

The Soliton-Stripe Pattern in the Seul-Andelman Membrane ^{*†}

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Abstract

The Seul-Andelman membrane is a system of two coupled fields: The composition ϕ of one of the two (A and B) constitutive molecules, and the height profile h of the flexible membrane. The free energy of the system consists of two parts. The first part is the usual Ginzburg-Landau free energy of ϕ ; the second part is attributed to the bending of the membrane and the coupling of ϕ to h . The coupling term models the tendency that the two molecular constituents display an affinity for regions of the membrane of different local curvature. In a particular parameter range we prove the existence of the soliton-stripe pattern, using the Γ -limit theory in perturbative variational calculus. This pattern, modelled by one-dimensional local minimizers of the free energy of the system, consists of A-rich and B-rich stripes covering the membrane, delineated by sharp domain walls. The optimal spacing between domain walls is determined from the global minimizer of the Γ -limit.

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1 Introduction

We study a membrane problem considered by Seul and Andelman [28]. In a 2-D sheet there are two partially incompatible molecular species, say A and B, which can diffuse laterally. We assume that A and B molecules form an incompressible film that fully covers the sheet. The state of the

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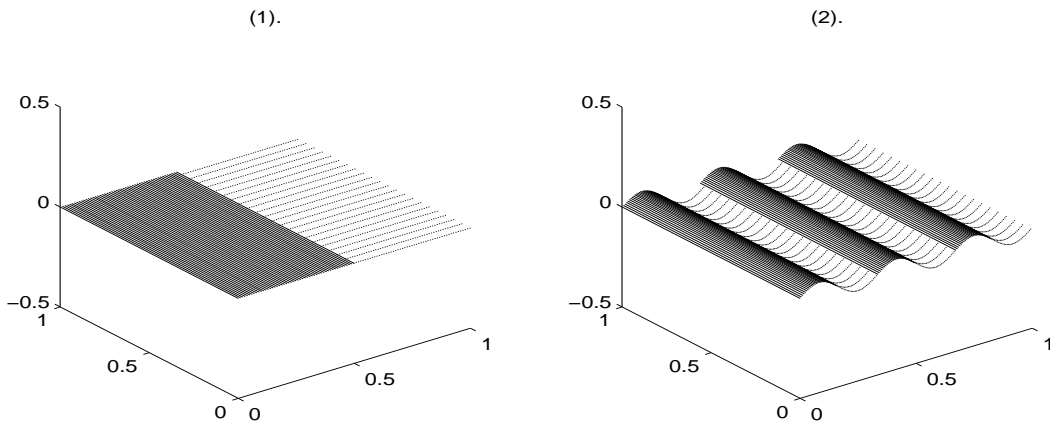


Figure 1: (1). In the absence of bending, the A and B molecules form a large A-rich domain and a large B-rich domain. (2). With (1.2), A and B molecules form a lamellar pattern on the bending membrane.

system is then characterized by selecting the relative composition ϕ to serve as an order parameter: $\phi = 1$ indicates pure A composition, and $\phi = 0$ corresponds to pure B composition. A value of ϕ that is between 0 and 1 represents a mixture of the two types of molecules. The incompatibility of the molecular constituents will favor segregation into large coexisting A-rich and B-rich domains, Figure 1 (1). This situation is modelled by the familiar Ginzburg-Landau free energy

$$\int_{\Omega} (W(\phi(r)) + \frac{b}{2} |\nabla\phi(r)|^2) dr, \quad (1.1)$$

where we may take $W(\phi) = (1/4)((\phi - 1/2)^2 - 1/4)^2$, and $\Omega \subset \mathbf{R}^2$ is the sheet. Because the number of A molecules and the number of the B molecules are conserved quantities, we assume that $\bar{\phi} = m$, where $\bar{\phi} = \frac{1}{|\Omega|} \int_{\Omega} \phi(r) dr$ is the average of ϕ , and $m \in (0, 1)$, the average relative composition of A molecules, is given and fixed.

The situation is substantially altered when we allow for out-of-plane (bending) distortions of the sheet. Specifically we assume that the two molecular constituents display an affinity for regions of different local curvature of the sheet, Figure 1 (2). The molecules separate into A-rich and B-rich micro-domains. The tendency can be modelled by introducing a coupling term between the local composition of ϕ and the curvature of the sheet. Provided that distortions remain small, we may add to (1.1)

$$\int_{\Omega} (\frac{\sigma}{2} |\nabla h(r)|^2 + \frac{\kappa}{2} |\Delta h(r)|^2 + \Lambda\phi(r)\Delta h(r)) dr, \quad (1.2)$$

where h represents the height profile of the sheet relative to a flat reference plane and Ω now becomes the projection of the sheet to the reference plane. σ is its surface tension, and κ is its bending modulus; Λ measures the strength of the coupling of local curvature Δh and local composition ϕ . The free energy is now a functional of both ϕ and h .

The soliton-stripe pattern is a lamellar pattern for ϕ which varies in one direction. It is characterized by sharp domain walls delineating fully segregated A-rich and B-rich regions, Figure 2

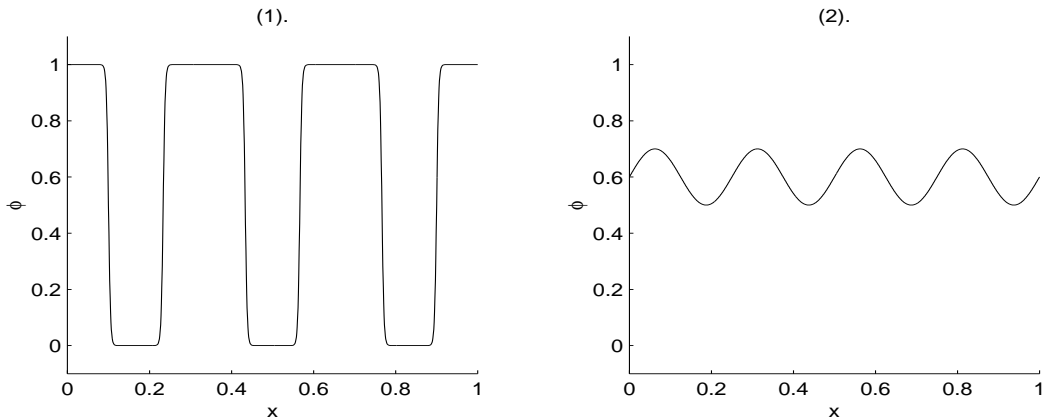


Figure 2: (1). A soliton-stripe pattern for ϕ where sharp domain walls separate A-rich and B-rich regions. (2). A sinusoidal pattern which has no sharp domain walls. A and B molecular constituents are more mixed in (2) than in (1).

