Fréedericksz transition thresholds in pretilted nematic slabs

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The appearance of periodically distorted director structures in pretilted nematic slabs with rigid boundary conditions above the Fréedericksz transition is determined as a function of the Frank elastic constant ratios K_2/K_1, K_3/K_1, and the pretilt angle. It is found that the periodically distorted state can be reached either directly from the undistorted state on increasing the magnetic field or indirectly through the homogeneously distorted state. A new threshold field for the transition undistorted state, homogeneously distorted state was found for specific ranges of the Frank elastic constant ratios K_2/K_1, K_3/K_1, and the pretilt angle.
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I. INTRODUCTION

It has been known for some time that periodically distorted nematic director structures may occur above the magnetic field driven Fréedericksz transition in a uniform nematic slab [1–3]. In the bend geometry the so called stripe phase was analyzed by several authors [1,4,5] who proposed different mechanisms for its appearance. Among those Allender *et al.* [5] have put forward a stability analysis study of the director field based on the usual Frank free energy that predicts the stripe phase to appear at a magnetic field that can be only marginally higher than the usual bend Fréedericksz transition field. In the splay geometry Lonberg and Meyer [3] found that a periodic distorted nematic director state could appear at a field smaller than the usual splay Fréedericksz transition field for nematics of sufficiently high elastic anisotropy. A similar situation can in principle also occur in the twist geometry as noticed by Kini [6].

In this study we focus our attention on magnetic field driven Fréedericksz transitions in pretilted nematic slabs with rigid boundary conditions in the intermediate geometries between the pure bend and splay geometries. This subject has been studied by several authors [6–12] but a complete account was not given until now. It was shown by several authors [7–9] that in pretilted nematics when $K_3 \neq K_1$ the usual magnetic field driven Fréedericksz transition from the uniform to the homogeneously distorted state ($\mathcal{H}_d$) is discontinuous. It was also found [6] that for a certain range of the pretilt angle around the pure splay geometry the undistorted state ($\mathcal{U}$) may become unstable against a periodically distorted director state ($\mathcal{P}_d$) in sufficiently anisotropic nematics. The consideration of both findings in a consistent picture has not been obtained yet and is the subject of this work.

II. CALCULATION METHOD

The nematic director field can in principle be obtained from the solution of the appropriate set of Euler-Lagrange equations that follow from the minimization of the usual Frank free energy plus the magnetic contribution [13]. Unless special symmetry considerations can be used to simplify the structure of the director field, the Euler-Lagrange equations are in general not amenable to an analytical solution and numerical methods must be employed. In this work we are going to follow the approach of [14] which consists in parametrizing the two nematic director field defining angles θ and ϕ in terms of their lowest order Fourier components allowing for the existence of $\mathcal{P}_d$ with wave vector in (x,y) plane. The nematic-director–magnetic-field geometry studied is shown in Fig. 1. The director considered is

$$n_x = \cos(\theta+\gamma)\cos(\phi),$$

$$n_y = \cos(\theta+\gamma)\sin(\phi), \tag{1}$$

$$n_z = \sin(\theta+\gamma),$$

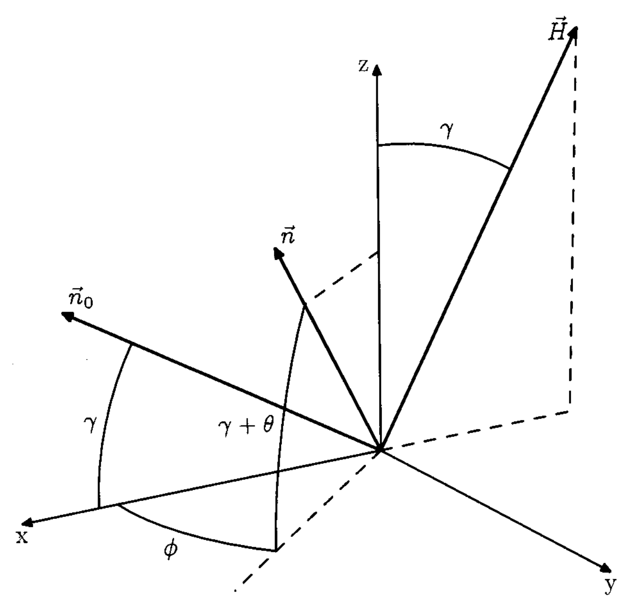

FIG. 1. Nematic-director-magnetic-field Fréedericksz transition geometries analyzed in this study. The plates are at $z = \pm l/2$.

