi'} + \frac{\partial \gamma_1}{\partial \psi_1} \right]_{-d/2} u(-d/2) \right\}\,. \end{aligned}$$

By imposing, as usual, Eq. (1.101) for all $v(z)$, $u(z)$ belonging to the C_1-class, from the previous expression for $\delta_1 F$, we obtain again the bulk equations (1.102), and the boundary conditions

$$-\frac{\partial f}{\partial \phi'} + \frac{\partial \gamma_1}{\partial \phi_1} = 0\,, \quad -\frac{\partial f}{\partial \psi'} + \frac{\partial \gamma_1}{\partial \psi_1} = 0\,, \tag{1.105}$$

for $z = -d/2$ and

$$\frac{\partial f}{\partial \phi'} + \frac{\partial \gamma_2}{\partial \phi_2} = 0\,, \quad \frac{\partial f}{\partial \psi'} + \frac{\partial \gamma_2}{\partial \psi_2} = 0\,, \tag{1.106}$$

for $z = d/2$. Hence, the functions $\phi(z)$ and $\psi(z)$ extremizing Eq. (1.104) are solutions to the ordinary differential Eqs. (1.102) and they satisfy the boundary conditions (1.105) and (1.106).

As an example, determine the functions $\phi(z)$ and $\psi(z)$ extremizing the functional

$$F = \int_{-d/2}^{d/2} \left[\frac{1}{2} K {\psi'}^2 + \frac{1}{2} K \sin^2(\psi) {\phi'}^2 - Kq \sin^2(\psi) \phi' \right] \mathrm{d}z\,, \tag{1.107}$$

where $K > 0$ and $q > 0$, in the strong-anchoring case in which Eq. (1.98) holds. Since f does not depend on ϕ, the quantity $\partial f / \partial \phi'$ is z independent. It is given by

$$\frac{\partial f}{\partial \phi'} = K \sin^2 \psi \phi' - Kq \sin^2 \psi = K(\phi' - q) \sin^2 \psi = KB\,,$$

where B is a constant. Hence,

$$(\phi' - q) \sin^2 \psi = B\,. \tag{1.108}$$

Furthermore, by taking into account that f does not depend explicitly on z, the quantity p introduced in Eq. (1.103) is also z independent. In the present case, p given by Eq. (1.103) reads

$$p = \frac{K}{2} ({\psi'}^2 + \sin^2 \psi {\phi'}^2)\,,$$

that we rewrite in the form

$$\psi^2 + \sin^2 \psi {\phi'}^2 = A^2\,, \tag{1.109}$$

where $A^2 = p/K > 0$. It follows that the functions extremizing Eq. (1.107) in the strong-anchoring case (Eq. (1.98)) are solutions of the differential Eqs. (1.108) and (1.109).

1.12. The Junction Problem

Determine the function $\phi(z)$ extremizing the functional

$$F[\phi_1(z),\phi_2(z)] = \int_{-\infty}^{0} f_2[\phi_2(z),\phi_2'(z)]\mathrm{d}z + \int_{0}^{\infty} f_1[\phi_1(z),\phi_1'(z)]\mathrm{d}z + M[\phi_2(0),\phi_1(0)]\,, \tag{1.110}$$

where $f_i[\phi_i(z),{\phi'}_i(z)]$ are the bulk energy densities of the two media. Furthermore, $M[\phi_2(0),\phi_1(0)]$ takes into account the localized interaction between the medium 2 with the medium 1 at the interface localized at $z=0$. Let $\tilde{\phi}_2(z)=\tilde{\phi}(z<0)$ and $\tilde{\phi}_1(z)=\tilde{\phi}(z>0)$ be the functions extremizing F given by Eq. (1.110). By operating in the usual manner, we consider a function $\phi(z)$ close to $\tilde{\phi}(z)$ given by

$$\begin{aligned} \phi_2(z) &= \tilde{\phi}_2(z) + \alpha v_2(z)\,, \qquad z<0 \\ \phi_1(z) &= \tilde{\phi}_1(z) + \alpha v_1(z)\,, \qquad z>0\,, \end{aligned} \tag{1.111}$$

where the arbitrary functions $v_i(z) \in C_1$ in general are different for $z=0$: $v_1(0) \neq v_2(0)$. This follows from the fact that $\tilde{\phi}(z)$ is, in general, discontinuous for $z=0$. By substituting Eq. (1.111) into Eq. (1.110), and deriving with respect to α, one obtains

$$\begin{aligned} \frac{dF}{d\alpha} = &\int_{-\infty}^{0}\left[\frac{\partial f_2}{\partial\phi_2} - \frac{d}{dz}\frac{\partial f_2}{\partial\phi_2'}\right]v_2(z)\mathrm{d}z + \int_{0}^{\infty}\left[\frac{\partial f_1}{\partial\phi_1} - \frac{d}{dz}\frac{\partial f_1}{\partial\phi_1'}\right]v_1(z)\mathrm{d}z \\ &+ \left(\frac{\partial f_2}{\partial\phi_2'} + \frac{\partial M}{\partial\phi_2}\right)v_2(z) - \lim_{z\to-\infty}\frac{\partial f_2}{\partial\phi_2'}v_2(z) \\ &+ \left(-\frac{\partial f_1}{\partial\phi_1'} + \frac{\partial M}{\partial\phi_1}\right)v_1(z) + \lim_{z\to\infty}\frac{\partial f_1}{\partial\phi_1'}v_1(z)\,. \end{aligned} \tag{1.112}$$

Since $(dF/d\alpha)_0 = 0$, $\forall\, v_i(z) \in C_1$, we deduce that

$$\frac{\partial f_2}{\partial\phi_2} - \frac{d}{dz}\frac{\partial f_2}{\partial\phi_2'} = 0 \quad \text{and} \quad \frac{\partial f_1}{\partial\phi_1} - \frac{d}{dz}\frac{\partial f_1}{\partial\phi_1'} = 0\,, \tag{1.113}$$

for $-\infty < z \leq 0$ and $0 \leq z < \infty$, respectively. They have to be solved with the boundary conditions

$$\frac{\partial f_2}{\partial\phi_2'} + \frac{\partial M}{\partial\phi_2} = 0 \quad \text{and} \quad -\frac{\partial f_1}{\partial\phi_1'} + \frac{\partial M}{\partial\phi_1} = 0\,, \tag{1.114}$$

at $z = 0$, and

$$\lim_{z\to-\infty}\frac{\partial f_2}{\partial \phi_2'} = 0 \quad \text{and} \quad \lim_{z\to\infty}\frac{\partial f_1}{\partial \phi_1'} = 0\,. \tag{1.115}$$