(1). The similar phenomenon occurs in many other systems including diblock copolymers (Leibler [11] and Ohta and Kawasaki [15]), Langmuir monolayers of polar molecules (Andelman *et al* [1]), and smectic films (Selinger *et al* [27]). In the diblock copolymer theory this pattern, which occurs in systems with large polymerization indexes at low temperature, is called the strongly segregated lamellar pattern, and in [27] it is called the soliton-stripe pattern. Here we follow the terminology of [27]. We will show the existence of this pattern using the Γ -limit theory of De Giorgi [5], which is a rigorous singular perturbation theory in variational calculus. More specifically we will prove that the free energy of the system in one-dimension has local minimizers that have soliton-stripe shape. This argument was first used by the authors to study strongly segregated lamellar patterns in di- and tri-block copolymers [17, 18, 22]. We will also determine the optimal thickness of an A-rich, or B-rich, region by studying the global minimizer of the free energy functional in one-dimension.

There is another lamellar pattern which has no sharp domain walls. ϕ forms a partially segregated, sine-like function in space, Figure 2 (2). This type is termed the weakly segregated lamellar pattern in the diblock copolymer theory [11], and the sinusoidal pattern in [27]. It may be studied by the standard bifurcation theory. We will give a sketch of this method in Section 6.

Mathematical studies on periodic patterns with sharp domain walls started rather recently. Many works have been done to the block copolymer problem. The literature there includes Nishiura and Ohnishi [13], Ohnishi *et al* [14], Ren and Wei [17, 19, 18, 21, 22, 20, 25], Choksi [2], Fife and Hillhorst [7], Henry [8], and Choksi and Ren [3]. Elsewhere Ren and Wei [23] studies this phenomenon in charged monolayers, and [24] in chiral liquid crystals.

2 Soliton-stripe pattern

To study a lamellar pattern, it is natural to take the sample Ω to be a square. Let $\Omega = (0, L) \times (0, L)$. The size L of the sample will be determined mathematically. The consequence is that L is several

times greater than but still comparable to the thickness of one A-rich, or B-rich, region. Next we scale Ω to $D = (0, 1) \times (0, 1)$ to separate the size effect of the sample from its shape effect. Namely we let $(x, y) = (r_1/L, r_2/L) \in D$ for $r = (r_1, r_2) \in \Omega$. Then the sum of (1.1) and (1.2) divided by L^2 becomes

$$\int_D [W(\phi) + \frac{b}{2L^2} |\nabla \phi|^2 + \frac{\sigma}{2L^2} |\nabla h|^2 + \frac{\kappa}{2L^4} |\Delta h|^2 + \frac{\Lambda}{L^2} \phi \Delta h] dx dy. \quad (2.1)$$

Here we have regarded ϕ and h as functions of the new variables x and y .

Since lamellar patterns vary in one direction we assume that ϕ and h depend on x only. So (2.1) becomes an integral on $(0, 1)$. To eliminate the boundary effect we identify 0 and 1 to turn $(0, 1)$ to \mathbf{R}/\mathbf{Z} , i.e. we assume the periodic boundary condition, throughout this paper. This is the simplest boundary condition here. However we do pay a price of taking care of the translation invariance. On \mathbf{R}/\mathbf{Z} there is the action by the translation group,

$$\phi(\cdot) \rightarrow \phi(\cdot - y), \quad \forall y \in \mathbf{R}/\mathbf{Z},$$

so we will often use phrases like ‘modulo translation’ and ‘up to translation’. We rewrite (2.1) as

$$F_\epsilon(\phi, q) = \int_0^1 [W(\phi) + \frac{\epsilon^2}{2} \phi_x^2 + \frac{\epsilon \omega^2}{2} q^2 + \frac{\epsilon}{2} q_x^2 + \epsilon \gamma \phi q_x] dx \quad (2.2)$$

where

$$\phi, q \in W^{1,2}(\mathbf{R}/\mathbf{Z}), \quad \bar{\phi} - m = \bar{q} = 0. \quad (2.3)$$

We have introduced new positive parameters ϵ , ω , and γ to replace the original physical parameters in (2.1). The new parameters are related to the original parameters through

$$\epsilon = \frac{b^{1/2}}{L}, \quad \omega = \frac{\sigma^{1/2} L}{\kappa^{1/2}}, \quad \gamma = \frac{\Lambda L^{1/2}}{b^{1/4} \kappa^{1/2}}. \quad (2.4)$$

The new function q is proportional to h_x , i.e.

$$q = \frac{\kappa^{1/2}}{b^{1/4} L^{3/2}} h_x. \quad (2.5)$$

Here h_x stands for the derivative of h with respect to x . In (2.2) q is the second variable of the functional. Now $\bar{\phi}$ is the average of ϕ on $(0, 1)$. $\bar{q} = 0$ because of (2.5). The function W may be generalized from the exact formula mentioned after (1.1). We assume that W is smooth, it has a global minimum value 0 achieved at exactly two points: 0 and 1, and it grows to ∞ at least quadratically fast as its argument approaches $\pm\infty$.

We will show mathematically that the soliton-stripe pattern exists if

$$\epsilon \rightarrow 0, \quad \text{and } \omega, \gamma \text{ remain positive and fixed.} \quad (2.6)$$

This condition may be interpreted in terms of the original parameters with the help of (2.4). More specifically (2.6) is equivalent to

$$\frac{b^{1/2} \sigma^{1/2}}{\kappa^{1/2}} \rightarrow 0, \quad \frac{b^{1/2} \sigma^{1/2} \kappa^{1/2}}{\Lambda^2} \sim 1. \quad (2.7)$$

Note that L does not appear in (2.7). This is natural since L , the size of the membrane, is a chosen parameter, while b , σ , κ and Λ are intrinsic physical parameters of the membrane. Once the physical parameters b , σ , κ and Λ are in the right range (2.7), we take

$$L \sim \frac{\kappa^{1/2}}{\sigma^{1/2}}. \quad (2.8)$$

The condition (2.6) is then satisfied.

Our main result is the following theorem regarding the existence of the soliton-stripe pattern as local minimizers of F_ϵ . The proof of the theorem will span Sections 3, 4, and 5.

