MODULATIONAL INSTABILITY AND TWO-DIMENSIONAL DYNAMICAL STRUCTURES

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A process of nonlinear structure formation on a two-dimensional lattice is proposed. The basic model consists of a two-dimensional lattice equipped at each node with a molecule or dipole rotating in the lattice plane. The interactions involved in the model are reduced to a periodic potential and nonlinear couplings between first-nearest molecules in the two directions of the lattice. Such a discrete system can be applied to the problem of molecule adsorption on a substrate crystal surface, for instance. The continuum approximation of the model leads to a 2-D sine-Gordon system including nonlinear couplings, which itself can be reduced to a 2-D nonlinear Schrödinger equation in the low amplitude limit. Spatio-temporal structure formation is investigated by means of numerical simulations. These nonlinear structures are caused by modulational instabilities of initial steady states of the two-dimensional system. Moreover, the analogy between the numerically generated patterns and vortex-like excitations in a lattice is also discussed.

1. - INTRODUCTION

Particular interest has been devoted, recently, to the **dynamics of structures on two dimensional nonlinear systems** [1,2]. These structures (dislocations, domain walls, vortices, etc. ....) play an important role in the material properties and they become crutial in nonlinear physics involved in the problem of adsorbates deposited on crystal surfaces [3], in superlattices of ultra thin layers or in large area Josephson jonctions [4], for instance. Here, a particular emphasis is placed on the **dynamical pattern formation mediated by modulational instability** on a two-dimensional Hamiltonian model.

The paper is divided as follows : in Section 2 we introduce our model and show how the basic equation for the lattice model can be reduced to a 2-D nonlinear Schrödinger equation which can exhibit modulational instabilities under certain conditions. In Section 3 we study a particular dynamical regime by means of numerical simulations which then place the role of the modulational instability in evidence for the pattern formation. Then, beyond the instability a self-organisation of 2-D coherent structures takes place.

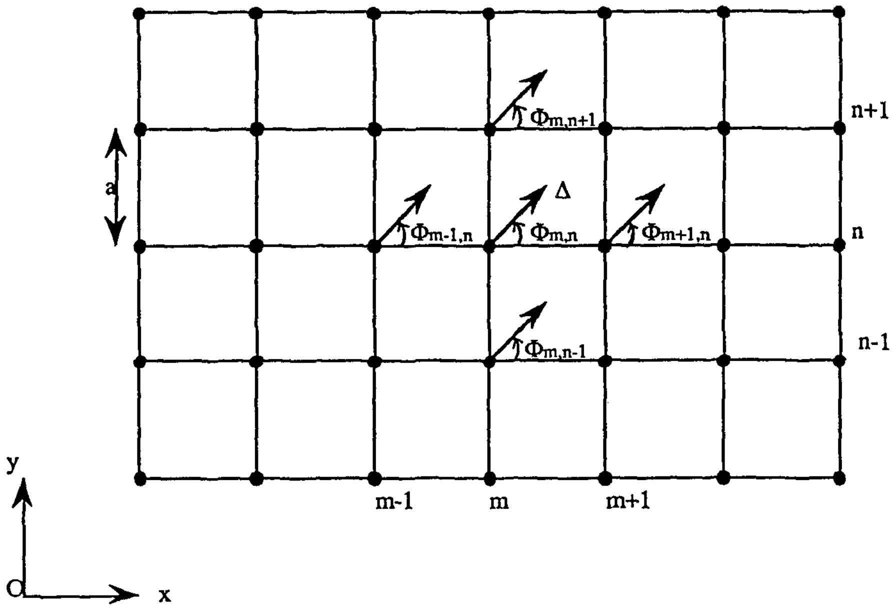


Fig. 1 : *the two – dimensional lattice model equipped, at each node, with rotating molecule (the arrow indicates the molecule orientation).*