with θ and ϕ given by

$$\theta=[\theta_0+\theta_2\cos(\vec{q}\cdot\vec{\rho}/l)]\cos(\pi z/l) +[\theta_1+\theta_3\cos(\vec{q}\cdot\vec{\rho}/l)]\cos(3\pi z/l) +[\theta_4\sin(2\pi z/l)+\theta_5\sin(4\pi z/l)]\sin(\vec{q}\cdot\vec{\rho}/l), \quad (2)$$

$$\phi=[\phi_0+\phi_2\cos(\vec{q}\cdot\vec{\rho}/l)]\cos(\pi z/l) +[\phi_1+\phi_3\cos(\vec{q}\cdot\vec{\rho}/l)]\cos(3\pi z/l) +[\phi_4\sin(2\pi z/l)+\phi_5\sin(4\pi z/l)]\sin(\vec{q}\cdot\vec{\rho}/l), \quad (3)$$

$$\vec{q}=q_x\hat{e}_x+q_y\hat{e}_y, \quad \vec{\rho}=x\hat{e}_x+y\hat{e}_y$$

where γ is the pretilt angle, l is slab thickness, $\vec{q}$ is the normalized wave vector of the $\mathcal{P}_d$ distortion, and the amplitudes $\theta_0,\ldots,\theta_5$, and $\phi_0,\ldots,\phi_5$ parametrize the director field. The magnetic field is

$$H_x=-H\sin(\gamma),$$

$$H_y=0, \quad (4)$$

$$H_z=H\cos(\gamma).$$

The average free energy per unit volume is given by

$$F=\frac{1}{l\lambda}\int_0^{\lambda}\int_{-l/2}^{l/2} f \ \ dz \ \ ds, \quad (5)$$

where

$$f=\frac{1}{2}\{K_1(\vec{\nabla}\cdot\vec{n})^2+K_2(\vec{n}\cdot\vec{\nabla}\times\vec{n})^2 +K_3(\vec{n}\times\vec{\nabla}\times\vec{n})^2-\chi_a(\vec{n}\cdot\vec{H})^2\},$$

$$\vec{s}=s\frac{\vec{q}}{||\vec{q}||},$$

$$\lambda=\frac{2\pi}{||\vec{q}||}l.$$

Upon substitution of $\vec{n}$ by Eq. (1) and θ and ϕ by Eqs. (2) and (3), F becomes a function of $\theta_0,\ldots,\theta_5$, $\phi_0,\ldots,\phi_5$, q_x, and q_y that parametrize the director field and the control parameters H, K_1, K_2, K_3, χ_a, and γ. For the calculations we used an adimensional form of F, given by $F_a=Fl^2/K_3$ and worked with the reduced magnetic field

$$h\equiv H\frac{l}{\pi}\frac{\sqrt{\chi_a/K_3}}{\sqrt{1-\cos^2(\gamma)(1-K_1/K_3)}}, \quad (6)$$

which corresponds for $h=1$ to the stability limit of $\mathcal{U}$ against the onset of $\mathcal{H}_d$ as is shown in [15]. In view of the results quoted earlier for the onset of $\mathcal{P}_d$, in the limiting geometries, respectively, pure splay and pure bend [3,5], our analysis of the intermediate geometry begins with the calculation of the relation between h, K_3/K_1, K_2/K_1, and γ at the stability limit of $\mathcal{U}$ against the onset of $\mathcal{P}_d$.

In order to obtain the Hessian or stability matrix of F_a with respect to the amplitudes connected with the existence of a $\mathcal{P}_d$, we need not consider the full form of F_a but it is enough to have its expansion about the desired point up to second order in those amplitudes which are θ_2, θ_3, θ_4, θ_5, ϕ_2, ϕ_3, ϕ_4, and ϕ_5. This is advantageous for the implementation of the integrations that appear in F_a. The stability matrix in $\mathcal{U}$ is

$$S_{ij}\equiv\left.\frac{\partial^2 F_a}{\partial x_i\partial x_j}\right|_{x_k=0}, \quad x_i=\theta_i, \quad \phi_i \quad (i=2,\ldots,5). \quad (7)$$

At the stability limit of $\mathcal{U}$ the determinant of S_{ij} is zero and this yields an implicit equation that relates the reduced critical magnetic field h with K_3/K_1, K_2/K_1, γ, and the wave vector of the distortion $\vec{q}$. The selected wave vector $\vec{q}$ minimizes $|S_{ij}|$ and from

$$|S_{ij}|_{\min}(h_{\mathrm{I}},K_3/K_1,K_2/K_1,\gamma)=0 \quad (8)$$

we obtain the desired relation between h_{I}, K_3/K_1, K_2/K_1, and γ, valid at the stability limit of $\mathcal{U}$ for the onset of a $\mathcal{P}_d$. h_{I} is hereafter defined as the value of the reduced magnetic field above which $\mathcal{U}$ loses stability to $\mathcal{P}_d$.