Theorem 2.1 *Under the condition (2.6) for each positive even integer K the functional F_ϵ has a local minimizer $(\phi_\epsilon, q_\epsilon)$ when ϵ is sufficiently small. It satisfies the Euler-Lagrange equation*

$$-\epsilon^2 \phi_{xx} + W'(\phi) + \epsilon \gamma q_x = \text{Const.} \quad (2.9)$$

$$-q_{xx} + \omega^2 q - \gamma \phi_x = 0 \quad (2.10)$$

and has the properties $\lim_{\epsilon \rightarrow 0} \|\phi_\epsilon - \phi_0\|_2 = 0$ and $\lim_{\epsilon \rightarrow 0} \|q_\epsilon - q_0\|_{2,2} = 0$ modulo translation, and

$$\lim_{\epsilon \rightarrow 0} \epsilon^{-1} F_\epsilon(\phi_\epsilon, q_\epsilon) = \tau K - \frac{\gamma^2 K \sinh \frac{\omega m}{K} \sinh \frac{\omega(1-m)}{K}}{2\omega \sinh \frac{\omega}{K}}. \quad (2.11)$$

The *Const.* in (2.9) is a Lagrange multiplier coming from the constraint $\bar{\phi} = m$. $\|\cdot\|_2$ denotes the L^2 -norm and $\|\cdot\|_{2,2}$ the $W^{2,2}$ -norm. τ in (2.11) is a positive constant defined by

$$\tau = \int_0^1 \sqrt{2W(u)} du. \quad (2.12)$$

It is called the interfacial tension, not to be confused with the surface tension σ in (1.2). That ϕ_ϵ develops a Soliton-Stripe pattern as $\epsilon \rightarrow 0$ lies in the fact that the limiting profile ϕ_0 of ϕ_ϵ is a step function with K regularly distributed jump points:

$$\phi_0(x) = \begin{cases} 0 & \text{on } (0, (1-m)/K), \\ 1 & \text{on } ((1-m)/K, (1+m)/K), \\ 0 & \text{on } ((1+m)/K, (3-m)/K), \\ 1 & \text{on } ((3-m)/K, (3+m)/K), \\ \dots & \\ 1 & \text{on } ((K-1-m)/K, (K-1+m)/K), \\ 0 & \text{on } ((K-1+m)/K, 1). \end{cases} \quad (2.13)$$

The limiting profile of q_ϵ is q_0 which is the solution of (2.10) with $\phi = \phi_0$. While ϕ_0 is discontinuous, q_0 is of class $W^{2,2}$.

One of the local minimizers of F_ϵ in Theorem 2.1 is a global minimizer. Our second result describes this global minimizer and gives the number of its domain walls. The existence of a global minimizer follows from the standard argument. Let $[c]$ denote the greatest integer less than or equal to c .

Theorem 2.2 *Let $(\phi_\epsilon, q_\epsilon)$ be a global minimizer of F_ϵ . Then under the condition (2.6) $\lim_{\epsilon \rightarrow 0} \|\phi_\epsilon - \phi_{opt}\|_2 = 0$ up to translation. ϕ_{opt} is (2.13) whose number of jumps K_{opt} is either $[t_*]$ or $[t_*] + 1$, where t_* is the minimum of the function*

$$h(t) := \tau t - \frac{\gamma^2 t \sinh \frac{\omega m}{t} \sinh \frac{\omega(1-m)}{t}}{2\omega \sinh \frac{\omega}{t}}$$

defined on $[1, \infty)$.

Straight calculations show that $h(t)$ is convex in t . Hence there is a unique t_* . For large t we can expand $h(t)$ and obtain, up to an additive constant, that

$$h(t) \approx \tau t + \frac{\gamma^2 \omega^2 m^2 (1-m)^2}{6t^2}. \quad (2.14)$$

We then find

$$t_* \approx \left(\frac{\gamma^2 \omega^2 m^2 (1-m)^2}{3\tau} \right)^{1/3}. \quad (2.15)$$

From (2.15) the optimal spacing may now be determined in terms of the original parameters

$$\frac{2L}{K_{opt}} \approx \frac{2L}{t_*} \approx \frac{2(3\tau)^{1/3} b^{1/6} \kappa^{2/3}}{\Lambda^{2/3} \sigma^{1/3} m^{2/3} (1-m)^{2/3}}, \quad (2.16)$$

which is the optimal thickness of a cycle of an A-rich layer plus a B-rich layer. Note, as it should be, the last quantity in (2.16) is independent of L .

Even though the last quantity in (2.16) is an approximate formula in this context, it is indeed a physically accurate description of optimal spacing. As L expands in the range (2.8), both γ and ω increase. The approximation (2.14) becomes more accurate near t_* . Then (2.15) is more effective. The right side of formula (2.16) is actually the optimal spacing in the thermodynamic limit ($L \rightarrow \infty$).

Now we begin to prove the two theorems. We hold ϕ and minimize F_ϵ with respect to q . The unique minimizer q satisfies (2.10). Substituting this q into (2.2) and using (2.10), we turn the local variational problem (2.2) of two variables ϕ and q to a nonlocal variational problem I_ϵ of one variable ϕ :

$$I_\epsilon(\phi) := \min_q F_\epsilon(\phi, q) = \int_0^1 (W(\phi) + \frac{\epsilon^2}{2} \phi_x^2 - \frac{\epsilon \gamma^2}{2} \phi_x G[\phi_x]) dx \quad (2.17)$$

where

$$\phi \in W^{1,2}(\mathbf{R}/\mathbf{Z}), \quad \bar{\phi} = m. \quad (2.18)$$

Here $G = G(x, y)$ is the Green function of

$$-q_{xx} + \omega^2 q = \delta(\cdot - y), \quad (2.19)$$

which is also viewed as a nonlocal, solution operator, i.e.

$$G[\phi_x](x) = \int_0^1 G(x, y) \phi'(y) dy.$$

For technical reasons I_ϵ is trivially extended to X_m :

$$X_m = \{\phi \in L^2(\mathbf{R}/\mathbf{Z}) : \bar{\phi} = m\} \quad (2.20)$$

by taking $I_\epsilon(\phi) = \infty$, for $\phi \in X_m \setminus W^{1,2}(\mathbf{R}/\mathbf{Z})$.