Let us consider now the particular case in which

$$f_i[\phi_i(z),\phi_i'(z)] = \frac{1}{2}K_i\phi_i'^2(z) + H_i[\phi_i(z)]\,, \tag{1.116}$$

and

$$M[\phi_2(0),\phi_1(0)] = \frac{1}{2}\beta[\phi_2(0)-\phi_1(0)]^2\,. \tag{1.117}$$

Expression (1.116) for f_i is the usual one used for NLC. Expression (1.117) for M concerns a situation in which the media 1 and 2 tend to be oriented at the same angle ϕ at the interface. β is a measure of the localized surface interaction. By means of Eqs. (1.116) and (1.117), Eqs. (1.113) become

$$\frac{dH_2}{d\phi_2} - K_2\phi_2'' = 0 \quad \text{and} \quad \frac{dH_1}{d\phi_1} - K_1\phi_1'' = 0\,,$$

which are equivalent to

$$\frac{1}{2}K_2\phi_2'^2 - H_2(\phi_2) = p_2 \quad \text{and} \quad \frac{1}{2}K_1\phi_1'^2 - H_1(\phi_1) = p_1\,, \tag{1.118}$$

where p_2 and p_1 are two integration constants. As we have discussed in Sec. 1.2, Eqs. (1.118) hold because z does not enter explicitly into f_i. Furthermore, in the present case, the boundary conditions (1.114) read

$$K_2\phi_2' + \beta(\phi_2-\phi_1) = 0 \qquad \text{and} \qquad K_1\phi_1' + \beta(\phi_2-\phi_1) = 0\,, \tag{1.119}$$

at $z = 0$, and

$$\lim_{z\to\infty}\phi_2' = 0 \quad \text{and} \quad \lim_{z\to\infty}\phi_1' = 0\,. \tag{1.120}$$

From Eqs. (1.119), it follows that $K_2\phi_2'(0) = K_1\phi_1'(0)$, i.e. the torque is continuous at $z = 0$, even if $\tilde{\phi}$ has a discontinuity point at $z = 0$. From Eqs. (1.120), we derive that for $z \to -\infty$, $\phi_2(z)$ tends to a constant value ϕ_{2_∞}, and for $z \to \infty$, $\phi_1(z)$ tends to ϕ_{1_∞}. Consequently, from Eqs. (1.118), we can deduce that for the integration constants $p_i (i = 1,2)$, the expressions

$$p_i = -H_i(\phi_{i_\infty})\,, \qquad i = 1,2\,. \tag{1.121}$$

A simple analysis shows that ϕ_{i_∞} are given by

$$\frac{dH_i(\phi_{i_\infty})}{d\phi_{i_\infty}} = 0\,.$$

In fact, if $\phi_i' = 0$ and $\phi_i = \phi_{i_\infty}$, F is given by

$$F(\phi_{2_\infty}, \phi_{1_\infty}) = \int_{-\infty}^{0} H_2(\phi_{2_\infty})\mathrm{d}z + \int_{0}^{\infty} H_1(\phi_{1_\infty})\mathrm{d}z\,.$$

It follows that the extrema of F, given by

$$\frac{\partial F(\phi_{2_\infty}, \phi_{1_\infty})}{\partial \phi_{2_\infty}} = \int_{-\infty}^{0} \frac{dH_2(\phi_{2_\infty})}{d\phi_{2_\infty}}\mathrm{d}z,$$

$$\frac{\partial F(\phi_{2_\infty}, \phi_{1_\infty})}{\partial \phi_{1_\infty}} = \int_{0}^{\infty} \frac{dH_1(\phi_{1_\infty})}{d\phi_{1_\infty}}\mathrm{d}z\,,$$

coincide with the extrema of $H_2(\phi_{2_\infty})$ and of $H_1(\phi_{1_\infty})$. By substituting Eq. (1.121) into Eqs. (1.118), we obtain

$$\phi_i'(z) = \sqrt{\frac{2}{K_i}\{H_i[\phi_i(z)] - H_i(\phi_{i_\infty})\}}\,, \tag{1.122}$$

in the hypothesis that $\phi_{2_\infty} < \phi_{1_\infty}$. The solutions of Eq. (1.122) are

$$\int_{\phi_i(0)}^{\phi_i(z)} \frac{\mathrm{d}\phi_i}{\sqrt{\frac{2}{K_i}\{H_i[\phi_i(z)] - H_i(\phi_{i_\infty})\}}} = z\,.$$

The value of $\phi_i(0)$ can be found by means of the boundary conditions (1.119), that rewrite in the form

$$\sqrt{2K_2\{H_2[\phi_2(0)] - H_2[\phi_{2_\infty}]\}} + \beta[\phi_2(0) - \phi_1(0)] = 0\,,$$

$$\sqrt{2K_1\{H_1[\phi_1(0)] - H_1[\phi_{1_\infty}]\}} + \beta[\phi_2(0) - \phi_1(0)] = 0\,,$$

by taking into account Eq. (1.122) (see Fig. 6).

There are problems in which ϕ has to be continuous at the interface between the two media. For instance, if ϕ is an electrical potential, it has to be continuous at the interface between the two dielectric media. This case can be analyzed by means of the equations reported above, performing the limit $\beta \to \infty$.

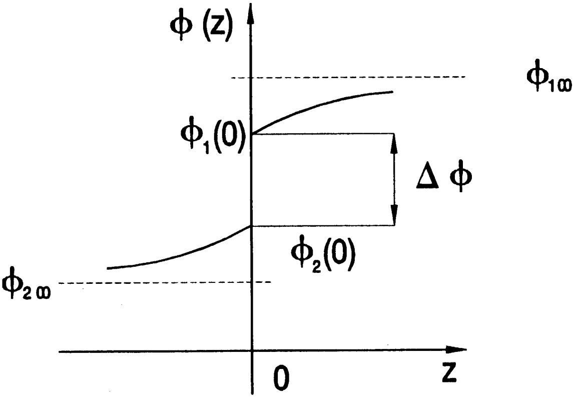

Fig. 6. Profile of the extremizing functions of a functional relevant to a junction of the kind considered in the text. Note that $\phi_1(0) \neq \phi_2(0)$. Only in the case of $M \to \infty$, $\phi_1(0) = \phi_2(0)$.

