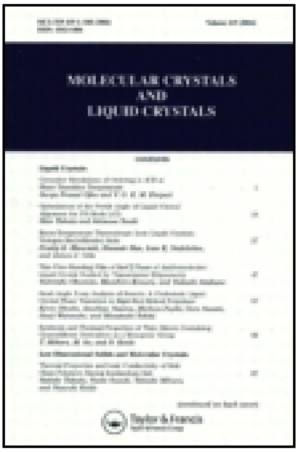


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# Surface Elastic Constant Problems for NLC Confined to Cylindrical Cavity: Stability of Axial Configuration

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# SURFACE ELASTIC CONSTANT PROBLEMS FOR NLC CONFINED TO CYLINDRICAL CAVITY: STABILITY OF AXIAL CONFIGURATION

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Abstract In this paper we consider nematic liquid crystal (NLC) confined to cylindrical cavity under the homeotropic anchoring conditions. Saddle-splay and splay-bend terms influence on the axial director configuration stability in the presence of magnetic field applied along the cavity axis is investigated. By using the Fourier expansion of director fluctuations over azimuth angle our analytical method of attack enables the stability conditions to be found in terms of the stability to each fluctuation mode. The dependence of the resultant stability threshold on the surfacelike elastic constant values is calculated. We have obtained the restrictions imposed on the constants to make possible the stabilization of the axial structure by the magnetic field.

## INTRODUCTION

As it have been shown in the papers of Oseen[1] and Frank[2] and, 40 years later, by Nehring and Saupe[3] in addition to the usual Frank terms ( splay plus twist plus bend ) the nematic free energy contains so-called surfacelike elastic terms ( comment on the terminology is made in Sec. III ), that is, two terms of divergence form which can be transformed into integrals over the boundary surface and are proportional to the saddle-splay elastic constant, $K_{24}$, and the splay-bend one, $K_{13}$. They may be taken in the following forms:

$$F_{24} = -\frac{K_{24}}{2}\int_V dv\, \mathrm{div}\left[\underline{n}\,\mathrm{div}\,\underline{n} + [\,\underline{n}\,\mathrm{curl}\,\underline{n}\,]\right] \qquad (1)$$

$$F_{13} = \frac{K_{13}}{2}\int_V dv\, \mathrm{div}\left[\underline{n}\,\mathrm{div}\,\underline{n}\right] \qquad (2)$$

where $\underline{n}$ is the nematic director field.

The surface terms are irrelevant if we are interested in the bulk properties of nematic liquid crystal (NLC), but they are of considerable importance in the understanding of the physical properties of NLC confined in geometries more restrictive than bulk. Dealing with the surface elastic constant problem one comes up against two questions: Is it possible to incorporate the surfacelike elastic terms into the framework of the liqiud crystal continuum theory unambiguously ? What are the effects caused by the presence of $K_{24}$- and $K_{13}$- terms ?

Let us take up first the $K_{24}$- problem with the $K_{13}$- term being disregarded. At the moment it is safe to say that the answer to the first question is affirmative and the problem of minimizing the free energy with the $K_{24}$- term was shown to be always well posed[4,5] for the term doesn't contain the director derivatives along the directions normal to the boundary surface. Hence the only effect is that the $K_{24}$- term affects the standard boundary conditions. Recently the second question has been received much attention: physical effects whose very occurrence critically depends on the value of $K_{24}$ has been shown to exist[5-9], and even estimates of the value of $K_{24}$ has been made[10-12].

In contrary to the $K_{24}$- problem, the issue relative to the $K_{13}$- term is much more questionable. In the strict sence, the free energy functional with the $K_{13}$- term is unbounded below and that is the reason why strong spontaneous substrate director deformations were found to be possible[13]. One way to avoid such an unphysical effect is to search the director distrbution minimizing the free energy functional among the solutions to the Euler-Lagrange equations[14-15]. Recently the estimate of the value of $K_{13}$, obtained on the basis of this method, have been reported[16]. We are not to discuss another ways of looking at the problem[17-18] and shall employ the above approach to study how the surfacelike terms affect the stability threshold of axial director configuration in NLC confined to cylindrical cavity in the presence of stabilizing magnetic field under the homeotropic anchoring conditions.