3 Γ -limit

The Γ -limit theory is a singular perturbation theory in the calculus of variations. An introduction to the theory may be found in Dal Maso [4]. In this theory there is a perturbed variational problem, which is often a standard one with a small parameter, say ϵ . The Euler-Lagrange equation of this problem is often a differential equation, although in our case the Euler-Lagrange equation is an integro-differential equation (6.2). The limiting problem, as $\epsilon \rightarrow 0$, is usually a geometric problem, whose Euler-Lagrange equation is a free boundary problem. Certain properties of the limiting problem are carried over to the perturbed problem. In this sense the perturbed problem is reduced to the limiting problem.

In this paper we need the property, Corollary 3.2, that near isolated local minimizers of the limiting problem there exist local minimizers of the perturbed problem. Then the construction of local minimizers of I_ϵ becomes the search for local minimizers of the limiting problem.

The singular limit (the Γ -limit) of $\epsilon^{-1}I_\epsilon$, denoted by J in this paper, is a variational problem initially defined in

$$A = \{\phi \in BV(\mathbf{R}/\mathbf{Z}, \{0, 1\}) : \bar{\phi} = m\}. \quad (3.1)$$

Here $BV(\mathbf{R}/\mathbf{Z})$ is the class of periodic functions of bounded variation with values in $\{0, 1\}$. Each function in A has a finite number of jumps between 0 and 1. A more formal description of these functions may be found in Evans and Gariepy [6, chapter 5]. Naturally for each positive, even integer K we set

$$A_K = \{\phi \in A : \phi \text{ has } K \text{ jumps}\}. \quad (3.2)$$

Then we have a decomposition

$$A = \bigcup_{K=2}^{\infty, \text{ even}} A_K. \quad (3.3)$$

For each ϕ in A we define

$$J(\phi) = \tau K - \frac{\gamma^2}{2} \int_0^1 \phi_x G[\phi_x] dx, \text{ if } \phi \in A_K. \quad (3.4)$$

Here the positive constant τ is defined in (2.12). Again we extend J trivially to X_m by taking $J(\phi) = \infty$ if $\phi \in X_m \setminus A$.

Unless otherwise indicated, convergence of functions in X_m means convergence under the L^2 -norm.

Proposition 3.1 *Let X_m be equipped with the L^2 metric.*

1. *As $\epsilon \rightarrow 0$, $\epsilon^{-1}I_\epsilon$ Γ -converges to J in the following sense.*

(a) *For every family $\phi_\epsilon \subset X_m$ with $\lim_{\epsilon \rightarrow 0} \phi_\epsilon = \phi$, $\liminf_{\epsilon \rightarrow 0} \epsilon^{-1}I_\epsilon(\phi_\epsilon) \geq J(\phi)$;*

(b) *For every $\phi \in X_m$, there is $\{\phi_\epsilon\} \subset X_m$ such that $\lim_{\epsilon \rightarrow 0} \phi_\epsilon = \phi$ and $\limsup_{\epsilon \rightarrow 0} \epsilon^{-1}I_\epsilon(\phi_\epsilon) \leq J(\phi)$.*

2. *Let ϵ_j be a sequence of positive numbers converging to 0, and $\{\phi_j\}$ a sequence in X_m . If $\epsilon_j^{-1}I_{\epsilon_j}(\phi_j)$ is bounded above in j , then $\{\phi_j\}$ is relatively compact in X_m and its cluster points belong to A .*

Proof. We view $\epsilon^{-1}I_\epsilon$ as a sum of a local part

$$K_\epsilon(\phi) := \int_0^1 \left[\frac{1}{\epsilon} W(\phi) + \frac{\epsilon}{2} \phi_x^2 \right] dx. \quad (3.5)$$

and an ϵ -independent, perturbative, nonlocal part

$$L(\phi) := -\frac{\gamma^2}{2} \int_0^1 \phi_x G[\phi_x] dx. \quad (3.6)$$

Regarding L , we note that $\phi \rightarrow L(\phi)$ is continuous from $L^2(\mathbf{R}/\mathbf{Z})$ to \mathbf{R} by the elliptic regularity theory.

After making some minor modifications (change L^1 to L^2) in the proof of Propositions 1 and 2 of Modica [12], we find that K_ϵ Γ -converges to K_0 . Here

$$K_0(\phi) := \tau K, \text{ if } \phi \in A_K. \quad (3.7)$$

Since $L : X_m \rightarrow \mathbf{R}$ is a continuous functional, by the definition of Γ -convergence $\epsilon^{-1}I_\epsilon = K_\epsilon + L$ Γ -converges to $J = K_0 + L$.

Part 2 of the proposition is type of uniform coercivity property. If we rewrite

$$-\frac{\gamma^2}{2} \int_0^1 \phi_x G[\phi_x] dx = \frac{\gamma^2}{2} \int_0^1 (-\phi^2 + \omega^2 \phi G[\phi]) dx,$$

then the property follows from Ren and Truskinovsky [16, Lemma A.3]. \square

The next result proved by Kohn and Sternberg [9] asserts that as a corollary of Proposition 3.1 near every isolated local minimizer of J there exists a local minimizer of I_ϵ . The original result in [9] deals with a domain with a boundary. Here on \mathbf{R}/\mathbf{Z} we must take care of the translation invariance of I_ϵ and state the result a little differently. Define a manifold of translates of ϕ_0

$$M(\phi_0) := \{ \phi \in X_m : \phi(\cdot) = \phi_0(\cdot - y), y \in \mathbf{R}/\mathbf{Z} \}$$

and a tube like neighborhood of $M(\phi_0)$

$$N_\delta(\phi_0) := \{ \phi \in X_m : \|\phi(\cdot) - \phi_0(\cdot - y)\| < \delta, \text{ for some } y \text{ in } \mathbf{R}/\mathbf{Z} \}.$$

Corollary 3.2 *Let $\delta > 0$ and $\phi_0 \in X_m$ be such that $J(\phi_0) < J(\phi)$ for all $\phi \in N_\delta(\phi_0) \setminus M(\phi_0)$. Then there exist $\epsilon_0 > 0$ and $\phi_\epsilon \in N_{\delta/2}(\phi_0)$ for all $\epsilon < \epsilon_0$ such that $I_\epsilon(\phi_\epsilon) \leq I_\epsilon(\phi)$ for all $\phi \in N_{\delta/2}(\phi_0)$. In addition $\phi_\epsilon \rightarrow \phi_0$ up to translation.*

Proposition 3.3 *If (x_1, x_2, \dots, x_K) strictly minimizes J in A_K locally, up to translation, then the corresponding ϕ is a strict local minimizer of J in X_m , modulo translation.*