However, if ϕ is continuous at the interface, the functional (1.110) reads

$$F[\phi_1(z), \phi_2(z)] = \int_{-\infty}^{0} f_2[\phi_2(z), \phi_2'(z); z]\mathrm{d}z + \int_{0}^{\infty} f_1[\phi_1(z), \phi_1'(z); z]\mathrm{d}z\,,$$

with the condition

$$\phi_1(0) = \phi_2(0)\,. \tag{1.123}$$

From Eq. (1.123), it follows that the arbitrary functions appearing in Eqs. (1.111) are such that

$$v_1(0) = v_2(0) = v(0)\,.$$

Consequently, $dF/d\alpha$ given by Eq. (1.112) becomes

$$\frac{dF}{d\alpha} = \int_{-\infty}^{0} \left[\frac{\partial f_2}{\partial \phi_2} - \frac{d}{dz}\frac{\partial f_2}{\partial \phi_2'}\right] v_2(z)\mathrm{d}z + \int_{0}^{\infty} \left[\frac{\partial f_1}{\partial \phi_1} - \frac{d}{dz}\frac{\partial f_1}{\partial \phi_1'}\right] v_1(z)\mathrm{d}z$$
$$+ \left(\frac{\partial f_2}{\partial \phi_2'} - \frac{\partial f_1}{\partial \phi_1'}\right) v(0) - \lim_{z\to-\infty} \frac{\partial f_2}{\partial \phi_2'} + \lim_{z\to\infty} \frac{\partial f_1}{\partial \phi_1'}\,.$$

From the condition $(dF/d\alpha) = 0$, $\forall\, v_i(z) \in C_1$, we derive again for the bulk Eq. (1.113) and the boundary conditions (1.114), and furthermore

$$\frac{\partial f_2}{\partial \phi_2'} - \frac{\partial f_1}{\partial \phi_1'} = 0\,. \tag{1.124}$$

Hence, the boundary conditions (1.114) are in this case substituted by Eqs. (1.123) and (1.124).

1.13. Generalized Junction Problem

Determine the function $\phi(z)$ extremizing the functional

$$F[\phi(z)] = \int_0^d \left[\frac{1}{2}K(z)\phi'^2 + \frac{1}{2}U(z)\phi^2\right] \mathrm{d}z\,, \tag{1.125}$$

in the case in which $K(z)$ or $U(z)$ presents a discontinuity point ρ in $[0, d]$. Discuss then the case in which $K(z)$ or $U(z)$ are continuous functions presenting a sharp variation localized in a very small range ϵ around ρ. Show that in this case the problem can be easily solved by using the continuity of the function ϕ and of $K(z)\phi'$ for $z = \rho$, and neglecting the abrupt variation of $U(z)$ or $K(z)$ over ϵ.

Solution

This problem is a generalization of the one presented above. The special form for f used in Eq. (1.125) is useful to analyze real problems important in the physics of liquid crystals. In the following, we shall present particular cases before to derive general conclusions. The first example is not really connected with a generalized junction problem, but it is presented to facilitate the understanding of the following cases.

1.13.1. *First example*

Determine the function $\phi(z)$ extremizing the functional (1.125), by assuming

$$U(z) = U_0\,, \qquad K(z) = K\,,$$

with free anchoring for $z = 0$ and strong anchoring for $z = d$,where $\phi(d) = \Phi$. In this case, the Euler–Lagrange equation is

$$K\phi'' - U_0\phi = 0\,, \tag{1.126}$$

which has to be solved with the boundary conditions

$$\phi'(0) = 0\,, \qquad \phi(d) = \Phi\,. \tag{1.127}$$

The first condition is the transversality condition for the present case (see Eq. (1.24)). A general solution of Eq. (1.126) is

$$\phi(z) = A\cosh(z/\lambda) + B\sinh(z/\lambda)\,, \tag{1.128}$$

where we have put $\lambda^{-1} = \sqrt{U_0/K}$. The integration constants A and B in Eq. (1.128) are determined by conditions (1.127). Simple calculations give $B = 0$, $A = \Phi/\cosh(d/\lambda)$. Hence, the function $\phi(z)$ we are looking for is

$$\phi(z) = \Phi\frac{\cosh(z/\lambda)}{\cos(d/\lambda)}\,,$$

which is, obviously, continuous in $[0, d]$.

1.13.2. *Second example*

Determine the function $\phi(z)$ extremizing functional (1.125) when $K(z) = K$ and (see Fig. 7(a))

$$U(z) = \begin{cases} U_0\,, & 0 \le z \le \rho \\ 0\,, & \rho \le z \le d\,, \end{cases} \tag{1.129}$$

with the same boundary conditions of the first example.

In this case, the functional (1.125) reads

$$F = \int_0^\rho \left[\frac{1}{2}K\phi_1'^2 + \frac{1}{2}U_0\phi_1^2\right]\mathrm{d}z + \int_\rho^d \frac{1}{2}K\phi_2'^2\,\mathrm{d}z\,, \tag{1.130}$$

where $\phi_1(z) = \phi(z)$ for $0 \le z \le \rho$, and $\phi_2(z) = \phi(z)$ for $\rho \le z \le d$. This problem is similar to the junction problem analyzed above, where no conditions

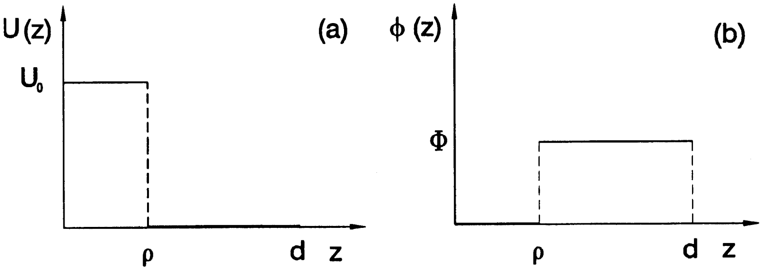

Fig. 7. (a) Discontinuous $U(z)$. (b) Discontinuous extremizing function relevant to the functional (1.125), when the border at $z = 0$ is free and the one at $z = d$ imposes strong anchoring at $\phi(d) = \Phi$.

at $z = \rho$ are imposed. Hence, the point $z = \rho$ has to be considered as a free border. In this case, the minimization of Eq. (1.130) gives

$$K\phi_1'' - U_0\phi_1 = 0 \qquad \text{and} \qquad K\phi_2'' = 0\,,$$

with the boundary conditions

$$\phi_1'(0) = 0\,, \quad \phi_1'(\rho) = 0\,, \quad \phi_2'(\rho) = 0 \quad \text{and} \quad \phi_2(\rho) = \Phi\,. \tag{1.131}$$

The second and third boundary conditions represent the transversality conditions at the border at $z = \rho$. $\phi_1(z)$ is now given by

$$\phi_1(z) = A\cosh(z/\lambda) + B\sinh(z/\lambda)\,,$$

where $\lambda^{-1} = \sqrt{U_0/K}$, and $\phi_2(z)$ by

$$\phi_2(z) = \frac{\Phi - \phi_2(\rho)}{d - \rho}(z - \rho) + \phi_2(\rho)\,.$$

By imposing the boundary conditions (1.131), one obtains

$$A = B = 0 \qquad \text{and} \qquad \phi_2(l) = \Phi\,.$$

Hence, the function extremizing Eq. (1.130) is the discontinuous function

$$\phi(z) = 0\,, \quad \text{for} \quad 0 \le z \le \rho \qquad \text{and} \qquad \phi(z) = \Phi\,, \quad \text{for} \quad \rho \le z \le d\,,$$

shown in Fig. 7(b).