2. - THE MODEL

2.1. - Basic discrete equations

The basic model is made of a two-dimensional lattice equipped, at each node, with a **rotator** or **rigid rotating molecule**. Namely, each molecule can rotate in the lattice plane. At site (m, n) the angle of rotation is $\Phi(m, n)$ (see Fig.1). Each molecule interacts **nonlinearly** with its first-nearest neighbors and with a **periodic substrate potential**. Under these conditions the equations of the rotational motion of the molecules can be written as

$$\begin{aligned}\ddot{\Phi}(m,n) = \; & A_L(\Phi(m+1,n) - 2\Phi(m,n) + \Phi(m-1,n)) + A_T(\Phi(m,n+1) - 2\Phi(m,n) \\ & + \Phi(m,n-1)) + B_L\left[(\Phi(m+1,n) - \Phi(m,n))^3 - (\Phi(m,n) - \Phi(m-1,n))^3\right] \\ & + B_T\left[(\Phi(m,n+1) - \Phi(m,n))^3 - (\Phi(m,n) - \Phi(m,n-1))^3\right] \\ & - \omega_0^2 sin(\Phi(m,n)) \quad . \end{aligned} \tag{1}$$

The inertia of the molecules has been set to unit for ease of presentation. The coefficients A_L and A_T are the linear couplings in the longitudinal and transverse directions while the parameters B_L and B_T are the nonlinear couplings in the longitudinal and transverse directions, respectively. At length, the last term in Eq.(1) is due to the substrate potential where ω_0^2 is the strength of the potential barrier and ω_0 can be interpreted as the frequency of small oscillations in the bottom of the potential wells. Note, if the nonlinear coupling is removed ($B_L = 0$ and $B_T = 0$) Eq.(1) casts in the 2-D Frenkel-Kontorova model (or the 2-D discrete sine-Gordon model [5]). In the following section we restrict our study to the isotropic case, i.e. $A_L = A_T = A$ and $B_L = B_T = B$.

2.2. - Continuum approximation

On using a classical procedure we consider the long wave-length limit and reach the continuum approximation of the discrete equations (1) (*i.e.* by expanding in Taylor series $\Phi(m,n)$ in terms of its derivatives about the point $(x = ma, y = na)$). Then Eq.(1) becomes

$$\Phi_{tt} = A(\Phi_{xx} + \Phi_{yy}) + (A/12)(\Phi_{4x} + \Phi_{4y}) + B\left(\left(\Phi_x^3\right)_x + \left(\Phi_y^3\right)_y\right) - \omega_0^2 sin(\Phi) \quad , \quad (2)$$

where the variable changes x/a and y/a have been considered (a being the lattice spacing). We notice that if, first, the nonlinear coupling ($B = 0$) and, second, the fourth order derivatives are dropped we recover the usual 2-D sine-Gordon equation [6]. On the other hand, if the substrate potential is removed, Eq.(2) is then somewhat similar to a 2-D Boussinesq equation. Nevertheless, the case for which the substrat potential and nonlinear coupling are both considered is of particular interest for pattern formation.

From Eq.(2), we now look for **plane wave solutions** with a slowly varying envelope of the form

$$\Phi(x,y,t) = \psi(X,Y,T)e^{i(\mathbf{k}.\mathbf{r}-\omega t)} + \; c.c. \quad , \quad (3)$$

where the wave vector is $\mathbf{k} = (k_L, k_T)$ and ω is the circular frequency of the carrier part of the plane wave and we have also set $\mathbf{r} = (x, y)$. Moreover the envelope ψ is a function of the **slow space and time variables** defined by

$$X = \epsilon x \; , \qquad Y = \epsilon y \qquad \text{and} \;\; T = \epsilon t \quad . \quad (4)$$

Where ϵ is a small parameter. In addition, the small amplitude limit has been considered (this allows us to expand the sine function up to the third order with respect to Φ). On inserting (3) into (2) we obtain the **nonlinear dispersion relation**

$$\omega^2 = \omega_0^2 + A\left(k_L^2 + k_T^2\right) - (A/12)\left(k_L^4 + k_T^4\right) + \left(3Bk_L^4 + 3Bk_T^4 - \omega_0^2/2\right)|\psi|^2 \quad . \quad (5)$$

This relation represents the key equation which allows us to reduce Eq.(2) to a 2-D nonlinear Schrödinger equation. It must be noticed that the first three terms in the right hand side of Eq.(5) are the linear part whereas the last term is the nonlinear contribution to the dispersion relation.