Proof. Suppose that the conclusion is false. There would be a sequence of ϕ_j such that $\phi_j \neq \phi \text{ mod } \mathbf{R}/\mathbf{Z}$, $\phi_j \rightarrow \phi$ and $J(\phi_j) \leq J(\phi)$. The L^2 -continuity of L implies $\lim_{j \rightarrow \infty} L(\phi_j) = L(\phi)$. Therefore

$$\limsup_{j \rightarrow \infty} K_0(\phi_j) \leq K_0(\phi).$$

On the other hand the lower semicontinuity theorem of BV functions ([6], Theorem 1, p. 172) states

$$\liminf_{j \rightarrow \infty} K_0(\phi_j) \geq K_0(\phi).$$

We deduce that

$$\lim_{j \rightarrow \infty} K_0(\phi_j) = K_0(\phi). \quad (3.8)$$

Hence for large j , ϕ_j has exactly K jumps and is in A_K . But this is inconsistent with $\phi_j \rightarrow \phi$, $J(\phi_j) \leq J(\phi)$, and the assumption of the proposition. \square

Now the study of J in X_m is reduced to the study in A_K . View the jumps of ϕ : x_1, x_2, \dots, x_K as K points on $(0, 1)$, with $0 < x_1 < x_2 < \dots < x_K \leq 1$, so that

$$\phi(x) = \begin{cases} 0 & \text{on } (0, x_1), \\ 1 & \text{on } (x_1, x_2), \\ 0 & \text{on } (x_2, x_3), \\ \dots & \\ 1 & \text{on } (x_{K-1}, x_K), \\ 0 & \text{on } (x_K, 1). \end{cases} \quad (3.9)$$

Then

$$\phi_x = \delta_{x_1} - \delta_{x_2} + \delta_{x_3} - \dots - \delta_{x_K}. \quad (3.10)$$

The constraint $\bar{\phi} = m$ becomes

$$x_2 - x_1 + x_4 - x_3 + \dots + x_K - x_{K-1} = m. \quad (3.11)$$

L is now viewed as a function of x_j , and

$$L(x_1, \dots, x_K) = -\frac{\gamma^2}{2} \sum_{j=1}^K \sum_{k=1}^K (-1)^{j+k} G(x_j, x_k). \quad (3.12)$$

Proposition 3.4 *Any critical point (x_1, \dots, x_K) of L (3.12) in A_K is $x_1 = \frac{1-m}{K}$, $x_2 = \frac{1+m}{K}$, $x_3 = \frac{3-m}{K}$, $x_4 = \frac{3+m}{K}$, $x_5 = \frac{5-m}{K}$, \dots , $x_{K-1} = \frac{K-1-m}{K}$, $x_K = \frac{K-1+m}{K}$, modulo translation.*

We postpone the proof of this proposition to Section 4.

Proposition 3.5 *At (2.13) or any of its translates, we have $z^T L''(x_1, \dots, x_K) z \geq 0$ for all vectors $z = (z_1, z_2, \dots, z_K)$ satisfying $z_2 - z_1 + z_4 - z_3 + \dots + z_K - z_{K-1} = 0$, and the equality holds if and only if $z \propto (1, 1, \dots, 1)^T$. So (2.13) is a strict local minimum of L in A_K , modulo translation.*

The constraint on z_j is a consequence of the constraint (3.11). We postpone the proof of this proposition to Section 5.

Proof of Theorem 2.1. The existence of a local minimizer ϕ_ϵ of K jumps follows from Corollary 3.2, Propositions 3.3 and 3.5. ϕ_ϵ satisfies that $\phi_\epsilon \rightarrow \phi_0$ and $\epsilon^{-1} I_\epsilon(\phi_\epsilon) \rightarrow J(\phi_0)$ as $\epsilon \rightarrow 0$. $J(\phi_0)$ is calculated in (5.19):

$$J(\phi_0) = \tau K - \frac{\gamma^2 K \sinh \frac{\omega m}{K} \sinh \frac{\omega(1-m)}{K}}{2\omega \sinh \frac{\omega}{K}}. \quad (3.13)$$

The convergence of q_ϵ to q_0 under the $W^{2,2}$ -norm follows from the elliptic regularity theory for (2.10). \square

Proof of Theorem 2.2. Let ϕ_ϵ be a global minimizer of I_ϵ . Then Part 2 of Proposition 3.1 implies that $\phi_\epsilon \rightarrow \phi_{opt} \in A$ in L^2 . From part 1 of the same proposition we conclude that ϕ_{opt} is a global minimizer of J . By Proposition 3.4, ϕ_{opt} must be a critical point of J , i.e. one of the ϕ_0 's. K_{opt} must minimize the right side of (3.13) among all positive integers K . Hence $K_{opt} = [t_*]$ or $[t_*] + 1$. \square

4 Proof of Proposition 3.4

The Green function of (2.10) is

$$G(x, z) = \frac{\cosh(\omega(1/2 - |x - z|))}{2\omega \sinh(\omega/2)}, \quad x, z \in [0, 1]. \quad (4.1)$$

At a critical point of L , because of the constraint (3.11), we have

$$2 \sum_{k=1, \neq j}^K G_{x_j}(x_j, x_k)(-1)^k = \lambda \quad (4.2)$$

where λ is the Lagrange multiplier. Let

$$P(x) = \sum_{k=1}^K G(x, x_k)(-1)^k. \quad (4.3)$$

Then P satisfies

$$-P'' + \omega^2 P = \sum_{k=1}^K (-1)^k \delta_{x_k} \quad (4.4)$$

At each x_k ,

$$P'(x_{k-}) - P'(x_{k+}) = (-1)^k. \quad (4.5)$$

From (4.3) we also have

$$P'(x_{k-}) + P'(x_{k+}) = 2 \sum_{j=1, \neq k}^K G_{x_k}(x_k, x_j)(-1)^j. \quad (4.6)$$

By (4.2) we deduce

$$P'(x_{k-}) + P'(x_{k+}) = \lambda. \quad (4.7)$$

Solving (4.5) and (4.7) we obtain

$$P'(x_{k-}) = \frac{\lambda + (-1)^k}{2}, \quad P'(x_{k+}) = \frac{\lambda - (-1)^k}{2}. \quad (4.8)$$

