Quasicrystals and strong interactions between square modes

H. G. Solari and G. B. Mindlin
Department of Physics, FCEN University of Buenos Aires, Pab I, 1428 Buenos Aires, Argentina
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We analyze the possibility of finding almost hexagonal and quasicrystalline patterns, in finite square containers, as the result of the nonlinear interaction of four-dimensional and eight-dimensional representations of D_4. We report the possibility of sustained oscillations between simple and nonsimple squares as the result of these interactions. [S1063-651X(97)04403-6]

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I. INTRODUCTION

Very often the description of physical problems in two-dimensional pattern forming systems is performed with integro-differential equations which are homogeneous and isotropic and therefore present the full symmetry of the Euclidean plane, $E2$. This symmetry is constrained by the boundary conditions to a subsymmetry of $E2$ (for example, think of convection in square containers, with symmetry $D_4 \subset E2$).

At a first glance we would expect the primary bifurcations to be dominated by the arising of patterns bearing symmetries that are subsymmetries of the complete problem (boundary conditions included). Indeed, for low aspect ratio this is often the case. (Here by aspect ratio we mean the quotient between the characteristic length of the vessel and an intrinsic length of the problem.) However, for large aspect ratio, the pattern emerging presents symmetries that are subsymmetries of $E2$ but not of the complete problem (think, for example, in hexagons in the convection problem).

The standard approach for the case of large aspect ratio is to neglect the restrictions imposed by the boundary conditions and to solve the problem in a support (of the space of solutions) compatible with the experimentally observed symmetries of the solutions [1,2]. This approach cannot explain why the observed patterns are preferred to those compatible with the full symmetry, since the selection of the support directly rules out the latter set of solutions.

The problem becomes even more intriguing when the transition from small to large aspect ratio is considered. What happens in the transition region where, presumably, the selection is not determined solely by the interactions or solely by the boundary conditions?

In the present work we address the problem of pattern formation for intermediate aspect ratio by considering the strong interaction of square modes in a D_4 problem. We have limited our study to the interactions between one mode supported in a four-dimensional symmetric subspace and one mode supported in an eight-dimensional symmetric subspace, leaving aside other possible cases such as interactions between two eight-dimensional subspaces. The emphasis is placed on the transitional solutions which can be present and include (as will be shown) almost hexagonal and quasicrystalline duodecagonal symmetries, as well as (simple and nonsimple) squares, rolls, and modulated rolls (D_2 symmetry). We will also show that dynamic alternation between some of these patterns is possible.

The appearance of hexagonal shapes as the result of mode interactions in square vessels has been observed in experimental studies of the Faraday instability [3]. In [4] the presence of D_{12} quasicrystalline patterns is reported at the transition region between table hexagons and stable squares in a numerical study of the Benard-Marangoni instability. Duodecagonal quasicrystals have also been reported in Faraday experiments [5] in transition regions between rolls and hexagons. However, these experiments should be interpreted in terms of the interaction of modes with substantially different wave numbers and its analysis is beyond the scope of this work. Nevertheless, the analysis performed here can be extended to such situations.

The presentation is organized as follows. In Sec. II we discuss the single modes in a D_4 problem with Newmann and Dirichlet conditions. Section III addresses the possible equivariant normal forms that describe the interaction between these modes and their solutions. Finally, Sec. IV contains our conclusions.

II. THE SQUARE MODES

The general homogeneous problem we are going to tackle is of the following form:

$$\partial \psi / \partial t = Q(\psi;\lambda) + N(\psi). \tag{1}$$

Here $\psi = \psi(x): \mathbb{R}^2 \to \mathbb{R}$ is a real function of physical interest (e.g., a temperature field in a convective problem), Q is the linear term dominant at the onset of the pattern formation, λ is the bifurcation parameter with critical value $\lambda = 0$, and N stands for the nonlinear terms.