In Sec.II the stability analysis is given in the one-constant approximation. By using the Fourier expansion of director fluctuation over azimuth angle we derive unequalities that yield the stability of the axial structure to every fluctuation harmonics. It is found that one has to impose the restrictions on the values of $K_{24}$ and $K_{13}$ to make possible the stabilization of the structure by the magnetic field. In particular, the value of $K_{24}/2K$ must fall in the range from zero to unity provided $K_{13} = 0$. The same result had been obtained in the case of spherical cavity[9] and we have the $K_{24}$- term being of great importance to the axial structure stability. Taking into account the $K_{13}$- term the stabilization appears to be possible provided that the quantity $K_{13}/4K$ lies between $q_{24} - (q_{24})^{1/2}$ and $q_{24} + (q_{24})^{1/2}$, where the notation $q_{24}$ stands for $K_{24}/2K$. We also discuss whether the number of fluctuation mode, which defines the resultant stability threshold, could be changed by the magnetic field at a given $K_{24}$ and $K_{13}$ . The results of numerical calculations are presented.

Some additional comments on the $K_{13}$- problem are made in Sec. III . The stability threshold to zero-numbered fluctuation mode is shown to describe the transition between the axial structure and the escape-radial one. A comparison of the energies reveals that there are the values of $K_{13}$ such that the stability condition doesn't provide the global stability of the axial pattern .

Some calculations are detailed in Appendix.

## STABILITY OF AXIAL DIRECTOR CONFIGURATION

Let us consider NLC confined to the cylindrical cavity of radius R in the presence of magnetic field applied along the cavity axis, $\underline{H} = H\, \underline{e}_z$. The NLC free energy may be taken in its standard form:

$$F = \frac{K}{2} \int_V dv \left[ ( \operatorname{div} \underline{n} )^2 + ( \operatorname{curl} \underline{n} )^2 - q^2 n_z^2 \right] +$$

$$+ F_{24} + F_{13} - \frac{W}{2} \int_S ds\, ( \underline{n}, \underline{e} )^2 \qquad (3)$$

where the one-constant approximation is used and $q^2 = \chi_a H/K$ ( $q^{-1}$ is the magnetic coherent length, $\chi_a$ is the anisotropic part of magnetic susceptibility ), W is the anchoring energy, $\underline{e}$ is the unit vector directed along the axis of easy orientation on the confining surface. The last addend of Eq.(3) represents the energy of the interaction between NLC and the cavity wall written in the Rapini- Papoular form[19]. To begin with the stability analysis it is convenient to present the director in the cylindrical coordinate system ( OZ axis is paralell to the cavity axis ) as follows:

$$\underline{n} = \cos\Theta \cos\Phi\, \underline{e}_z + \cos\Theta \sin\Phi\, \underline{e}_R + \sin\Theta\, \underline{e}_\varphi \qquad (4)$$

where $\Theta = \Theta(r,\varphi)$ and $\Phi = \Phi(r,\varphi)$. Evidently, the axial director distribution ( $\underline{n}_o = \underline{e}_z$ ) can be obtained from Eq.(4) on putting $\Theta = \Phi = 0$. Hereinafter we shall use the notations $\theta$ and $\phi$ for small deviations of the angles $\Theta$ and $\Phi$ from zero and assume the anchoring conditions to be homeotropic, $\underline{e} = \underline{e}_R$.

To study the axial configuration stability one has to substitute the director field given by Eq.(4) into the expression for the NLC free energy Eq.(3) and derive the second-order variation of the free energy functional $\delta^2 F$ as a bilinear part of the energy in the angle fluctuations $\theta$ and $\phi$. The result is given by Eq.(A1) in Appendix, where after the fluctuations expanded in Fourier series over azimuth angle and the Euler-Lagrange equations solved the second-order variation of the free energy is shown to be a sum of quadratic forms $\delta^2 F_m(A)$, each associated with fluctuation mode specified by number m ( see Eqs.(A10-A11) ).