We solve (4.4) on (x_{k-1}, x_k) to find

$$P(x) = P'(x_{k-1+}) \frac{\cosh \omega(x - x_k)}{\omega \sinh \omega(x_{k-1} - x_k)} + P'(x_{k-}) \frac{\cosh \omega(x - x_{k-1})}{\omega \sinh \omega(x_k - x_{k-1})}, \quad (4.9)$$

which, together with (4.8), yields

$$\begin{aligned}
P(x_k) &= -P'(x_{k-1+})\frac{1}{\omega \sinh \omega l_k} + P'(x_k-)\frac{\cosh \omega l_k}{\omega \sinh \omega l_k} \\
&= -\frac{\lambda - (-1)^{k-1}}{2}\frac{1}{\omega \sinh \omega l_k} + \frac{\lambda + (-1)^k}{2}\frac{\cosh \omega l_k}{\omega \sinh \omega l_k} \\
&= \frac{\lambda + (-1)^k}{2\omega} \coth \frac{\omega l_k}{2}.
\end{aligned} \tag{4.10}$$

We have set $l_1 = x_1$, $l_2 = x_2 - x_1$, $l_3 = x_3 - x_2$, ..., $l_K = x_K - x_{K-1}$, $l_{K+1} = 1 - x_K$. Similarly if we consider P on (x_k, x_{k+1}) ,

$$P(x_k) = \frac{\lambda + (-1)^{k+1}}{2\omega} \coth \frac{\omega l_{k+1}}{2}. \tag{4.11}$$

From (4.10) and (4.11) we conclude that $\frac{\lambda + (-1)^k}{2\omega} \coth \frac{\omega l_k}{2}$, $k = 2, 3, \dots, K$, is independent of k . Therefore

$$l_2 = l_4 = \dots l_{K-2} = l_K, \quad l_3 = l_5 = \dots = l_{K-1}. \tag{4.12}$$

l_1 and l_{K+1} are handled differently. Translating x_1, \dots, x_K if necessary, we may assume $P'(0) = 0$. Then

$$P(x_1) = P'(x_1-)\frac{\cosh \omega l_1}{\omega \sinh \omega l_1} = \frac{\lambda - 1}{2\omega} \coth \omega l_1. \tag{4.13}$$

On the other hand (4.11) implies

$$P(x_1) = \frac{\lambda + 1}{2\omega} \coth \frac{\omega l_2}{2} = \frac{\lambda - 1}{2\omega} \coth \frac{\omega l_3}{2}. \tag{4.14}$$

Combining (4.13) and (4.14) we find $l_1 = l_3/2$. Similarly we have $l_{K+1} = l_{K-1}/2 = l_3/2$.

5 Proof of Proposition 3.5

In this section we translate (2.13) to

$$y_0 = 0, \quad y_1 = \frac{1-m}{\nu}, \quad y_2 = \frac{1}{\nu}, \quad y_3 = \frac{2-m}{\nu}, \quad y_4 = \frac{2}{\nu}, \quad \dots, \quad y_{2\nu-1} = \frac{\nu-m}{\nu}, \tag{5.1}$$

where $\nu = K/2$. For (5.1)

$$\phi_0(y) = \begin{cases} 0 & \text{if } y \in (y_0, y_1) \\ 1 & \text{if } y \in (y_1, y_2) \\ 0 & \text{if } y \in (y_2, y_3) \\ \dots & \\ 1 & \text{if } y \in (y_{2\nu-1}, 1) \end{cases}. \tag{5.2}$$

The second derivatives of L of (3.12) with respect to x_j are

$$\frac{\partial L}{\partial x_j \partial x_k} = \begin{cases} \gamma^2 \omega^2 (-1)^{j+k} G(x_j, x_k) & \text{if } j \neq k \\ -\gamma^2 \omega^2 \sum_{l \neq j} (-1)^{j+l} G(x_j, x_l) & \text{if } j = k \end{cases}. \tag{5.3}$$

It is more convenient to study the spectrum of L'' in the complex space \mathbf{C}^K . In this context i is the imaginary unit. We decompose

$$\frac{1}{\gamma^2 \omega^2} L'' = \mathbf{E} + \mathbf{F} \quad (5.4)$$

at (5.1). The (j, k) entry of \mathbf{E} is $(-1)^{j+k} G(y_j, y_k)$. The matrix \mathbf{F} is a scalar multiple of the identity matrix, i.e.

$$\mathbf{F} = \left(- \sum_{l=0}^{K-1} (-1)^{j+l} G(y_j, y_l) \right) \mathbf{I}_K. \quad (5.5)$$

Note that the sum in (5.5) is independent of j . Let us divide \mathbf{E} into 2 by 2 blocks:

$$\mathbf{E} = \begin{bmatrix} \mathbf{e}_{00} & \mathbf{e}_{01} & \dots & \mathbf{e}_{0(\nu-1)} \\ \mathbf{e}_{10} & \mathbf{e}_{11} & \dots & \mathbf{e}_{1(\nu-1)} \\ \dots & \dots & \dots & \dots \\ \mathbf{e}_{(\nu-1)0} & \mathbf{e}_{(\nu-1)1} & \dots & \mathbf{e}_{(\nu-1)(\nu-1)} \end{bmatrix}. \quad (5.6)$$

These blocks are labelled by indices $\beta, \xi \in \{0, 1, \dots, \nu - 1\}$. A typical $\mathbf{e}_{\beta\xi}$ is

$$\mathbf{e}_{\beta\xi} := \begin{bmatrix} G(y_{2\beta}, y_{2\xi}) & -G(y_{2\beta}, y_{1+2\xi}) \\ -G(y_{1+2\beta}, y_{2\xi}) & G(y_{1+2\beta}, y_{1+2\xi}) \end{bmatrix}. \quad (5.7)$$

The spectral analysis is done in two steps. First we perform a ‘‘coarse’’ discrete Fourier transform to convert L'' to a matrix with vanishing off-diagonal 2 by 2 blocks. In the second step we study the spectra of the diagonal blocks.

The coarse discrete Fourier transform, used in [22] for triblock copolymers, treats a cycle of two interfaces as a single unit. It is given by the matrix \mathbf{P} whose (α, β) block is

$$\frac{1}{\sqrt{\nu}} \exp(-2\pi i \frac{\alpha\beta}{\nu}) \mathbf{I}_2, \quad \alpha, \beta \in \{0, 1, \dots, \nu - 1\}, \quad (5.8)$$

where \mathbf{I}_2 is the 2 by 2 identity matrix. \mathbf{P} is unitary so its inverse \mathbf{P}^{-1} is its adjoint, i.e. (5.8) with the $-2\pi i$'s replaced by $2\pi i$'s in the exponents.