The problem (1) is assumed to be $E2$ equivariant if no boundary conditions are taken into account. Hence the linear term reads

$$Q(\psi;\lambda) = \int q(|x-y|;\lambda)\,\psi(y)\,d^2y, \tag{2}$$

or

$$\overline{Q(\psi;\lambda)} = \overline{q(k;\lambda)}\,\overline{\psi(k)} \tag{3}$$

in reciprocal space, where $\overline{\psi}$ stands for the Fourier transform of ψ and k is the conjugate of the variable x.

TABLE I. Normal forms for different mode interactions and boundary conditions. ''even'' means even integer number, ''odd'' means odd integer number.

4D representation	8D representation	Boundary condition	Wave numbers	(example)	Equation
sin	sin×sin	Dirichlet	even,even:even,even	2*(3,3:4,1)	(5)
sin	cos×cos	Dirichlet	even,even:odd,odd	(8,8:11,3)	(5)
cos	sin×cos	Dirichlet	odd,odd:even,odd	(5,5:2,7)	(5)
cos	cos×cos	Newmann	even,even:even,even	2*(3,3:4,1)	(6)
cos	sin×sin	Newmann	even,even:odd,odd	(8,8:11,3)	(6)
sin	cos×sin	Newmann	odd,odd:even,odd	(5,5:2,7)	(7)
cos	sin×sin	Newmann	even,0:odd,odd	(10,0:9,5)	(8)
cos	cos×cos	Newmann	even,0:even,even	(12,0:10,6)	(8)

For a pattern forming system in which a characteristic length exists, the bifurcation takes place when the models within the ring defined by $|k|\approx|k_c|$ lose stability. A further restriction is imposed by the boundary conditions. Let us focus on the case of a square container. The linear problem can be further split into the product of two one-dimensional problems. The solutions with a single growth rate can be written as $\psi=\exp(\mu t)\cos(k_1x+\phi_1)\cos(k_2y+\phi_2)$ (in the case of other containers with D_4 symmetry the bifurcating solutions still have support on a ring of wave vectors but the support is no longer a set of isolated dots. Such a situation does not imply important changes for the coming discussion). Whenever a mode with wave vector $\mathbf{k}=(k_1,k_2)$ loses stability, so do all the modes associated to wave vectors obtained from $\mathbf{k}$ through an application of the symmetry operations. As the eight operations in the square symmetry group are generated by the reflections about the x axis and the reflections about one diagonal of the square, the subspace of simultaneously bifurcating modes is spanned by eight functions in general. However, if the vector $\mathbf{k}$ lies on one of the reflection's axis, the subspace of bifurcating modes is four dimensional.

We will further restrict ourselves to real functions ψ. Hence our bifurcating solutions are of the form

$$\psi(x)=\sum_{i=1}^{x} c_i(t)\sin(\mathbf{k}_i\cdot\mathbf{x}+\phi_i), \tag{4}$$

where $c_i(t)$ are real, time dependent coefficients. For the boundary condition $0=a|\partial\psi(x)/\partial x|_{x=L}-b\psi(L)$ the wave vectors satisfy the equation

$$0=a\ \sin(k_nL+n\pi/2)+bk_n\sin(k_nL+n\pi/2),$$

where L is the side of the box, and the phase reads

$$0=a\ \sin(\phi_n)+bk_n\cos(\phi_n).$$

Notice that the dimensions of the resulting subspaces are two for the representation spanned by eight wave vectors, and either one or two for the one spanned by four wave vectors.

III. INTERACTION BETWEEN SQUARE MODES

In the preceding section we have reviewed the possible bifurcations to patterns associated to single irreducible representations of the underlying $E2$ symmetry group, restricted by the D_4 (square) symmetric boundary conditions.

Now we will discuss the possibility of strong interactions between those modes. The motivation for this study is that as a result of these interactions, it is possible to find solutions which give rise to patterns resembling hexagons or even quasicrystals.

By strong interactions we consider those that involve terms of degree smaller than three in the normal form. The invariance of Eq. (1) under arbitrary translations implies that $|\mathbf{k}_i+\mathbf{k}_j|\sim k_c$. When this condition is met for two sets of modes which bifurcate for similar control parameters ($|k|\sim|k'|$), the angle between the wave vectors is approximately 60°.