For the axial configuration to be stable all the quadratic forms $\delta^2 F_m(A)$ should be positive definite, so that the condition of the axial structure stability is given by a set of inequalities descriptive of the stability to each fluctuation harmonics. Standard algebraic analysis provides the conditions for $\delta^2 F_m$ to be positive definite which are taken in the form suitable for subsequent discussion:

$$m = 0: \quad \begin{cases} w < ( 1 + 2q_{13} ) \, \gamma_{+1}(x) - q_{24} = T_0(x) \\ 0 < \gamma_{+1}(x) - q_{24} = p_0(x) \end{cases} \tag{5a}$$

$$m > 0: \quad \begin{cases} w < T_m(x) = t_m(x)/(2p_m(x)) \\ 0 < p_m(x) = \alpha_m(x) + \beta_m(x) - 2q_{24} \end{cases} \tag{5b}$$

where
$$\gamma_{m+1}(x) = \frac{x\, I_m(x)}{2\,(m+1)\, I_{m+1}(x)} = \frac{\beta_m(x)}{m+1} \tag{6a}$$

$$\gamma_{m-1}(x) = \frac{2\, m\, I_m(x)}{x\, I_{m-1}(x)} = 4\, m\, \alpha_m(x)\, x^{-2} \tag{6b}$$

$$\begin{aligned} t_m(x) = &- q_{13}^2 \left( \alpha_m(x) - \beta_m(x) \right)^2 + \\ &+ 4\, q_{13} \left( \alpha_m(x) \, [\, 2\, \beta_m(x) - (\, m + 1\, )\, q_{24}\, ] + \right. \\ &\left. + q_{24}(\, m - 1\, )\, \beta_m(x) \right) + \\ &+ 4 \left( \alpha_m(x) + (\, m - 1\, )\, q_{24} \right) \left( \beta_m(x) - (\, m + 1\, )\, q_{24} \right). \end{aligned} \tag{7}$$

The following designations for four dimensionless parameters were used: $w = WR/2K$, $q_{24} = K_{24}/2K$ , $q_{13} = K_{13}/2K$ and $x = qR$.

Since parameter w is nonnegative, we can determine the resultant stability threshold as a greatest lower bound of the quantities, that govern the stability to each fluctuation mode:

$$W_c(x) = \inf_m \{ TR_m(x) \} \tag{8}$$

$$TR_m(x) = \begin{cases} T_m(x), \text{ if } T_m(x) > 0 \text{ and } p_m(x) > 0 \\ 0, \text{ otherwise} \end{cases} \tag{9}$$

Then the stability condition is given by

$$w < W_c(x) \ . \tag{10}$$

In what follows we consider the possibility for the axial director configuration to be stabilized by applying the magnetic field. Mathematically, the magnetic field fails to stabilize the structure if $W_c(x) = 0$ for all $x > 0$.

## $K_{24}$-Term Influence On The Stability Threshold

In this subsection we explore the case of $K_{13} = 0$. First it is useful to point out some simplest properties of the functions $\gamma_{m\pm1}(x)$: a. $\gamma_{m\pm1}(0) = 1$; b. $\gamma_{m+1}(x) > 1$, $\gamma_{m-1}(x) < 1$ for nonzero values of $x$; c. $\gamma_{m\pm1}(x)$ monotonically tend to unity as m goes to infinity. There is no need to make numerical calculation to arrive at the conclusion that the axial structure cannot be stabilized by the magnetic field if the value of $q_{24}$ doesn't lie within the interval (0, 1). In other words, if $q_{24}$ takes a value, which is outside the interval (0, 1), then for a given value of x there is a number m, such that either $p_m(x) < 0$ or $T_m(x) < 0$. To prove our contention let $q_{24}$ initially be negative, so that $p_m(x) > 0$ for any m. The expression for $t_m(x)$ can be rewritten as follows:

$$t_m(x) = 4\,(m+1) \left[ \alpha_m + (m-1)\, q_{24} \right] \left[ \gamma_{m+1} - q_{24} \right] \tag{11}$$