2.3. - 2-D nonlinear Schrödinger equation and modulational instability

Now, if we consider slow modulations in space and time of a carrier wave with wave numbers k_{Lc} and k_{Tc}, we can formally expand the dispersion relation (5) around the carrier parameters ($k_L = k_{Lc}$, $k_T = k_{Tc}$ and $|\psi| = 0$) and we arrive at

$$\begin{aligned} \omega - \omega_c \;=\; & (k_L - k_{Lc})\left(\frac{\partial\omega}{\partial k_L}\right)_c + (k_T - k_{Tc})\left(\frac{\partial\omega}{\partial k_T}\right)_c + \frac{1}{2}(k_L - k_{Lc})^2\left(\frac{\partial^2\omega}{\partial k_L^2}\right)_c \\ & + \frac{1}{2}(k_T - k_{Tc})^2\left(\frac{\partial^2\omega}{\partial k_T^2}\right)_c + (k_L - k_{Lc})(k_T - k_{Tc})\left(\frac{\partial^2\omega}{\partial k_L \partial k_T}\right)_c \\ & + \left(\frac{\partial\omega}{\partial|\psi|^2}\right)_c |\psi|^2 \; . \end{aligned} \quad (6)$$

The subscript c means that all partial derivatives are taken for the carrier wave features. Then, let the operators $k_L - k_{Lc} : -i\partial/\partial X$, $k_T - k_{Tc} : -i\partial/\partial Y$ and $\omega - \omega_c : i\partial/\partial T$. The frequency

ω_c is the carrier frequency and it is provided by the linear part of the dispersion relation (5). On applying these operators to the amplitude function $\psi(X,Y,T)$, we obtain then the following equation

$$2i\left(\psi_T + v_{gL}\psi_X + v_{gT}\psi_Y\right) + P_1\psi_{XX} + P_2\psi_{YY} + P_3\psi_{XY} + Q|\psi|^2\psi = 0 \quad , \qquad (7.a)$$

where we have set

$$P_1 = \left(A/\omega_c^3\right)\left[\omega_0^2 + Ak_{Tc}^2 - \left(3Ak_{Lc}^4 + Ak_{Tc}^4 + 6Ak_{Lc}^2k_{Tc}^2 + 6\omega_0^2k_{Lc}^2\right)/12\right] \quad , \qquad (7.b)$$

$$P_2 = \left(A/\omega_c^3\right)\left[\omega_0^2 + Ak_{Lc}^2 - \left(3Ak_{Tc}^4 + Ak_{Lc}^4 + 6Ak_{Lc}^2k_{Tc}^2 + 6\omega_0^2k_{Tc}^2\right)/12\right] \quad , \qquad (7.c)$$

$$P_3 = -\,A^2\left(1 - k_{Lc}/6\right)\left(1 - k_{Tc}/6\right)k_{Lc}^2k_{Tc}^2/2\omega_c \quad , \qquad (7.d)$$

$$Q = \left(\omega_0^2 - 6Bk_{Lc}^4 - 6Bk_{Tc}^4\right)/2\omega_c \quad . \qquad (7.e)$$

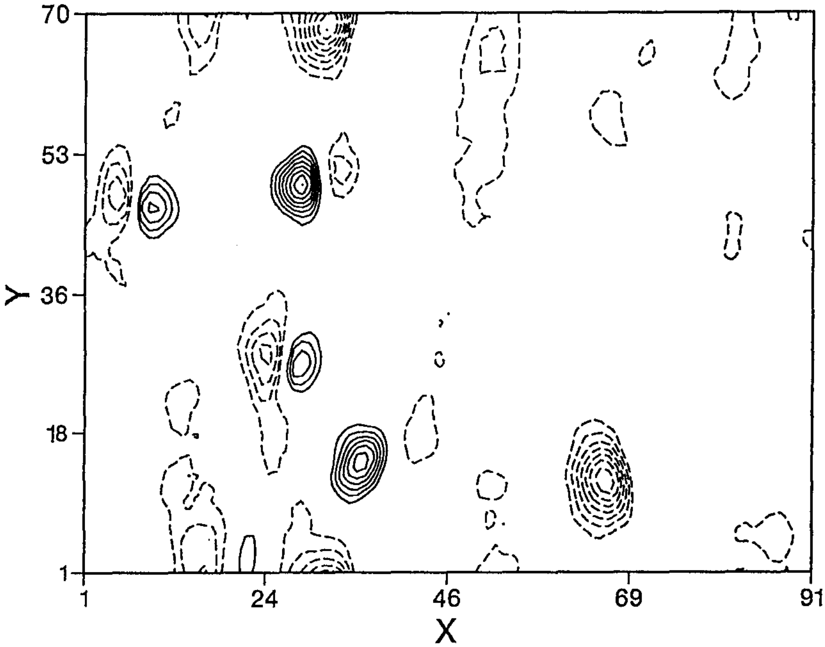
On considering a frame moving with the wave and using the transformations $\xi = X - v_{gL}T$, $\eta \doteq Y - v_{gT}T$, next (v_{gL} and v_{gT} being the group velocities in the longitudinal and transverse directions), we can rewrite Eq.(7.a) in the standard **2-D nonlinear Schrödinger equation.** The latter equation has been extensively studied especially in plasma physics [7]. With the help of this 2-D nonlinear Schrödinger equation we can investigate the stability of a plane wave traveling on the lattice. A linear analysis of small pertubations of the elementary plane wave solution leads to a criterion of stability or instability maned **modulational instability** [8]. Skipping all the analytic details, the region of instability are given by