1.13.3. *Third example*

Determine the function $\phi(z)$ extremizing the functional (1.125) when $K(z) = K$ and (see Fig. 8(a))

$$U(z) = \begin{cases} U_0\,, & 0 \le z \le \rho \\ u(z)\,, & \rho \le z \le \rho + \epsilon \\ 0\,, & \rho + \epsilon \le z \le d\,. \end{cases}$$

Since in this case, $U(z)$ is continuous in $[0, d]$, the function extremizing Eq. (1.125) is continuous too, as we have discussed at the end of Sec. 1.2.

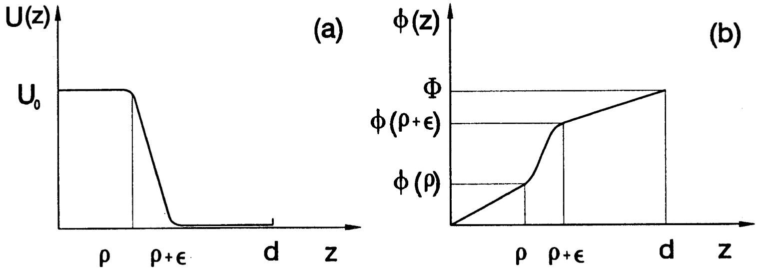

Fig. 8. (a) Function $U(z)$ presenting a sharp variation localized over ϵ around ρ. (b) Extremizing function. Note that $\phi(z)$ is continuous, with its first derivative ϕ', for $z = \rho$ and $z = \rho + \epsilon$. The boundary conditions at $z = 0$ and $z = d$ are as in Fig. 7.

In this case, the functional (1.125) may be rewritten in the form

$$F[\phi(z)] = \int_0^d \left[\frac{1}{2}K\phi_1'^2 + \frac{1}{2}U_0\phi_1^2\right] \mathrm{d}z$$

$$+ \int_\rho^{\rho+\epsilon} \left[\frac{1}{2}K\varphi'^2 + \frac{1}{2}u(z)\varphi^2\right] \mathrm{d}z + \int_{\rho+\epsilon}^d \left[\frac{1}{2}K\phi_2'^2\right] \mathrm{d}z\,, \qquad (1.132)$$

where

$$\phi(z) = \begin{cases} \phi_1(z)\,, & 0 \le z \le \rho \\ \varphi(z)\,, & \rho \le z \le \rho + \epsilon \\ \phi_2(z)\,, & \rho + \epsilon \le z \le d\,. \end{cases}$$

Since $\phi(z)$ has to be continuous in $[0, d]$, we have that

$$\phi_1(\rho) = \varphi(\rho) \quad \text{and} \quad \varphi(\rho + \epsilon) = \phi_2(\rho + \epsilon)\,.$$

By minimizing (1.131), we obtain

$$K\phi_1'' - U_0\phi_1 = 0\,, \quad K\varphi'' - u(z)\varphi = 0 \quad \text{and} \quad K\phi_2'' = 0\,, \qquad (1.133)$$

with the boundary conditions

$$\phi_1'(0) = 0\,, \quad \phi_1'(\rho) = \varphi'(\rho)\,, \quad \varphi'(\rho + \epsilon) = \phi_2'(\rho + \epsilon)\,, \quad \phi_2(d) = \Phi\,, \qquad (1.134)$$

the second and third of which follows from Eq. (1.124) written for the present case. We have now three differential equations of second order and six boundary conditions. The problem is well-posed and it can be solved. The solution will be a continuous function of the kind shown, schematically, in Fig. 8(b).

Let us consider now the second equation of Eqs. (1.133). From it we have

$$\varphi''(z) = \frac{u(z)}{K}\varphi(z)\,,$$

and hence, integrating between $z = \rho$ and $z \leq \rho + \epsilon$,

$$\varphi'(z) - \varphi'(\rho) = \int_\rho^z \frac{u(z')}{K}\varphi(z')\mathrm{d}z' = \psi(\rho, z)\,, \tag{1.135}$$

where $\psi(\rho, z)$ is a continuous function. By putting $z = \rho + \epsilon$, Eq. (1.135) becomes

$$\varphi'(\rho + \epsilon) = \varphi'(\rho) + \psi(\rho, \rho + \epsilon)\,. \tag{1.136}$$

Furthermore, from Eq. (1.135), integrating again from $z = \rho$ to $z \leq \rho + \epsilon$, we have

$$\varphi(z) - \varphi(\rho) = \varphi'(\rho)(z - \rho) + \int_\rho^z \psi(\rho, z')\mathrm{d}z'\,,$$

and in particular,

$$\varphi(\rho + \epsilon) - \varphi(\rho) = \varphi'(\rho)\epsilon + \int_\rho^{\rho+\epsilon} \psi(\rho, z')\mathrm{d}z'\,. \tag{1.137}$$

In the case in which ϵ is negligible with respect to the other lengths present in the problem, i.e. ρ and d, we can perform the limit $\epsilon \to 0$, and forget the region over which the $U(z)$ variation takes place. In this case, from Eqs. (1.136) and (1.137), we obtain

$$\lim_{\epsilon\to 0} \varphi'(\rho + \epsilon) = \varphi'(\rho)\,, \tag{1.138}$$

and

$$\lim_{\epsilon\to 0} \varphi(\rho + \epsilon) = \varphi(\rho)\,. \tag{1.139}$$

Hence, in the case under consideration, if $\epsilon \ll \rho$ and $\epsilon \ll d$, we can find $\phi_1(z)$ and $\phi_2(z)$ by minimizing the functional

$$F = \int_0^\rho \left[\frac{1}{2}K\phi_1'^2 + \frac{1}{2}U_0\phi_1^2\right]\mathrm{d}z + \int_\rho^d \frac{1}{2}K\phi_2'^2\,\mathrm{d}z\,,$$

in which the $U(z)$ variation is neglected, and imposing the boundary conditions $\phi_1'(0) = 0$, $\phi_2(d) = \Phi$, and furthermore

$$\phi_1(\rho) = \phi_2(\rho)\,, \qquad \phi_1'(\rho) = \phi_2'(\rho)\,, \tag{1.140}$$

following from Eqs. (1.138) and (1.139), and from the second and third of conditions (1.134). In the special case we are considering, $\phi_1(z)$ and $\phi_2(z)$ are solution of the first and third differential Eq. (1.134). Hence,

$$\phi_1(z) = A\cosh(z/\lambda)\,,$$

$$\phi_2(z) = \frac{\Phi - \phi_2(\rho)}{d-\rho}(z-\rho) + \phi_2(\rho)\,,$$

which satisfy the $\phi_1'(0) = 0$ and $\phi_2(d) = \Phi$. By means of Eqs. (1.140), we find then

$$A = \frac{\lambda}{\lambda\cosh(\rho/\lambda) + (d-\rho)\sinh(\rho/\lambda)}\,,$$

$$\phi_2(\rho) = \frac{\lambda\cosh(\rho/\lambda)}{\lambda\cosh(\rho/\lambda) + (d-\rho)\sinh(\rho/\lambda)}\,.$$