Clearly $\mathbf{P}\mathbf{F}\mathbf{P}^{-1} = \mathbf{F}$. The calculation of $\mathbf{P}\mathbf{E}\mathbf{P}^{-1}$ is more involved. The (α, η) block of this product is

$$\sum_{\beta, \xi} \frac{1}{\nu} \exp(-2\pi i \frac{\alpha\beta}{\nu} + 2\pi i \frac{\xi\eta}{\nu}) \mathbf{e}_{\beta\xi}. \quad (5.9)$$

The computation of (5.9) is done on the entries of $\mathbf{e}_{\beta\xi}$ individually, so for any $s, t \in \{0, 1\}$ the (s, t) entry of (5.9) is

$$\frac{(-1)^{s+t}}{\nu} \sum_{\beta, \xi} \exp(-2\pi i \frac{\alpha\beta}{\nu} + 2\pi i \frac{\xi\eta}{\nu}) G(y_{s+2\beta}, y_{t+2\xi}). \quad (5.10)$$

Let us first set

$$g(z) = \frac{\cosh(\omega(1/2 - z))}{2\omega \sinh(\omega/2)} \quad (5.11)$$

on $[0, 1]$ and periodically extended to \mathbf{R} , and define

$$Q(\alpha, s, t) = \begin{cases} \sum_{\sigma} \exp(-2\pi i \frac{\alpha\sigma}{\nu}) g(\frac{\sigma}{\nu}) & \text{if } s = t \\ \sum_{\sigma} \exp(-2\pi i \frac{\alpha\sigma}{\nu}) g(\frac{\sigma}{\nu} - \frac{1-m}{\nu}) & \text{if } s = 0, t = 1 \\ \sum_{\sigma} \exp(-2\pi i \frac{\alpha\sigma}{\nu}) g(\frac{\sigma}{\nu} + \frac{1-m}{\nu}) & \text{if } s = 1, t = 0 \end{cases}. \quad (5.12)$$

Straight calculations show that

$$\begin{aligned} Q(\alpha, 0, 0) &= Q(\alpha, 1, 1) = \frac{1}{2\omega} \left(\frac{e^{\frac{\omega}{\nu}}}{e^{\frac{\omega}{\nu}} - e^{-2\pi i \frac{\alpha}{\nu}}} - \frac{e^{-\frac{\omega}{\nu}}}{e^{-\frac{\omega}{\nu}} - e^{-2\pi i \frac{\alpha}{\nu}}} \right) \\ Q(\alpha, 0, 1) &= \frac{1}{2\omega} \left(\frac{e^{-\frac{\omega m}{\nu}}}{e^{2\pi i \frac{\alpha}{\nu}} - e^{-\frac{\omega}{\nu}}} - \frac{e^{\frac{\omega m}{\nu}}}{e^{2\pi i \frac{\alpha}{\nu}} - e^{\frac{\omega}{\nu}}} \right) \\ Q(\alpha, 1, 0) &= \frac{1}{2\omega} \left(\frac{e^{\frac{\omega m}{\nu}}}{e^{\frac{\omega}{\nu}} - e^{-2\pi i \frac{\alpha}{\nu}}} - \frac{e^{-\frac{\omega m}{\nu}}}{e^{-\frac{\omega}{\nu}} - e^{-2\pi i \frac{\alpha}{\nu}}} \right). \end{aligned} \quad (5.13)$$

Note that $Q(0, 0, 1) = Q(0, 1, 0) = g(y_1) + g(y_3) + \dots + g(y_{K-1}) > 0$ and $Q(\alpha, 0, 1)$ is conjugate to $Q(\alpha, 1, 0)$. Then

$$\frac{(-1)^{s+t}}{\sqrt{\nu}} \sum_{\beta} \exp(-2\pi i \frac{\alpha\beta}{\nu}) G(y_{s+2\beta}, y_{t+2\xi}) = \frac{(-1)^{s+t}}{\sqrt{\nu}} \exp(-2\pi i \frac{\alpha\xi}{\nu}) Q(\alpha, s, t) \quad (5.14)$$

is the (s, t) entry of the (α, ξ) block of \mathbf{PE} . From (5.9) we conclude that the (α, η) block of \mathbf{PEP}^{-1} vanishes if $\alpha \neq \eta$ and the (α, α) block is

$$\begin{bmatrix} Q(\alpha, 0, 0) & -Q(\alpha, 0, 1) \\ -Q(\alpha, 1, 0) & Q(\alpha, 1, 1) \end{bmatrix}.$$

This way $\frac{1}{\gamma^2 \omega^2} L'' = \mathbf{E} + \mathbf{F}$ is diagonalized to 2 by 2 blocks, where the α 'th diagonal one is

$$\mathbf{m}_{\alpha} = \begin{bmatrix} Q(\alpha, 0, 0) & -Q(\alpha, 0, 1) \\ -Q(\alpha, 1, 0) & Q(\alpha, 1, 1) \end{bmatrix} - (Q(0, 0, 0) - Q(0, 0, 1)) \mathbf{I}_2. \quad (5.15)$$

Here we have used the fact that

$$\sum_k (-1)^{j+k} G(y_j, y_k) = Q(0, 0, 0) - Q(0, 0, 1) = \frac{\sinh \frac{\omega m}{K} \sinh \frac{\omega(1-m)}{K}}{\omega \sinh \frac{\omega}{K}} \quad (5.16)$$

where the last quantity follows from (5.13).

In the second step of our spectral analysis we study \mathbf{m}_{α} . Note that

$$\mathbf{m}_0 = \begin{bmatrix} Q(0, 0, 1) & -Q(0, 0, 1) \\ -Q(0, 1, 0) & Q(0, 1, 0) \end{bmatrix}. \quad (5.17)$$

One of the eigenvalues of \mathbf{m}_0 is 0 and the second is $2Q(0, 0, 1)$. Although it is positive, the second eigenvalue is irrelevant. Note that an eigenvector of the eigenvalue 0 is $(1, 1, \dots, 1, 1)$, in the coordinates before the coarse Fourier transform. The invariant subspace corresponding to \mathbf{m}_0 is the linear span of the first two columns of \mathbf{P} in (5.8), i.e.

$$c_1(1, 0, 1, 0, \dots, 1, 0)^T + c_2(0, 1, 0, 1, \dots, 0, 1)^T.$$

In this two-dimensional subspace $(1, -1, 1, -1, \dots, 1, -1)$ is an eigenvector corresponding to the second eigenvalue of \mathbf{m}_0 . However this vector does not satisfy the condition $z_2 - z_1 + z_4 - z_3 + \dots + z_K - z_{K-1} = 0$ in Proposition 3.5. The vector is indeed normal to the condition hyperplane. Other eigenvectors of L'' all satisfy the condition.