In the following subsections we will explicitly write the normal forms for the mode interactions mentioned above.

The boundary conditions and the parity of the active modes determine the action of D_4 and the normal form. While Newmann boundary conditions allow for $(0,m)$ modes [the notation $(n_1,\ n_2)$ refers to the wave vector of the mode], Dirichlet conditions are incompatible with such modes. This situation determines the existence of a four-dimensional phase space in the case of Newmann boundary conditions not present for Dirichlet boundary conditions.

In Table I we present the different possible cases of normal forms corresponding to the different parity of the functions. The three cases resulting are as follows.

Case 1 of Table I (corresponding to Dirichlet even-even, Dirichlet odd-odd, and Dirichlet even-odd) reads

$$\begin{aligned}\dot{A}_1&=\mu_1A_1+A_1(a_1A_1^2+a_2A_2^2\pm B^2),\\ \dot{A}_2&=\mu_1A_2+A_2(a_1A_2^2+a_2A_1^2\pm B^2),\\ \dot{B}&=\mu_2B+B[-B^2+d(A_1^2+A_2^2)].\end{aligned} \tag{5}$$

This case does not differ from the general nonresonant case and will not be further considered.

Case 2 of Table I (corresponding to Newmann even-even and Newmann odd-odd) reads

$$\begin{aligned}\dot{A}_1&=\mu_1A_1+\alpha BA_2+A_1(a_1A_1^2+a_2A_2^2\pm B^2),\\ \dot{A}_2&=\mu_1A_2+\alpha BA_1+A_2(a_1A_2^2+a_2A_1^2\pm B^2),\\ \dot{B}&=\mu_2B+\beta A_1A_2+B[-B^2+d(A_1^2+A_2^2)].\end{aligned} \tag{6}$$

Case 3 (corresponding to Newmann even-odd) reads

$$\dot{A}_1=\mu_1 A_1+\alpha B A_2+A_1(a_1 A_1^2+a_2 A_2^2 \pm B^2),$$

$$\dot{A}_2=\mu_1 A_2+\alpha B A_1+A_2(a_1 A_2^2+a_2 A_1^2 \pm B^2), \tag{7}$$

$$\dot{B}=\mu_2 B-\beta A_1 A_2+B[-B^2+d(A_1^2+A_2^2)].$$

Case 3 differs from case 2 only in the sign of the quadratic terms. Therefore if no further restrictions on α and β are imposed, both of them are equivalent. We have distinguished the two cases having in mind the large aspect ratio limit in which the resonant modes span an, approximate, D_{12} invariant subspace.

The fourth case of Table I corresponds to Newmann boundary conditions with a $(0, n)$ mode,

$$\dot{A}_1=\mu_1 A_1-\alpha A_1 B_2+A_1[(g_1+g_3)A_1^2+(g_2+g_4)A_2^2+g_3(B_1^2+B_2^2)],$$

$$\dot{A}_2=\mu_1 A_2-\alpha A_2 B_1+A_2[(g_1+g_3)A_2^2+(g_2+g_4)A_1^2+g_3(B_1^2+B_2^2)],$$

$$\dot{B}_1=\mu_2 B_1-\beta A_2^2+B_1(g_1 B_1^2+g_4 B_2^2+2g_2 A_1^2+2g_3 A_2^2), \tag{8}$$

$$\dot{B}_2=\mu_2 B_2-\beta A_1^2+B_2(g_1 B_2^2+g_4 B_1^2+2g_2 A_2^2+2g_3 A_1^2).$$

As stated in the Introduction, our main motivation is the possibility of having stationary solutions with almost quasicrystalline (D_{12}) symmetry, therefore we will focus our attention on the bifurcation of steady state solutions in the symmetric invariant planes.

The normal form (6) is further reduced considering the case of near D_{12} symmetry in which the coefficients present the relations (with an adequate choice of scales)

$$a_1=-1, \tag{9}$$

$$a_2=d=\pm 1. \tag{10}$$

Hereafter we will take $d=-1$ in order to guarantee the existence of global attractors.