Hence, we can conclude that in the case in which $K(z) = K$ and $U(z)$ is of the kind shown in Fig. 8(b), the solution of the problem can be found neglecting the region over which $U(z)$ changes rapidly. The limiting solution is obtained by imposing the continuity of ϕ and ϕ' at the "discontinuity" point $z = \rho$, where $U(z)$ begins to change.

1.13.4. *Fourth example*

Determine the function $\phi(z)$ extremizing the functional

$$F = \int_0^d \frac{1}{2}K(z)\phi'^2 \mathrm{d}z\,, \tag{1.141}$$

when $K(z)$ is the discontinuous function (see Fig. 9(a))

$$K(z) = \begin{cases} K_1\,, & 0 \le z \le \rho \\ K_2\,, & \rho \le z \le d\,, \end{cases} \tag{1.142}$$

by supposing strong anchoring for $z = 0$ and $z = d$, where

$$\phi(0) = 0\,, \qquad \phi(d) = \Phi\,. \tag{1.143}$$

The given functional, taking into account function (1.142) may be rewritten as

$$F = \int_0^\rho \frac{1}{2}K_1\phi_1'^2\,\mathrm{d}z + \int_\rho^d \frac{1}{2}K_2\phi_2'^2\,\mathrm{d}z\,, \tag{1.144}$$

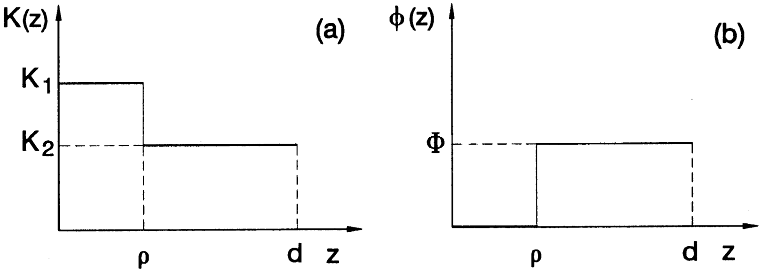

Fig. 9. Discontinuous $K(z)$ function (a), and relevant tilt angle minimizing the functional (1.141) (b). The solution refers to the case in which for $z = 0$ and $z = d$ the anchoring is strong and such that $\phi(0) = 0$ and $\phi(d) = \Phi$.

where $\phi_1(z) = \phi(z)$, for $0 \le z \le \rho$, and $\phi_2(z) = \phi(z)$, for $\rho \le z \le d$, without any conditions at $z = \rho$. The point at $z = \rho$ has then to be considered as a free point.

By minimizing Eq. (1.144), we obtain

$$\phi_1''(0) = 0 \qquad \text{and} \qquad \phi_2''(0) = 0\,, \tag{1.145}$$

with the transversality conditions at $z = \rho$ that in the present case read

$$\phi_1'(\rho) = 0\,, \qquad \phi_2'(\rho) = 0\,. \tag{1.146}$$

The solution of Eqs. (1.145) satisfying boundary conditions (1.143) and (1.146) is the discontinuous function

$$\phi(z) = 0\,, \quad \text{for} \quad 0 \le z < \rho\,, \quad \text{and} \quad \phi(z) = \Phi\,, \quad \text{for} \quad \rho < z \le d\,,$$

shown in Fig. 9(b). This solution is identical to the one deduced in the second example, where $U(z)$ was the discontinuous function (1.129).

1.13.5. *Fifth example*

Determine the function $\phi(z)$ extremizing the functional (1.141) when the function $K(z)$ is of the kind

$$K(z) = \begin{cases} K_1\,, & 0 \le z \le \rho \\ k(z)\,, & \rho \le z \le \rho + \epsilon \\ K_2\,, & \rho + \epsilon \le z \le d\,, \end{cases}$$

that is, it changes abruptly from K_1 to K_2 over ϵ. Discuss then the case in which $\epsilon \to 0$. Consider again the boundary condition of the fourth example, where $\phi(0) = 0$ and $\phi(d) = \Phi$.

Since in this case, $K(z)$ is a continuous function, the function minimizing the functional (1.141) is continuous too. Hence, by minimizing the functional (see Eq. (1.132)),

$$F = \int_0^\rho \frac{1}{2} K_1 {\phi_1'}^2 \mathrm{d}z + \int_\rho^{\rho+\epsilon} \frac{1}{2} k(z) {\varphi'}^2 \mathrm{d}z + \int_{\rho+\epsilon}^d \frac{1}{2} K_2 {\phi_2'}^2 \mathrm{d}z \,. \tag{1.147}$$

We have to take into account that

$$\phi_1(\rho) = \varphi(\rho) \qquad \text{and} \qquad \varphi(\rho+\epsilon) = \phi_2(\rho+\epsilon)\,,$$

which represent the continuity of $\phi(z)$ at $z = \rho$ and $z = \rho + \epsilon$. By operating in the standard manner from Eq. (1.147), we obtain for the bulk equations

$$K_1 \phi_1'' = 0\,, \quad \frac{d}{dz}[k(z)\varphi'(z)] = 0\,, \quad \text{and} \quad K_2 \phi_2'' = 0\,, \tag{1.148}$$

with the conditions

$$\begin{aligned} K_1 \phi_1'(\rho) &= k(\rho)\varphi'(\rho)\,, \\ k(\rho+\epsilon)\varphi'(\rho+\epsilon) &= K_2 \phi_2'(\rho+\epsilon)\,. \end{aligned} \tag{1.149}$$

From Eqs. (1.148) and the conditions (1.149), we derive that

$$K_1 \phi'(\rho) = k(\rho)\varphi'(\rho) = k(\rho+\epsilon)\varphi'(\rho+\epsilon) = K_2 \phi_2'(\rho+\epsilon) = c\,, \tag{1.150}$$

stating that $K(z)\phi'(z)$ is constant across the full range $[0, d]$ (see Fig. 10(b)).