Obviously, sign of $t_m(x)$ is dictated by the first factor enclosed in square brackets and it remains to see that the factor goes negative for sufficiently large number m, since $\alpha_m(x)$ tends to zero as $m \longrightarrow \infty$ ( see Eq.(6b) ). If $q_{24}$ is greater than unity it will suffice to note that $\gamma_{m+1}(x)$ is monotonically decreasing function of m , which tends to unity as $m \to \infty$ , and therefore the second factor of Eq.(11) enclosed in square brackets goes negative, beginning with sufficiently large number m, while the first one being positive.

The same restrictions on $q_{24}$ had been shown to hold in the case of spherical geometry[9] and ones are more rigid than those given by Ericksen[21]. The latter can be rewritten in our denotions as: $0 < q_{24} < 2$. Note that the values of $q_{24}$ extracted from the deuterium nuclear-magnetic-resonance experiments[11,12] on nematic submicrometer-sized cylindrical cavities typically fall in the range 0.4 to 0.6 for 5CB-$\beta d_2$ with $K = 5\ 10^{-12}$ J/m and $W = 3\ 10^{-5}$ J/m$^2$. The value of w had been varied between 0.1 and 10 in[11].

The plots of $TR_0 - TR_3$ in relation to $x = qR$ , arranged in w-qR plane, are presented in Fig.1a at $q_{24} = 0.8$ to show how the curves $TR_m$ form the threshold line $W_c$, which is the lowermost curve (see Eq.(8)) and its graph in w-qR plane yields the stability diagram.

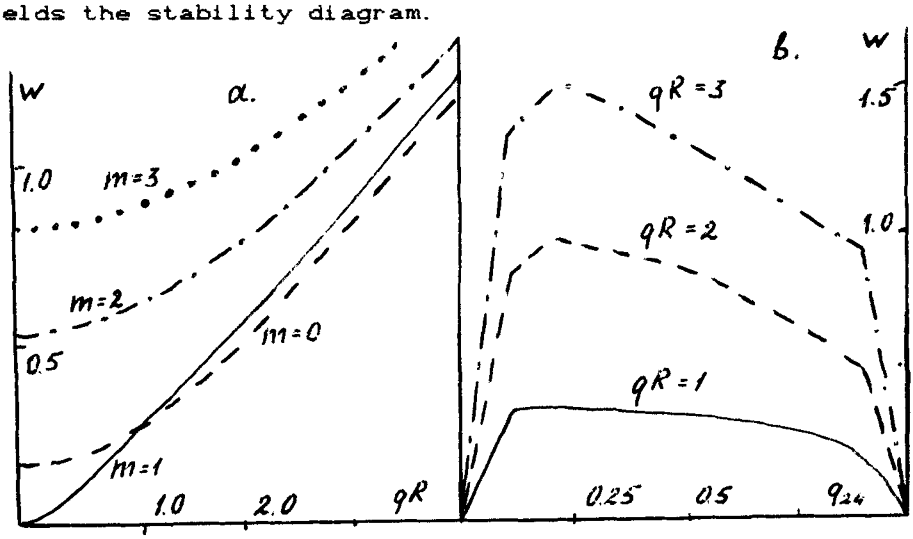


FIGURE 1 a. The plots of $TR_m$ versus qR in w - qR plane for m = 0 - 3 at $q_{24} = 0.8$. The stability region is arranged below the lowermost curves. b. The stability diagram in w - $q_{24}$ plane at qR = 1 - 3. For a given value of qR the area of the stability is enclosed by the curve and the $q_{24}$-axis.