As was seen in the pure bend geometry [5] $\mathcal{H}_d$ may become unstable against the onset of $\mathcal{P}_d$ and this constitutes another path for the appearance of a $\mathcal{P}_d$. At the stability limit of $\mathcal{H}_d$ against the onset of a $\mathcal{P}_d$, the determinant of the stability matrix (7), evaluated in the $\mathcal{H}_d$, goes to zero. The selected wave vector $\vec{q}$ of $\mathcal{P}_d$ minimizes $|S_{ij}|$ and as before from

$$|S_{ij}|_{\min}(h_{\mathrm{II}},K_3/K_1,K_2/K_1,\gamma)=0 \quad (9)$$

we obtain the relation between h_{II}, K_3/K_1, K_2/K_1, and γ valid at the stability limit of $\mathcal{H}_d$ relative to $\mathcal{P}_d$. Equation (9) represents surfaces of change of stability of $\mathcal{H}_d$ relative to $\mathcal{P}_d$ in the space of the control parameters. $h=h_{\mathrm{II}}^-$ and $h=h_{\mathrm{II}}^+$ characterize, respectively, the surfaces of loss and gain of stability of $\mathcal{H}_d$ relative to $\mathcal{P}_d$ on increasing the magnetic field.

The stability limiting surfaces of $\mathcal{P}_d$ in the space of control parameters $h,K_3/K_1,K_2/K_1,\gamma$ were determined from a minimization of F_a in the space of the director field parameters $\{\theta_0,\ldots,\theta_5,\phi_0,\ldots,\phi_5,q_x,q_y\}$ and are characterized by the lowest $(h=h_{\mathrm{III}}^-)$ and highest $(h=h_{\mathrm{III}}^+)$ fields at which a $\mathcal{P}_d$ could be found. h_{IV} gives the lowest field at which $\mathcal{H}_d$ is stable. h_{IV} was determined from the analytical solution of the apropriate Euler-Lagrange equation that exists for the $\mathcal{H}_d$ state.