$$0 < q_L^2 < 2\psi_0^2 Q/P_1 \;, \qquad 0 < q_T^2 < 2\psi_0^2 Q/P_2 \quad , \qquad (8)$$

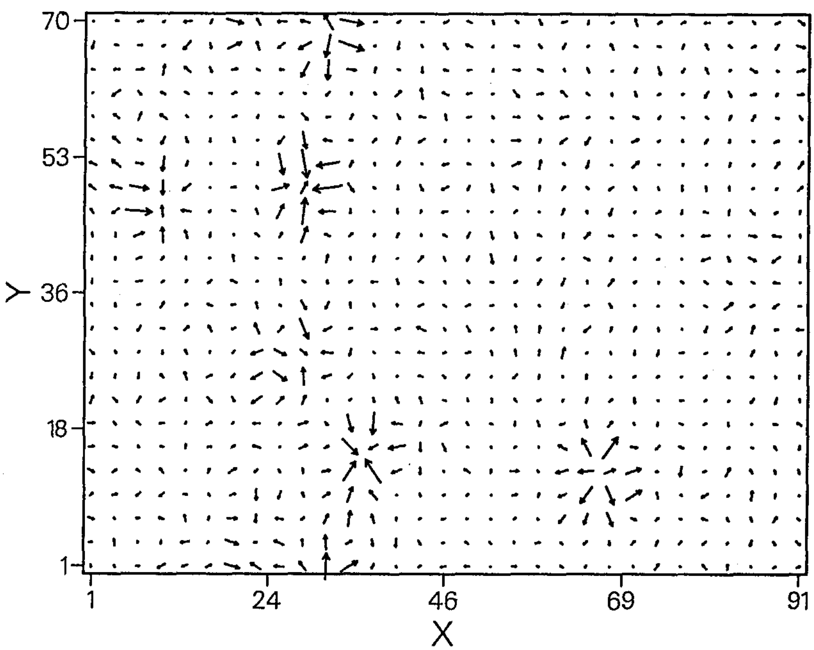
where ψ_0 is the constant amplitude of the carrier plane wave, q_L and q_T are the wave numbers of the **perturbation** in the longitudinal and transverse directions, respectively. Accordingly, a perturbation with a wave vector (q_L, q_T) satisfying (8) can trigger instabilities in both directions of the lattice. However, such conditions depend, of course, on the respective signs of the products QP_1 and QP_2.