The highest symmetry in Eq. (8) is achieved with the relation

$$\alpha=\beta, \tag{11}$$

$$g_3=g_2, \tag{12}$$

$$g_1=g_2=-1, \tag{13}$$

which yields an almost quasicrystalline symmetry (where a proper scaling of the time and variables have been chosen).

Equations (7) do not present additional symmetries for particular values of the coefficients.

A. Case 1

We discuss the symmetric solutions of Eq. (6).

There is an invariant, one-dimensional, subspace given by $A_1=A_2=0$ which corresponds to square patterns arising in pitchfork bifurcations from the zero solution at $\nu_2=0$. The solution with positive B loses stability to modulated squares with $A_1=A_2\neq 0$ in a typical inverse pitchfork bifurcation. The locus of the bifurcations is $\alpha\mu_2+\mu_1+\alpha\sqrt{\mu_2}=0$. These modulated squares are unstable and exist for $\mu_2<0$. They are born in saddle-node bifurcations with a second set of modulated squares that are stable. For these solutions, $\beta\sim\pm A_1\sim\pm A_2(\sim\alpha/3)$, and the resulting patterns for small μ_1 and μ_2 values look like (part of) duodecagons. For this reason, we will call them hereafter *quasicrystals*. There is yet another invariant space given by $A_2=B=0$ corresponding to *rectangular tile* patterns born in pitchfork bifurcations.

The full scheme is reproduced for the solution $A_1=A_2=0$ and $B<0$ which loses stability at $\alpha\mu_2+\mu_1-\alpha\sqrt{\mu_2}=0$. Thus at $\mu_1=0=\mu_2$ there are two attractors of the form $A_1=A_2, B\neq 0$ and $A_1=-A_2, B\neq 0$, as well as the zero solution which is critical.

Figure 1 shows a pattern quoted as *quasicrystals* in the previous paragraphs.

B. Case 3

In this case, the most relevant feature is the possibility of a dynamic alternation between different patterns.

It is instructive to study the case in which $\mu_1\approx 0$ and $\mu_2>0$. Within this parameter restriction, the fixed points located at $B=\pm\sqrt{\mu_2}$ are saddles. For $B>0$ ($B<0$), the local unstable manifold is contained in the $A_1=A_2$ ($A_1=-A_2$) plane, while the stable manifold is within the $A_1=-A_2$ ($A_1=A_2$) plane. So far, this scenario is common to cases 3 and 2. In case 3 (2), the line $B=0, A_1=A_2$ is crossed with B decreasing (increasing), and the line $B=0, A_1=-A_2$ with B increasing (decreasing). Therefore heteroclinic connections between the fixed points at $B=\pm\sqrt{\mu_2}$ are possible in the third case (see Fig. 2). Notice that these connections are possible due to the existence of invariant planes induced by the reflection symmetries [6,7]:

$$A_1\to -A_2,\quad A_2\to -A_1,\quad B\to B, \tag{14}$$

$$A_1\to A_2,\quad A_2\to A_1,\quad B\to B, \tag{15}$$

$$A_1\to A_1,\quad A_2\to -A_2,\quad B\to -B. \tag{16}$$

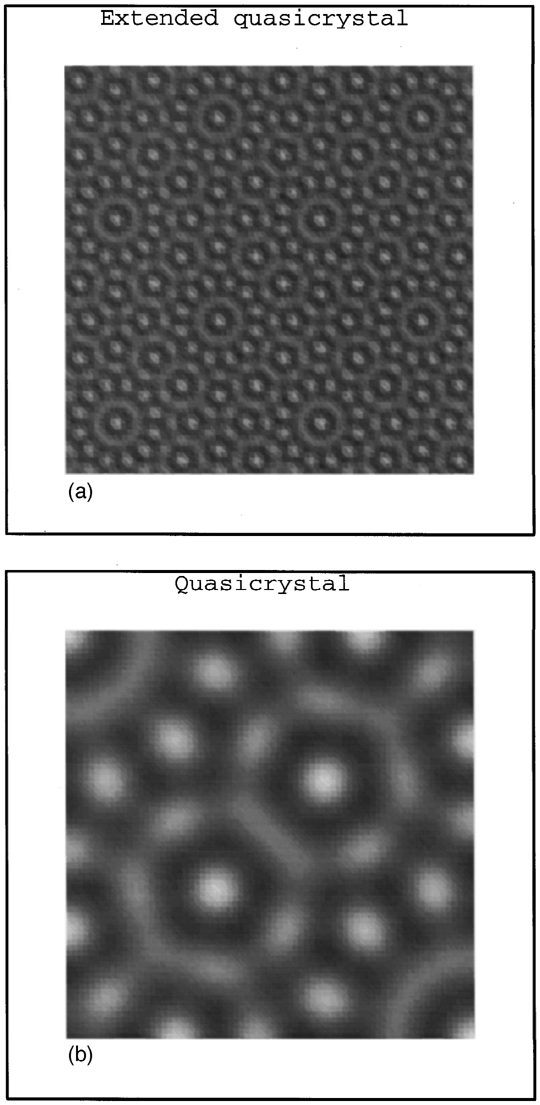

FIG. 1. Quasicrystals. The symmetric pattern expanded by the wave numbers (8,8) and (11,3)(3,11). (a) The pattern extended to 16 cells. (b) Pattern restricted to the cell.

The fixed points at $A_1=\sqrt{\mu_1}$, $A_2=0$, $B=0$ and $A_1=0$, $A_2=\sqrt{\mu_1}$, $B=0$ behave as stable focus for small μ_2 values. For μ_2 large enough, they lose stability against periodic orbits which eventually approach the heteroclinic cycle described above.

This scenario translates into a periodic alternation of patterns in the form of simple squares (when the trajectory visits the neighborhood of the fixed point in the $A_1=A_2=0$ axis) followed by nonsimple squares (see Fig. 2).

Other possible patterns associated to the fixed points of Eq. (7) are simple (stationary) squares and modulated rolls (A_1 or $A_2\neq0$). For parameter values close to the ones in which the Hopf bifurcation occurs, pulsating modulated rolls can be observed.

C. Case 4

Finally, we report the stationary solutions of Eq. (8). It is in this case that we find solutions that are slight deformations

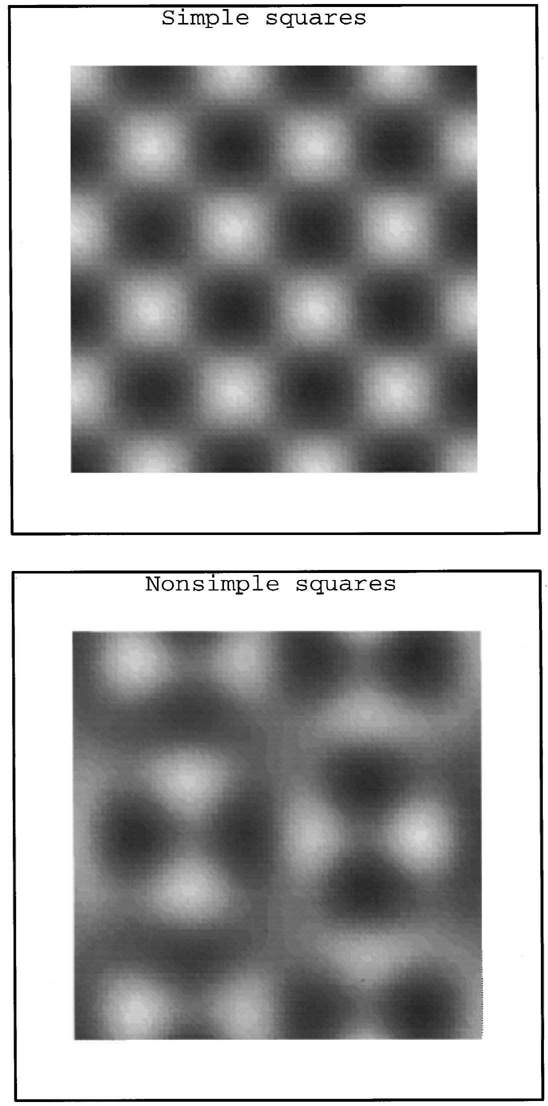

FIG. 2. Simple and nonsimple squares are part of the heteroclinic cycle.