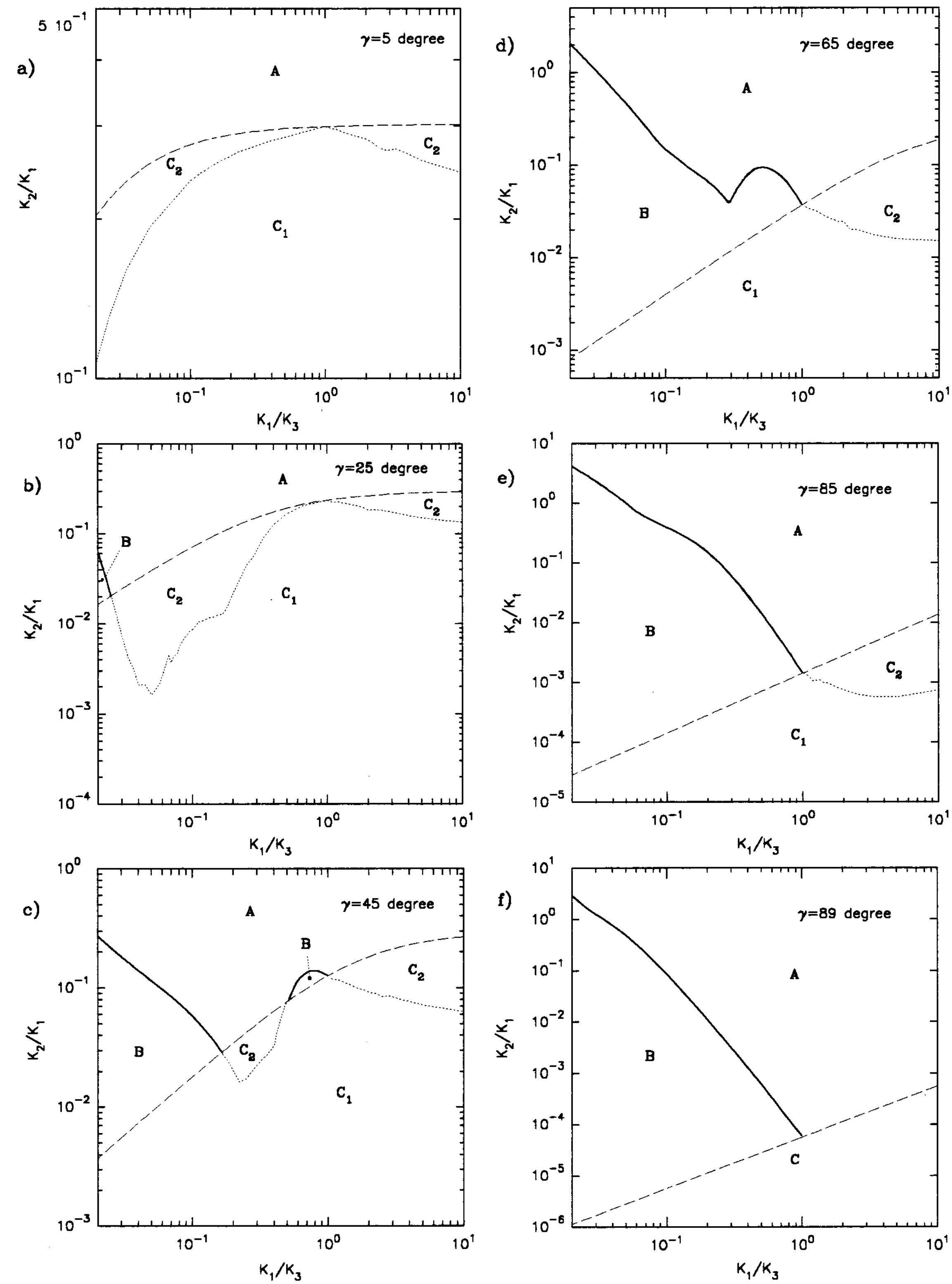

FIG. 2. (a)–(f) Diagrams defining in the K_1/K_3, K_2/K_1 plane the ranges of onset of the different states. In region *A*, $\mathcal{U}$ loses stability to $\mathcal{H}_d$, at $h=1$. In region *B*, $\mathcal{U}$ loses stability to $\mathcal{H}_d$, at $h=1$, which in turn is unstable against the formation of $\mathcal{P}_d$. The small dashed line separates two distinct behaviors in region *C* on increasing the magnetic field and corresponds to $h_{\mathrm{I}}=h_{\mathrm{III}}^{+}$. In subregion C_1, $\mathcal{U}$ loses stability directly to $\mathcal{P}_d$, at $h<1$. In subregion C_2, $\mathcal{U}$ loses stability directly to $\mathcal{P}_d$, which is unstable relative to $\mathcal{H}_d$. In (f) the small dashed line was not determined.

III. RESULTS

Depending on the values of h_{I}, h_{II}^{-}, h_{II}^{+}, and h_{III}^{+}, different behaviors are possible on increasing the magnetic field. When $h_{\mathrm{I}}<1$, $\mathcal{U}$ loses stability to a $\mathcal{P}_d$ at $h=h_{\mathrm{I}}$. When $h_{\mathrm{I}}=1$, $\mathcal{U}$ loses stability to $\mathcal{H}_d$ at $h=1$ (the usual Fréedericksz transition). $\mathcal{H}_d$ loses stability to $\mathcal{P}_d$ at $h=h_{\mathrm{II}}^{-}$.

In Figs. 2(a)–2(f) relations (8) and (9), dashed and full lines, respectively, are graphed as K_2/K_1 versus K_1/K_3 for

TABLE I. Definition of regions of different behavior on increasing magnetic field. Transitions occur at values of the reduced magnetic field indicated above the arrows ($\rightarrow$).