As illustrated, the first fluctuation mode ( $m = 1$ ) defines the stability threshold for a small magnetic field strength ( $TR_1(0) = 0$ ), but the number of the mode, governing the threshold, changes to zero as the field strength increases. The modes, that contribute to the resultant stability threshold, $W_c(x)$, are increasing in number when the quantity $q_{24}$ approaches zero or unity. Interestingly, $TR_m(x)$ are not equal to zero for all m at $q_{24} = 0$ or 1 and $x \neq 0$, but $\lim TR_m = 0$ as $m \to \infty$ and, as a consequence, $W_c(x) = 0$ for any x. It suggests that high order fluctuation modes play an important part in an immediate vicinity of the critical values of $q_{24}$ causing the destabilization of the structure as $q_{24}$ passes through its critical points. The effect of the destabilization is illustrated in Fig. 1b, where the graphs of $W_c$ as a function of $q_{24}$ are shown at qR = 1, 2, 3.

## $K_{13}$-Term Influence On The Stability Threshold

Here we find out how the surface elastic constant $K_{13}$ affects the axial pattern stability. As can be seen from Eqs.(5a-5b), the quantities $p_m(x)$ don't depend on $K_{13}$ and it is possible to meet the condition $p_m(x) > 0$ by choosing an appropriate magnitude of the field strength, that is x, even in the case of $q_{24} > 1$. Thus one has to analyze the expression for $t_m(x)$ as it has been done in the previous subsection. To this end let us consider the quantity $t_m(x)$ in the zero field limit:

$$t_m(0)/(m+1) = - q_{13}^2 (m+1) + 4 q_{13} (m-1) q_{24} + + 4 (m-1) q_{24} (1-q_{24}) \quad (12)$$

The stabilization can be proved to be possible only if the right-side part of Eq.(12) is an increasing function of m. It immediately follows that the parameter $q_{13}/2$ has to lie between $q_{24} - (q_{24})^{1/2}$ and $q_{24} + (q_{24})^{1/2}$ and $q_{24} > 0$:

$$2 [ q_{24} - (q_{24})^{1/2} ] < q_{13} < 2 [ q_{24} + (q_{24})^{1/2} ] \quad (13)$$

Omitting comprehensive proof of the statement, we just note that one is based on the observation that the coefficients of the quadratic polynomial in $q_{13}$ given by Eq.(12) will differ from ones in the case of nonzero magnetic field by quantities which tend to zero as $m \longrightarrow \infty$. Interestingly, there are no restrictions on $q_{24}$ bounded its value from above and $q_{24}$ just must be positive. From this point of view, one can say that $K_{13}$- term plays a stabilizing part in the problem. On the other hand, reffering to Fig. 2a, it can be seen that the axial pattern is unstable until the strength of magnetic field reaches its critical value, $x = x_c$, which strongly depends on $q_{24}$ and $q_{13}$. Indeed, coming back to Eq.(12), we find that $t_1(0) < 0$ and therefore it is necessary to apply the magnetic field of finite amplitude to make it positive. Here we have the effect to be tested experimentally.

Eq.(13) sets the limit on the value of $q_{13}$ from below: $q_{13}$ must be greater than $- 0.5$. The experimentally obtained estimate[16] of $K_{13}$ provides $q_{13} = - 0.2$ for submicron nematic films.