(needed to fit the square boundary conditions) of hexagonal and quasicrystalline structures. Analyzing the subspaces which are invariant under Eq. (8), we find the following families of solutions: (1) $A_1=A_2=B_1(B_2)=0$, rolls; (2) $A_1=A_2=0$, and $B_1=B_2$, squares; (3) $A_1=B_2=0$ $(A_2=B_1=0)$, giving rise to hexagons (antihexagons) if $A_2\sim\pm B_1$ $(A_1\sim\pm B_2)$, or some D_2 symmetric structures otherwise; (4) $A_1=B_2$, and $A_2=B_1$, *quasicrystals* and their deformations; and (5) $A_1=-B_2$, and $A_2=-B_1$ antiquasicrystals.

We focus our attention on the solutions that are characteristic of these mode interactions (namely, the ones associated to hexagonal and duodecagonal patterns). We will analyze separately the cases $g_4<0$ and $1>g_4>0$ (for $g_4>1$ the system has trajectories going to infinity and higher order terms are needed in the normal form). We used analytical techniques whenever it was possible, complementing them with numerical ones.

In the first case $(g_4<0)$, we observed the following structures.

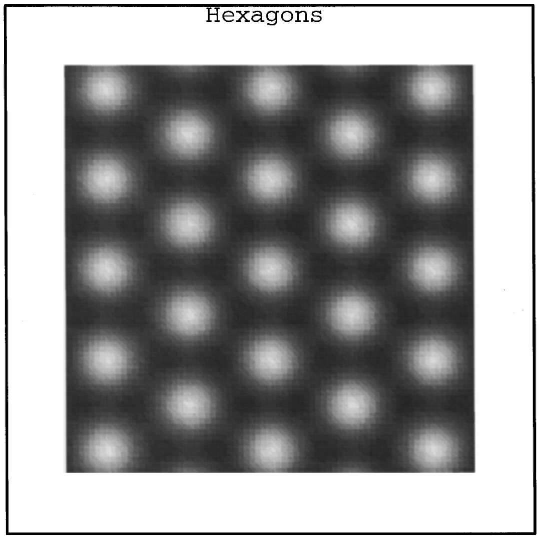

FIG. 3. Hexagonal pattern based in the modes (10,0) and (9,5).

Rolls are present for $\mu_2>0$. For small values of μ_1 they are stable if $g_4<-1$. Their eigenvalues are $(\mu_1-\alpha\sqrt{\mu_1}-\mu_1, \mu_1-\mu_2, \mu_2(1+g), -2\mu_2)$.

Squares (and antisquares) exist for $\mu_2>0$. These solutions are stable whenever $g_4>-1$, and μ_1 is small. The eigenvalues of the stability matrix are

$$\frac{-\mu_1(1-g)+\alpha(g-1)\sqrt{\mu_2/(1-g)}}{g-1}-2\mu_2,$$

with multiplicity 2,

$$-2\mu_2,$$

$$2\frac{\mu_2(1+g)}{g-1}. \tag{17}$$

The solutions with $A_1=B_2=0$ have, for small values of μ_1 and μ_2 compared to α, the following form:

$$A_2=\pm\sqrt{-2(\mu_1^2+\mu_2^2)+13\mu_1\mu_2}/3,$$

$$B_1=\pm\frac{\mu_2}{\alpha}. \tag{18}$$

These solutions look like hexagons for $\mu_1\sim\mu_2$ (see Fig. 3). Numerical simulations indicate that these solutions are stable over a wide range of parameters in the quadrant $\mu_1\mu_2>0$.

The quasicrystal-like solutions exist for $\mu_1\sim\mu_2>0$ but they are unstable towards the hexagons.

The most dramatic change for $1>g_4>0$ with respect to the previous case is that the hexagonal structures are no longer stable for $\mu_1\sim\mu_2>0$. They are unstable to solutions which are arbitrarily close to the quasicrystalline ones. An almost duodecagonal pattern is illustrated in Fig. 4.