When $\alpha > 0$, the two eigenvalues of \mathbf{m}_α are $Q(\alpha, 0, 0) + |Q(\alpha, 0, 1)| - Q(0, 0, 0) + Q(0, 0, 1)$ and $Q(\alpha, 0, 0) - |Q(\alpha, 0, 1)| - Q(0, 0, 0) + Q(0, 0, 1)$. From (5.13) we find them to be

$$\frac{\sinh \frac{\omega}{\nu} \pm \sqrt{\sinh^2 \frac{\omega m}{\nu} + 2 \sinh \frac{\omega m}{\nu} \sinh \frac{\omega(1-m)}{\nu} \cos \frac{2\pi\alpha}{\nu} + \sinh^2 \frac{\omega(1-m)}{\nu}}{2\omega(\cosh \frac{\omega}{\nu} - \cos \frac{2\pi\alpha}{\nu})} - \frac{\sinh \frac{\omega m}{2\nu} \sinh \frac{\omega(1-m)}{2\nu}}{\omega \sinh \frac{\omega}{2\nu}}. \quad (5.18)$$

Both of them are positive. To see this we consider the smaller one in (5.18) which is the one with $-$ in \pm . The quantity is minimized if $\cos \frac{2\pi\alpha}{\nu}$ is 1. When this happens, the entire (5.18) is exactly 0. However here we have $\alpha = 1, 2, \dots, \nu - 1$ and $\cos \frac{2\pi\alpha}{\nu} < 1$. Therefore (5.18) is positive.

One byproduct here is the value of J at (2.13). According to (3.12) and (5.16),

$$\begin{aligned} J(\phi_0) &= \tau K - \frac{\gamma^2}{2} \sum_{j,k=0}^{K-1} (-1)^{j+k} G(y_j, y_k) \\ &= \tau K - \frac{\gamma^2 K}{2} (Q(0, 0, 0) - Q(0, 0, 1)) \\ &= \tau K - \frac{\gamma^2 K \sinh \frac{\omega m}{K} \sinh \frac{\omega(1-m)}{K}}{2\omega \sinh \frac{\omega}{K}}. \end{aligned} \quad (5.19)$$

6 Remarks

Theorem 2.1 shows the existence of infinitely many solutions of (2.9) and (2.10) as local minimizers of the free energy. One of them is a global minimizer which is described in Theorem 2.2. All the local minimizers have the desired soliton-stripe shape, and hence model the soliton-stripe pattern in 1-D.

It is natural, as done by the authors in the diblock copolymer problem [20], to study the 2-D stability of the 1-D solutions viewed in 2-D. In the diblock copolymer problem only the 1-D local minimizers with sufficiently many domain walls are stable in 2-D. The 1-D global minimizer in the diblock copolymer problem is near the borderline between the stable ones and the unstable ones in 2-D. We suspect, based on our experience in [20], that not all the 1-D local minimizers constructed in Theorem 2.1 are stable in 2-D. It is interesting to see whether the 1-D global minimizer in Theorem 2.2 is stable in 2-D. There is also the possibility, as in the diblock copolymer problem (Ren and Wei [25]), that there could be stable lamellar solutions with wriggled domain walls in 2-D.

The approximate dependence of $J(\phi_0)$ on K , according to (2.14), is

$$J(\phi_0) \approx \tau K + \frac{CL^3}{K^2}$$

for some proper positive constant C independent of L , when K is large. This asymptotic formula that leads to the optimal spacing shows up in many other physical systems, including di- and tri-block copolymers [17, 22] and chiral liquid crystals [27, 24]. It is minimized at $K = (\frac{2C}{\tau})^{1/3}L$. Another important formula that leads to optimal spacing is

$$\tau K + \frac{CL^2}{K} \tag{6.1}$$

which is minimized at $K = (\frac{C}{\tau})^{1/2}L$. The difference between the exponents $1/3$ and $1/2$ may be significant. In [23] we showed that (6.1) appears in a charged Langmuir monolayer problem proposed by Andelman *et al* [1]. It is also found in the studies of the domain structures of ferromagnets, Landau, Lifshitz and Pitaevskii [10], and superconductors in the intermediate state, Tinkham [29].

The sinusoidal lamellar pattern, Figure 2 (2), is of very different nature. It bifurcates out of the constant state $(m, 0)$ of F_ϵ . Note that the Euler-Lagrange equation of (2.17) is

$$-\epsilon^2 \phi_{xx} + W'(\phi) - \overline{W'(\phi)} + \epsilon \gamma^2 G[\phi_x]_x = 0. \tag{6.2}$$

The eigenvalue problem of (6.2) at ϕ is

$$-\epsilon^2 \psi_{xx} + W''(\phi)\psi - \overline{W''(\phi)\psi} + \epsilon \gamma^2 G[\psi_x]_x = \lambda \psi. \tag{6.3}$$

Equation (6.2) is satisfied by $\phi = m$. At this solution m , we have, in (6.3),

$$\psi = \cos(2n\pi x), \text{ or } \psi = \sin(2n\pi x), \quad n = 1, 2, 3, \dots \tag{6.4}$$

and the corresponding

$$\lambda = 4\epsilon^2 n^2 \pi^2 + W''(m) - \epsilon \gamma^2 + \frac{\epsilon \gamma^2 \omega^2}{4n^2 \pi^2 + \omega^2}, \quad n = 1, 2, 3, \dots \tag{6.5}$$

In (6.5) λ is convex with respect to n^2 . Depending on the values of ϵ , γ , ω and m the principal eigenvalue (i.e. the smallest λ) may be positive, negative, or zero. This allows one to use the bifurcation theory to find solutions bifurcating out of m . Such solutions differ from m by a function proportional to (6.4), to the first order approximation. We then obtain a sinusoidal lamellar pattern. The stability of such solutions may also be determined.

This construction is rather standard, so we omit the details. The reader may find all the necessary tools in Sattinger [26]. It should be noted that this bifurcation phenomenon appears in a parameter range different from (2.6).

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