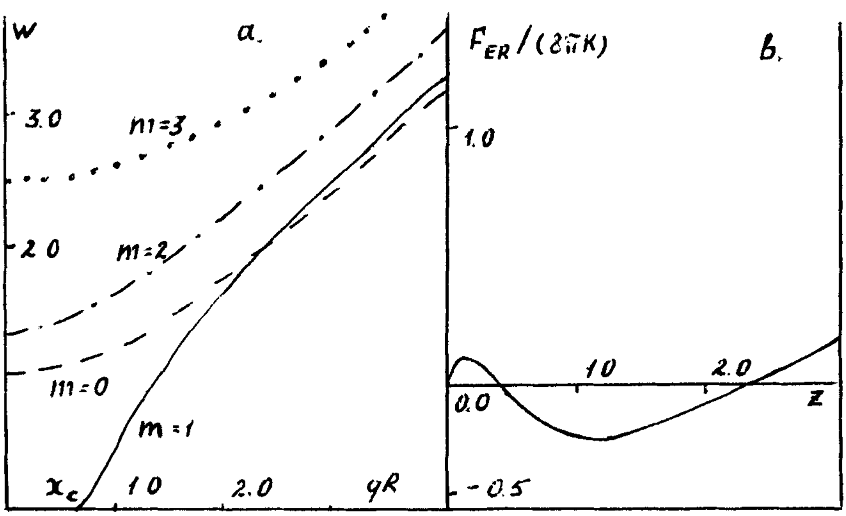


FIGURE 2 a. The qR - dependence of $TR_m$ in w-qR plane for $m = 0 - 3$ at $q_{24} = 0.8$ and $q_{13} = 0.5$ The axial structure is shown to be unstable at $qR < x_c$. b. The energy of the escaped-radial configuration as a function of parameter z at $q_{24} = 0.9$, $q_{13} = 1.2$ and $w = 2.0$ .

CONCLUSIONS

In this paper we study how the surfacelike elastic terms influence the stability of the axial configuration under the homeotropic anchoring conditions. It is reasonable to take the assumption that the axial pattern can be stabilized by magnetic field. If so, our analysis provides the restrictions on the values of $K_{24}$ and $K_{13}$. The $K_{13}$ - term is found to change the situation in both quantitative and qualitative ways. For instance, we saw the $K_{13}$ - term result in the appearence of the threshold for the magnetic field even if $W = 0$ ( no anchoring ). To clarify the role of $K_{13}$-term we now compare the value of the axial configuration energy , $F_A = 0$, with the free energy of the escaped-radial configuration[12,22]:

$$F_{ER}(z) = 4\pi K z (1+z)^{-3} \left[ z^2 + ( 3 - 2q_{24} - 2w + 4q_{13} ) z + + 2 ( 1 - q_{24} - w + 2q_{13} ) \right] \qquad (14)$$

where $z = (R/\rho)^2$, $\rho$ is the integration constant. It is easy to see from Eqs.(5a, 14) that the stability condition $w < T_0(0)$ implies an increase of $F_{ER}(z)$ at $z = 0$, i.e. it means the local stability of the axial configuration. But as evident from Fig. 2b , in the presence of the $K_{13}$-term the local stability doesn't imply the global one. Thus we encounter here the effect which looks like bistability and caused by the $K_{13}$- term. For definiteness sake, one has to point out the fact that the first fluctuation mode makes the axial structure unstable under the homeotropic anchoring conditions in the zero field limit. But after w is replaced by -w in Eq.(14), we get the expression for the difference in energy of two configurations under the planar anchoring conditions with the vector of easy orientation directed along the cavity axis and the same effect can be shown to be possible. More detailed discussion will be given elsewhere[23].

Let us make a comment on the terminology used throughout the paper. Although it is common practice we followed to use the terms 'surfacelike' and 'surface elastic constants', the term 'divergence elastic constants' recently proposed by V. Pergamenchshik ( report at 15th ILCC ) seems to be more appropriate.

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APPENDIX

Here we sketch the way to derive the expression for $\delta^2 F$ as a sum of quadratic forms associated with fluctuation modes. The bilinear part of the free energy functional may be written in the following form:

$$\delta^2 F = \frac{K}{2}\int_0^{2\pi} d\varphi \int_0^R r\ dr \left\{ \left[ \frac{\phi}{r} + \frac{\partial\phi}{\partial r} + \frac{1}{r}\frac{\partial\theta}{\partial\varphi} \right]^2 + \right.$$

$$\left. + \left[ \frac{\theta}{r} + \frac{\partial\theta}{\partial r} - \frac{1}{r}\frac{\partial\phi}{\partial\varphi} \right]^2 \right\} + \delta^2 F_{24} + \delta^2 F_{13} + \delta^2 F_s \qquad (A1)$$

where

$$\delta^2 F_{24} = -K_{24}/2 \int_0^{2\pi} d\varphi \left[ \phi^2 + \theta^2 + \phi\frac{\partial\theta}{\partial\varphi} - \theta\frac{\partial\phi}{\partial\varphi} \right]_{r=R} \qquad (A2)$$

$$\delta^2 F_{13} = K_{13}/2 \int_0^{2\pi} d\varphi \left[ \phi^2 + \phi\frac{\partial\theta}{\partial\varphi} + R\,\phi\frac{\partial\phi}{\partial r} \right]_{r=R} \qquad (A3)$$

$$\delta^2 F_s = -W\ R/2 \int_0^{2\pi} d\varphi\ \phi^2 \Big|_{r=R} \qquad (A4)$$