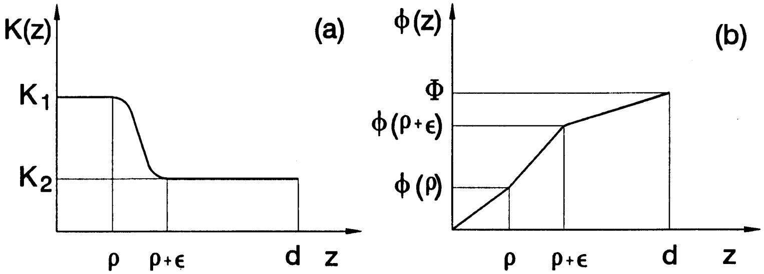

Fig. 10. (a) Function $K(z)$ presenting an abrupt variation localized over ϵ. (b) Function minimizing the functional (1.141). The boundary conditions at $z = 0$ and $z = d$ are as in Fig. 9.

From this result, we have in particular that

$$\varphi'(z) = \frac{c}{k(z)}\,,$$

showing that

$$\varphi'(\rho) = \frac{c}{K_1} \qquad \text{and} \qquad \varphi'(\rho+\epsilon) = \frac{c}{K_2}\,.$$

Consequently,

$$\lim_{\epsilon\to 0} \varphi'(\rho+\epsilon) \neq \varphi'(\rho)\,.$$

This result shows that in the limit $\epsilon \to 0$, ϕ' is discontinuous at $z = \rho$. From Eq. (1.150), we have furthermore

$$\varphi(z) - \varphi(\rho) = c\int_{\rho}^{z} \frac{dz'}{k(z')}\,, \tag{1.151}$$

and in particular

$$\varphi(\rho+\epsilon) - \varphi(\rho) = c\int_{\rho}^{\rho+\epsilon} \frac{dz}{k(z)}\,.$$

From Eq. (1.151), we deduce that

$$\lim_{\epsilon\to 0} \varphi(\rho+\epsilon) = \varphi(\rho)\,.$$

We can then conclude that $\phi_1(z)$ and $\phi_2(z)$ appearing in Eq. (1.147) may be deduced, in the case in which ϵ is negligible, by minimizing the functional

$$F = \int_0^{\rho} \frac{1}{2} K_1 \phi_1'^2 \,\mathrm{d}z + \int_{\rho}^{d} \frac{1}{2} K_2 \phi_2'^2 \,\mathrm{d}z\,, \tag{1.152}$$

by imposing the continuity of the function at $z = \rho$, i.e. $\phi_1(\rho) = \phi_2(\rho)$, and the continuity of $K_1\phi_1'(\rho) = K_2\phi_2'(\rho)$, as it follows from Eq. (1.150).

In this case, we obtain for the functions minimizing Eq. (1.152), and satisfying the above conditions

$$\phi_1(z) = \frac{\phi(\rho)}{\rho} z\,,$$

$$\phi_2(z) = \frac{\Phi - \phi(\rho)}{d-\rho}(z-\rho) + \phi(\rho)\,,$$

where

$$\phi(\rho) = \frac{\rho K_2}{\rho K_2 + (d-\rho)K_1}\Phi\,,$$

as it is easy to verify.

1.13.6. *Conclusions*

From the examples considered above, we can conclude that if $K(z)$ or $U(z)$ change abruptly over a range ϵ, negligible with respect to the lengths present in the problem, it is possible to solve the problem in an approximated manner. To do this we have to impose the continuity of ϕ and of $K\phi'$ at ρ, where the variations occur, and neglect the above-mentioned sharp variations.

1.14. Functional $F[\phi]$ in the Three-Dimensional Case

Determine the function $\phi(x, y, z) \in C_1$ extremizing the functional

$$F[\phi(x,y,z)] = \iiint_\tau f\left[\phi(x,y,z), \frac{\partial\phi}{\partial x}, \frac{\partial\phi}{\partial y}, \frac{\partial\phi}{\partial z}, x, y, z\right] \mathrm{d}\tau \,, \qquad (1.153)$$

where τ is a volume limited by a closed surface Σ over which $\phi(x, y, z)$ assumes the value $\phi(x, y, x) = \Phi(\Sigma)$, independent of the bulk values of $\phi(x, y, z \in \tau)$. This case corresponds to the strong-anchoring situation. Generalize the analysis to the weak-anchoring case.

Solution

Let us indicate by $\tilde{\phi}(x, y, z)$ the function extremizing Eq. (1.153) and assuming over Σ the value $\Phi(\Sigma)$,

$$\tilde{\phi}(x, y, z \in \Sigma) = \Phi(\Sigma) \,, \qquad (1.154)$$

imposed by the strong anchoring. A function $\phi(x, y, z)$ close to $\tilde{\phi}(x, y, z)$ is of the kind

$$\phi(x, y, z) = \tilde{\phi}(x, y, z) + \alpha v(x, y, z) \,, \qquad (1.155)$$

where, as usual, α is a small parameter and $v(x, y, z) \in C_1$. This function, in the strong-anchoring case, vanishes over Σ:

$$v(x, y, z \in \Sigma) = 0 \,.$$

As in the one-dimensional case, the differential equation satisfied by $\tilde{\phi}(x, y, z)$ is obtained by

$$\left(\frac{dF}{d\alpha}\right)_0 = 0 \,, \qquad \forall\, v(x, y, z) \in C_1 \,. \qquad (1.156)$$

To simplify the notation we indicate by x_i, $i = 1, 2, 3$, the coordinates x, y, z and by $\partial_i = \partial/\partial x_i$. Routine calculations give

$$\begin{aligned}\frac{dF}{d\alpha} &= \frac{d}{d\alpha}\iiint_\tau f[\phi(x_i), \partial_i\phi, x_i]\mathrm{d}\tau \\ &= \iiint_\tau \left[\frac{\partial f}{\partial\phi}\frac{\partial\phi}{\partial\alpha} + \frac{\partial f}{\partial(\partial_i\phi)}\frac{\partial}{\partial\alpha}(\partial_i\phi)\right]\mathrm{d}\tau \\ &= \iiint_\tau \left[\frac{\partial f}{\partial\phi}v + \frac{\partial f}{\partial(\partial_i\phi)}\partial_i v\right]\mathrm{d}\tau\,, \qquad (1.157)\end{aligned}$$

where the Einstein's convention has been used. By observing that

$$\frac{\partial f}{\partial(\partial_i\phi)}\partial_i v = \partial_i\left(\frac{\partial f}{\partial(\partial_i\phi)}v\right) - v\partial_i\frac{\partial f}{\partial(\partial_i\phi)}\,,$$