3. - NUMERICAL SIMULATIONS

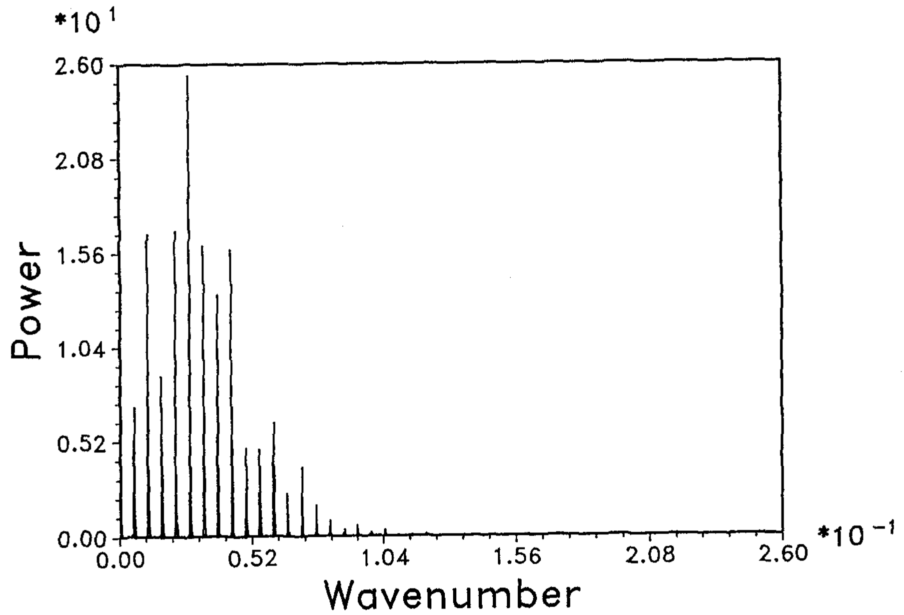
We now present the preliminary numerical investigations of the dynamics of structure formation initialized by modulational instabilities. Specifically, an initial carrier wave propagating in the x (or y) direction (5 periods in the propagating direction, the wave number of the carrier wave in x is $k_{Lc} \simeq 0.35$ corresponding to the long wave-length limit) is modulated by adding a random noise of small amplitude to the initial velocity field (the noise is removed afterwards). It is important to emphasize that the numerical simulations are directly performed on the **original lattice model** (see Eq.(1)). A lattice made of 91×70 points is considered and periodic boundary conditions in x and y directions are used for the numerical simulations. Under these conditions the 2-D nonlinear Schrödinger equation describes the dynamical behavior of the system in the very beginning of the instability (at the birth of the instability).



(a)



(b)



(c)

Fig. 2 : *Numerical simulations of the discrete system Eq.*(1) ($A = 0.1$, $B = 0.2$, $\omega_0^2 = 0.4$) *at* $t = 1200$, (*a*) *contour line graphe for the rotation* (*full line* $\Phi \geq 0$ *and dashed line* $\Phi < 0$), (*b*) *the corresponding pseudo – velocities and* (*c*) *the power spectrum exhibiting additional wave number components due to instabilities*

The most significant results are collected together in Fig.2. Figure 2.a represents the picture of the contour lines for the rotation Φ. This picture exhibits, after a long time, very clear localized structures, in fact these structures are moving on the lattice. We can observe small pertubations due to the phonon radiations but they remain rather weak. On introducing a "**pseudo-velocity**" associated with the rotation Φ (*i.e.* the gradient of Φ) as in perfect fluid hydrodynamics, we can plot a lattice of pseudo-velocity as shown in Fig.2b (each arrow corresponds to the velocity vector). The picture thus numerically generated exhibits sorts of **vortex-like structures.** Finally, the power spectrum of the lattice dynamics is given in Fig.2c showing then additional harmonic components around the high peak corresponding to the carrier frequency. These components are produced by the instabilities. From Fig.2.c, we can compare the range of the instability wave vectors to that given by the conditions (8) and a good agreement is obtained. It is worthwhile noting that, here, in contrast to the pure 2-D nonlinear Schrödinger equation the drastic collapse does not occur [7,9], this emerges from saturation effects because of the substrat potential and discreteness effects.

4. - CONCLUSIONS

We have studied the formation of nonlinear localized structures on a two- dimensional lattice model. We have also shown that these structures are the result of the modulational instabilities of a steady plane wave solution. The most significant idea, which can be underlined in the present work, is that we have been able to reduce the rather complicated dynamics of the lattice to the 2-D nonlinear Schrödinger equation in the long wave-length and small amplitude limits. Although the 2-D nonlinear Schrödinger equation is limited to the birth of the modulational instability, this informs us about the selection mechanism of wave vectors of the instabilities taking place both in longitudinal and transverse directions. In short, the modulational instability is a **natural vehicle** for the nonlinear structure formation. It seems that the characteristic radius of the coherent structures thus produced can be connected with the growth rate of the instabilities as well as the model parameters. This point should be clarified in a further work. In addition, extensions of the study to the specific problems of **vortex-like** and **spiral excitations** will be examined [1,10,11]. Finally, the relative influence of the substrat potential and nonlinear coupling (see the definition of the coefficients of the nonlinear Schrödinger equation, Eqs(7.a)-(7.e)) will be studied in more detail by means of an analytical approach and numerical simulations.

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