Name	Transitions	Conditions
A_1	$\mathcal{U}\xrightarrow{1}\mathcal{H}_d$	$h_{\rm II}^{+}<1,\ h_{\rm I}=1$
A_2	$\mathcal{U}\xrightarrow{1}\mathcal{H}_d\xrightarrow{h_{\rm II}^{-}}\mathcal{P}_d\xrightarrow{h_{\rm III}^{+}}\mathcal{H}_d$	$h_{\rm I}=1,\ h_{\rm II}^{-}>1$
B	$\mathcal{U}\xrightarrow{1}\mathcal{H}_d\xrightarrow{1}\mathcal{P}_d\xrightarrow{h_{\rm III}^{+}}\mathcal{H}_d$	$h_{\rm II}^{-}<1,\ h_{\rm I}=1,\ h_{\rm II}^{+}>1$
C_1	$\mathcal{U}\xrightarrow{h_{\rm I}}\mathcal{P}_d\xrightarrow{h_{\rm III}^{+}}\mathcal{H}_d$	$h_{\rm I}<1,\ h_{\rm I}<h_{\rm III}^{+}$
C_2	$\mathcal{U}\xrightarrow{h_{\rm I}}\mathcal{P}_d\xrightarrow{h_{\rm I}}\mathcal{H}_d$	$h_{\rm III}^{+}<h_{\rm I}<1$

$h=1$ and different values of the pretilt angle γ. As the plots of relations (8) and (9) were obtained for $h=1$, the lines plotted separate regions of different behavior. $\mathcal{U}$ loses stability to $\mathcal{H}_d$ at $h=1$ in region A. At least two subregions exist in region A, subregions A_1 and A_2. In subregion $A_2(A_1)$ $\mathcal{H}_d$ does (does not) lose stability relative to a $\mathcal{P}_d$ for $h>1$. Subregion A_2 repeats the results of [5]. In region B, $\mathcal{U}$ loses stability to $\mathcal{H}_d$ at $h=1$ that in turn is also unstable relative to $\mathcal{P}_d$. In region C, $\mathcal{U}$ loses stability to $\mathcal{P}_d$ at some value of $h=h_{\rm I}<1$. While in subregion C_1 a $\mathcal{P}_d$ is found when a minimization of F_a is carried out for the set of control parameters $\{K_3/K_1, K_2/K_1, \gamma, h_I\}$, in subregion C_2 when a minimization of F_a is carried out, no $\mathcal{P}_d$ is found for the set of parameters $\{K_3/K_1, K_2/K_1, \gamma, h_{\rm I}\}$ considered and we obtain instead $\mathcal{H}_d$ as the lowest energy stable state. Within subregion C_2, $\mathcal{U}$ loses stability directly to a $\mathcal{P}_d$, at $h=h_{\rm I}<1$, that in turn is unstable relative to $\mathcal{H}_d$. The transition field in region C_2 from $\mathcal{U}$ to $\mathcal{H}_d$ (through $\mathcal{P}_d$) at $h=h_{\rm I}$ is lower than 1 and so lower than the usual Fréedericksz transition field.

In Table I the complete definition of each region is given. The actual transitions between the different states will occur at the stability boundaries when they are continuous while the exact location of the discontinuous transitions is fluctuation dependent. In a mechanical system discontinuous transitions also occur at the stability boundaries. In Ref. [7] it is shown that the magnetic field driven discontinuous transition between the two stable homogeneously distorted nematic structures occurring in a nematic slab takes place at the stability limit of the configuration the system is in or within its experimental error. This result leads us to expect a similar type of behavior for the system studied here.

To characterize the type of transitions between the different director structures encountered, $\mathcal{U}$, $\mathcal{H}_d$, and $\mathcal{P}_d$, we begin by referring the transition from $\mathcal{U}$ to $\mathcal{H}_d$ which was shown to be discontinuous for a pretilted nematic when $K_3\neq K_1$ [7–9]. The transition from $\mathcal{U}$ to $\mathcal{P}_d$ at $h=1$ which is achieved through $\mathcal{H}_d$ is also discontinuous as in the previous case. To investigate the other possible transitions and the type of $\mathcal{P}_d$ structures, we have determined the amplitudes $\theta_0, \ldots, \theta_5$ and $\phi_0, \ldots, \phi_5$ as functions of the reduced magnetic field h for several sets of elastic constants ratios