Eq. (1.157) may be rewritten as

$$\frac{dF}{d\alpha} = \iiint_\tau \left[\frac{\partial f}{\partial\phi} - \partial_i\frac{\partial f}{\partial(\partial_i\phi)}\right]v\mathrm{d}\tau + \oint_\Sigma \nu_i\frac{\partial f}{\partial(\partial_i\phi)}v\mathrm{d}\Sigma\,, \qquad (1.158)$$

where we have used the Gauss theorem. In Eq. (1.158), ν_i are the Cartesian components of the surface geometrical normal to $\mathrm{d}\Sigma$. By imposing Eq. (1.156), $\forall\, v(x_i) \in C_1$ such that $v(x_i \in \Sigma) = 0$, from Eq. (1.158) we derive that

$$\frac{\partial f}{\partial\phi} - \partial_i\frac{\partial f}{\partial(\partial_i\phi)} = 0\,, \qquad \forall\, x_i \in \tau\,. \qquad (1.159)$$

The differential Eq. (1.159) defines the function ϕ extremizing F given by Eq. (1.153). The actual $\phi(x_i)$ satisfies the boundary condition (1.154).

In the case of weak anchoring, instead of the functional (1.153), it is necessary to consider the quantity

$$F[\phi(x_i)] = \iiint f[\phi(x_i), \partial_i\phi, x_i]\mathrm{d}\tau + \oint_\Sigma \gamma[\phi(x_i)]\mathrm{d}\Sigma\,,$$

where $\gamma[\phi(x_i \in \Sigma)]$ represents the surface contribution to F. In this case, we can still use the parametrization (1.155), but $v(x_i \in \Sigma) \neq 0$. By taking into account that

$$\frac{d}{d\alpha}\oint_\Sigma \gamma(\phi)\mathrm{d}\Sigma = \oint_\Sigma \frac{\partial\gamma}{\partial\phi}\frac{\partial\phi}{\partial\alpha}\mathrm{d}\Sigma = \oint_\Sigma \frac{\partial\gamma}{\partial\phi}v\mathrm{d}\Sigma\,,$$

Eq. (1.157) writes in the present case as

$$\frac{dF}{d\alpha} = \iiint_\tau \left[\frac{\partial f}{\partial \phi} - \partial_i \frac{\partial f}{\partial(\partial_i \phi)}\right] v\mathrm{d}\tau + \oint_\Sigma \left(\nu_i \frac{\partial f}{\partial(\partial_i \phi)} + \frac{\partial \gamma}{\partial \phi}\right) v\mathrm{d}\Sigma\,.$$

Since $dF/d\alpha = 0$, $\forall\, v(x_i) \in C_1$, we derive again Eq. (1.159) which has to be solved with the boundary condition

$$\nu_i \frac{\partial f}{\partial(\partial_i \phi)} + \frac{\partial \gamma}{\partial \phi} = 0\,, \qquad \forall\, x_i \in \Sigma\,,$$

due to the fact that $v(x_i \in \Sigma)$ is an arbitrary quantity.

1.15. Dirichlet Problem

Determine the function $\phi(x, z)$, which in the region $-d/2 \leq z \leq d/2$ and $-\infty < x < \infty$, minimizes the functional

$$F[\phi(x,z)] = \int_{-d/2}^{d/2} \int_{-\infty}^{\infty} \frac{1}{2} (\vec{\nabla}\phi)^2 \mathrm{d}x\mathrm{d}z\,, \tag{1.160}$$

and on the boundaries located at $z = \pm d/2$ assumes the values $\phi(x, -d/2) = \Phi_-(x)$ and $\phi(x, d/2) = \Phi_+(x)$. Consider, in particular, the case in which

$$\Phi_-(x) = \Phi_+(x) = \begin{cases} \Phi_1\,, & x < 0 \\ \Phi_2\,, & x > 0\,. \end{cases} \tag{1.161}$$

Solution

In the present case

$$f\left(\phi, \frac{\partial \phi}{\partial x}, \frac{\partial \phi}{\partial z}; x, z\right) = \frac{1}{2}\left[\left(\frac{\partial \phi}{\partial x}\right)^2 + \left(\frac{\partial \phi}{\partial z}\right)^2\right].$$

Consequently, Eq. (1.159)

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial z^2} = 0, \qquad \forall\, (x, z)\, \in [(-\infty, \infty), (-d/2, d/2)]\,. \tag{1.162}$$

It follows that the function extremizing Eq. (1.160) is a harmonic function, which satisfies the boundary conditions

$$\phi(x, -d/2) = \Phi_-(x) \quad \text{and} \quad \phi(x, d/2) = \Phi_+(x)\,. \tag{1.163}$$

To find the solution of Eq. (1.162) satisfying Eq. (1.163), we expand $\phi(x,z)$ as follows:

$$\phi(x,z) = \int_{-\infty}^{\infty} \left[\alpha(k)e^{ikx+kz} + \beta(k)e^{ikx-kz}\right] \mathrm{d}k\,, \tag{1.164}$$

where $\alpha(k)$ and $\beta(k)$ have to be determined by means of Eq. (1.163). By substituting Eq. (1.164) into Eq. (1.163) and exploiting the orthonormality of the set of functions e^{ikx}, one obtains

$$I_-(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ikx}\Phi_-(x)\mathrm{d}x = \alpha(k)e^{-kd/2} + \beta(k)e^{kd/2}\,,$$

$$I_+(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ikx}\Phi_+(x)\mathrm{d}x = \alpha(k)e^{kd/2} + \beta(k)e^{-kd/2}\,,$$

where $I_-(k)$ and $I_+(k)$ are known functions of k. From these equations for $I_\pm(k)$, we deduce for $\alpha(k)$ and $\beta(k)$ the expressions

$$\alpha(k) = \frac{I_+(k)e^{kd/2} - I_-(k)e^{-kd/2}}{2\sinh(kd)}\,,$$

$$\beta(k) = \frac{I_-(k)e^{kd/2} - I_+(k)e^{-kd/2}}{2\sinh(kd)}\,.$$

By substituting $I_\pm(k)$ into Eq. (1.164), we obtain

$$\phi(x,z) = \int_{-\infty}^{\infty} \left[G_+(x-x',z)\Phi_+(x') + G_-(x-x',z)\Phi_-(x')\right] \mathrm{d}x'\,, \tag{1.165}$$

where the kernels $G_\pm(x-x',z)$ are given by

$$G_\pm(x-x',z) = \pm\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik(x-x')}\frac{\sinh k(z \pm d/2)}{\sinh(kd)}\mathrm{d}k\,.$$

An integration allows to put $G_\pm(x-x',z)$ in the form

$$G_\pm(x-x',z) = \frac{1}{2d}\frac{\cos(\pi z/d)}{\cosh[\pi(x-x')/d] \mp \sin(\pi z/d)}\,. \tag{1.166}$$

Expression (1.165), in which $G_\pm(x-x',z)$ are given by Eq. (1.166), represents the general solution of our problem.