The Euler-Lagrange equations for the functional $\delta^2 F$ are given by:

$$\begin{bmatrix} \Delta - 1 - q^2 r^2 & 2\frac{\partial}{\partial\varphi} \\ -2\frac{\partial}{\partial\varphi} & \Delta - 1 - q^2 r^2 \end{bmatrix} \begin{bmatrix} \theta \\ \phi \end{bmatrix} = 0 \qquad (A5)$$

where

$$\Delta = \left( r \frac{\partial}{\partial r} \right)^2 + \left( \frac{\partial}{\partial\varphi} \right)^2 .$$

Since the angle fluctuations are $2\pi$-periodic functions of the azimuth angle, they can be expanded in the Fourier series over $\varphi$ .

$$\theta = (2\pi)^{-1/2} \sum_{m=-\infty}^{\infty} \theta_m(r) \exp(im\varphi) \qquad (A6a)$$

$$\phi = (2\pi)^{-1/2} \sum_{m=-\infty}^{\infty} \phi_m(r) \exp(im\varphi) \qquad (A6b)$$

To solve the Euler-Lagrange equations let us introduce new Fourier amplitudes in the following way:

$$\phi_m^1(r) = ( \phi_m(r) + i\, \theta_m(r) )/2 \qquad (A7a)$$

$$\theta_m^1(r) = ( \phi_m(r) - i\, \theta_m(r) )/2 \qquad (A7b)$$

By using Eqs.(A5-A7) it is not difficult to get the equations for these fluctuation mode amplitudes:

$$\Delta_{m+1}\phi_m^1 = 0; \quad \Delta_{m-1}\theta_m^1 = 0, \qquad (A8)$$

where $\Delta_{m\pm 1} = \left( r \frac{\partial}{\partial r} \right)^2 - ( m \pm 1 )^2 - q^2 r^2$ .

The solutions to the equations (A8) are expressed in terms of modified Bessel functions[20] :

$$\theta_m^1(r) = C_m^1 I_{|m-1|}( q r ); \quad \phi_m^1(r) = C_m^2 I_{m+1}( q r ), \qquad (A9)$$

where $C_m^j$ are the complex coefficients ( $\mathrm{Re}\, C_m^j = A_m^j$ and $\mathrm{Im}\, C_m^j = B_m^j$, $j = 1, 2;$ ), $I_m(x)$ is the modified Bessel function of order m .

After inserting Eqs.(A6, A7, A9) into Eq.(A1) and performing rather routine calculations we have

$$\delta^2 F = \sum_{m=0}^{\infty} \left[ \delta^2 F_m(A) + \delta^2 F_m(B) \right] \qquad (A10)$$

$$\delta^2 F_m(A) = (A_m^1)^2 \left\{ ( K + K_{13}/2 ) \times I_{|m-1|}(x)\, I_m(x) + \right.$$
$$\left. + I_{|m-1|}^2(x) ( K_{24}( m - 1 ) - W R/2 ) \right\} +$$
$$+ (A_m^2)^2 \left\{ ( K + K_{13}/2 ) \times I_{m+1}(x)\, I_m(x) - \right.$$
$$\left. - I_{m+1}^2(x) ( K_{24}( m + 1 ) + W R/2 ) \right\} +$$
$$+ A_m^1 A_m^2 \left\{ K_{13} \times I_m(x) ( I_{m+1}(x) + I_{|m-1|}(x) )/2 - \right.$$
$$\left. - I_{m+1}(x)\, I_{|m-1|}(x)\, W R \right\} , \qquad (A11)$$

where $x = q R$ .

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