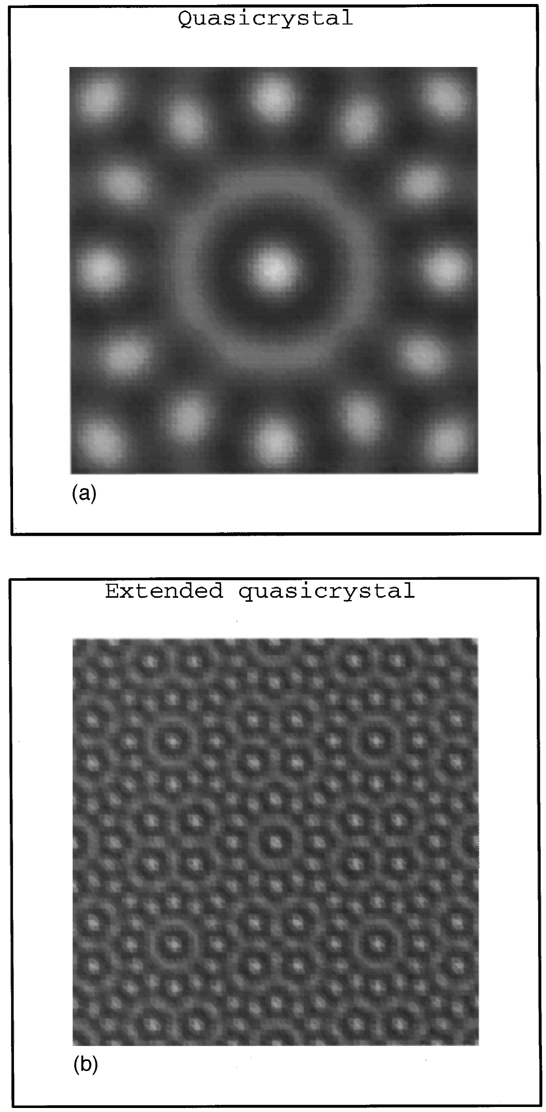

FIG. 4. A duodecagonal pattern based in the modes (10,0)(0,10) and (9,5)(5,9). (a) The pattern. (b) Extension of the pattern to 16 cells.

IV. CONCLUSIONS

In this work we have addressed the problem of pattern formation in intermediate aspect ratio problems where both boundary conditions and interactions determine (jointly) the emerging patterns.

The approach taken has been the study of strong interactions of eigenmodes in a square container. This presentation is more suitable for the present problem than first solving the problem in an infinite container and later singularly perturbing the solutions to match the boundary conditions (a program that in our knowledge has been enunciated but not successfully completed).

The normal forms for these interactions strongly depend on the boundary conditions (BC). In the case of Dirichlet BC there are no quadratic terms and the modes selected interact in the general form, hence the distinction between strong and weak interactions vanishes. It should be noticed that this situation is structurally unstable. The case of Newmann BC is substantially different: there are three different normal forms with stable solutions (for suitable parameter values) associated to ''unsuspected'' patterns. By ''unsuspected'' we mean patterns whose symmetries are not a subsymmetry of the problem and closely resemble hexagons, duodecagonal quasicrystals, and related patterns (here called antihexagons and antiquasicrystals).

One of the advantages of our approach with respect to standard methods is that hexagons and duodecagons are not imposed by a choice of the supported solutions (plan forms) but are eventually selected by the system despite the square boundary conditions.

In more strict terms, the patterns here found are (square based) crystalline approximants of quasicrystals and hexagons. For practical purposes (for example, in an experimental situation) they can be very well ''identified'' as hexagons and quasicrystals.

In addition to the existence of hexagons and other nonsquare patterns that could have been conjectured from the setup of the problem, we have found that periodic alternations between different kinds of squares (simple and nonsimple) is possible. This mechanism resembles the Kupper-Lortz instability [8].

Finally, we point out that the present study can be extended without major differences to the stroboscopic maps of forces systems (like the Faraday instability) and to mixed boundary conditions.

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