Let us consider now the simple case in which $\Phi_\pm(x)$ are given by Eq. (1.161). In this case Eq. (1.165) reads

$$\phi(x,z) = \Phi_1 \int_{-\infty}^{0} [G_+(x-x',z) + G_-(x-x',z)]\mathrm{d}x' + \Phi_2 \int_{0}^{\infty} [G_+(x-x',z) + G_-(x-x',z)]\mathrm{d}x' \,.$$

Since $G_\pm(x-x',z)$ are given by Eq. (1.166), we have

$$G_+(x-x',z) + G_-(x-x',z) = \frac{1}{d}\frac{\cos(\pi z/d)\cosh(\pi(x-x')/d)}{\cosh^2(\pi(x-x')/d) - \sin^2(\pi z/d)}\,,$$

which is even in z, as required by the present problem because $\Phi_-(x) = \Phi_+(x)$, and hence $\phi(x,z) = \phi(x,-z)$. By taking into account that

$$\begin{aligned} j_1(x,z) &= \frac{1}{d}\int_{-\infty}^{0} \frac{\cos(\pi z/d)\cosh[\pi(x-x')/d]}{\cosh^2[\pi(x-x')/d] - \sin^2(\pi z/d)}\mathrm{d}x' \\ &= \frac{1}{\pi}\left\{\frac{\pi}{2} - \arctan\left[\frac{\sinh(\pi x/d)}{\cos(\pi z/d)}\right]\right\} \\ j_2(x,z) &= \frac{1}{d}\int_{0}^{\infty} \frac{\cos(\pi z/d)\cosh[\pi(x-x')/d]}{\cosh^2[\pi(x-x')/d] - \sin^2(\pi z/d)}\mathrm{d}x' \\ &= \frac{1}{\pi}\left\{\frac{\pi}{2} + \arctan\left[\frac{\sinh(\pi x/d)}{\cos(\pi z/d)}\right]\right\}\,, \end{aligned} \tag{1.167}$$

we obtain that in the present case, $\phi(x,z)$ is given by

$$\phi(x,z) = \Phi_1 j_1(x,z) + \Phi_2 j_2(x,z)\,, \tag{1.168}$$

where $j_{1,2}(x,z)$ are given by Eq. (1.167). By substituting Eq. (1.167) into Eq. (1.168), we have finally, for $\phi(x,z)$ the expression

$$\phi(x,z) = \frac{1}{2}(\Phi_1 + \Phi_2) + \frac{1}{\pi}(\Phi_2 - \Phi_1)\arctan\left(\frac{\sinh(\pi x/d)}{\cos(\pi z/d)}\right)\,. \tag{1.169}$$

The function $\phi(x,z)$ given by Eq. (1.169) is a harmonic function which satisfies the boundary conditions (1.161). In the bulk, i.e. for $-d/2 < z < d/2$, $\phi(x,z)$ passes, in a continuous manner, from Φ_1 to Φ_2 (Fig. 11).

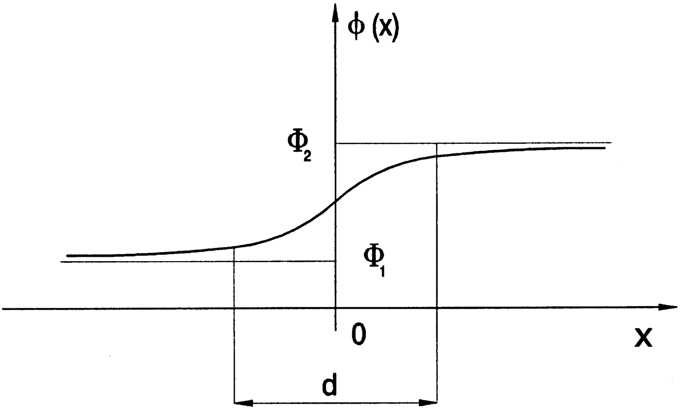

Fig. 11. Solution of the Dirichlet problem for the boundary conditions $\phi(x, \pm d/2) = \Phi_1$, $x < 0$ and $\phi(x, \pm d/2) = \Phi_2$, $x > 0$, for $z = \pm d/2$. Note that $\phi(x, z)$ varies in a region whose thickness is of the order of d, where d is the width of the band $(-d/2 \leq z \leq d/2)$.

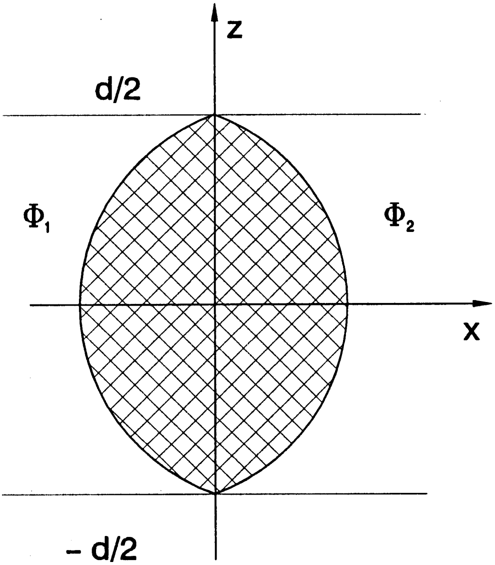

Fig. 12. The dashed region represents the zone in which is localized the variation of $\phi(x, z)$ for the Dirichlet problem. Note that for $z = \pm d/2$, $\phi(x, \pm d/2)$ present two discontinuity points. When ϕ represents an elastic deformation, the discontinuity points are called dislocations and the dashed region, wall of constraint.

Let us consider the straight-line at $z = 0$, and analyze the x dependence of $\phi(x, 0)$. A simple analysis shows that for small x, i.e. $|\pi x/d| \ll 1$, Eq. (1.169) reads

$$\phi(x,0) = \frac{1}{2}(\Phi_1 + \Phi_2) + (\Phi_2 - \Phi_1)\frac{x}{d}\,,$$

that is $\phi(x, 0)$ changes linearly with x. The spatial variations, along x, of $\phi(x, z)$ is localized in a region whose thickness is of the order of d. For a generic z coordinate, the thickness of the regions is of the order of $d\cos(\pi z/d)$. We can then conclude that the discontinuity of the surface values of $\Phi(x)$ induces a "wall" in which $\phi(x, z)$ depends on both the coordinate (x, z) of the kind shown in Fig. 12. The thickness of the wall for $z = \pm d/2$ is zero, due to the strong-anchoring hypothesis.

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