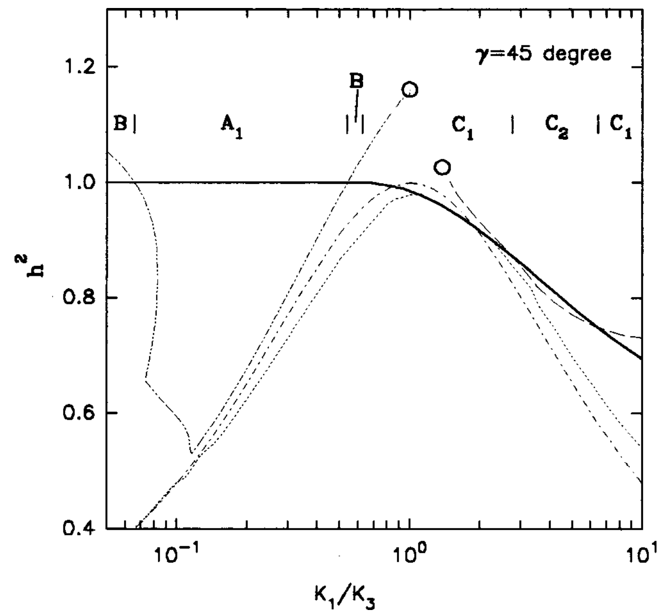

FIG. 3. K_1/K_3 dependence of the stability limit reduced fields squared for the three states involved, respectively, $\mathcal{U}$, $\mathcal{H}_d$, and $\mathcal{P}_d$ for $K_2/K_1=0.09$ and $\gamma=\pi/4$. Full line—$h_{\rm I}^2$; dash-double dotted line—$h_{\rm II}^{+2}$ coinciding with $h_{\rm III}^{+2}$; dash-dotted line—$h_{\rm IV}^2$, coinciding with $h_{\rm II}^{-2}$ for $K_1/K_3\leqslant 1$; small dashed line—$h_{\rm III}^{-2}$; large dash line—$h_{\rm III}^{+2}$. The circles mark the limiting values of K_1/K_3 beyond which the corresponding lines could not be found for fields up to $h^2=1.4$. The K_1/K_3 range of existence of the different regions is also indicated.

K_2/K_1, K_3/K_1, and pretilt angle in all regions, defined in Table I, by a straight minimization of F_a. In $\mathcal{U}$ all the amplitudes are zero while in $\mathcal{H}_d$ the amplitudes linked to $\mathcal{P}_d$, i.e., $\theta_2, \ldots, \theta_5$ and $\phi_2, \ldots, \phi_5$ are null.

Within the sets $\{K_2/K_1, K_3/K_1, \gamma\}$ studied, both continuous and discontinuous transitions from $\mathcal{U}$ directly to the $\mathcal{P}_d$ were encountered in region C_1 as the reduced magnetic field h at which $\mathcal{U}$ becomes unstable for the onset of a $\mathcal{P}_d$ is either equal to or higher than the reduced field at which $\mathcal{P}_d$ becomes stable. In Fig. 3 we present for $K_2/K_1=0.09$ and $\gamma=\pi/4$ the $h_{\rm I}$, $h_{\rm II}^{-}$, $h_{\rm II}^{+}$, $h_{\rm III}^{-}$, $h_{\rm III}^{+}$, and $h_{\rm IV}$ dependence on K_1/K_3.

The accuracy of the approach followed based on the use of an ansatz can be checked in the first part of the work where the stability matrix is calculated. The determination of the stability matrix either in $\mathcal{U}$ or in $\mathcal{H}_d$ requires the knowledge of the amplitudes that characterize that state. In $\mathcal{U}$ those amplitudes are zero but in $\mathcal{H}_d$ they are not and must be found from a minimization process on four parameters (θ_0, θ_1, ϕ_0, and ϕ_1). Fortunately, as mentioned previously, the exact director field of $\mathcal{H}_d$ can be found from the solution of the appropriate Euler-Lagrange equations; this calculation was carried out and both the energy and the maximum value of the distortion were compared with the values obtained from the ansatz solution and they agreed in better than 1% for the majority of the K_3/K_1 range explored. In $\mathcal{P}_d$ the amplitudes must be found from a minimization process on the parameters $\{\theta_0, \ldots, \theta_5, \phi_0, \ldots, \phi_5, q_x, q_y\}$.

IV. CONCLUSION

We found that in pretilted nematics with sufficiently high elastic anisotropy the homogeneously distorted state ($\mathcal{H}_d$) appearing above the magnetic field driven Fréedericksz transition may be replaced by a periodically distorted state ($\mathcal{P}_d$). When $K_3 \neq K_1$ the transitions between the different states are not continuous in general. For a particular range of the elastic constant ratios K_3/K_1, K_2/K_1, and the pretilt angle γ, a periodic state that appears at $h=1$ is not reached directly but through $\mathcal{H}_d$. In particular ranges of the elastic constant ratios K_3/K_1, K_2/K_1, and the pretilt angle γ, a transition field lower than the usual Fréedericksz transition field for the $\mathcal{U}$-$\mathcal{H}_d$ transition was also found, with the transition occurring through $\mathcal{P}_d$.

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