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Breaking of Analyticity in 2 Coupled Frenkel-Kontorova Chains.

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Abstract. – We investigated the destruction of a two-frequency torus in a 4D volume-preserving map and its influence on the solid-state properties of the related model. The hull functions associated with this solid-state model exhibit a transition from a smooth surface to a devil fragmentation with the increase of the chaos parameter. We also discuss the properties of the phonon spectrum of excitations in this regime.

In the last decade many efforts have been devoted to a deeper comprehension of the transition from commensurate to incommensurate structure in solid-state models. The model which became well known in the description of this phenomenon is the discrete Frenkel-Kontorova model. On the one side it is sufficiently simple, but on the other side it contains many significant and nontrivial features about the commensurate-incommensurate transitons in solid-state systems.

The study of this 1D solid-state model has close connections with the dynamical properties of the Chirikov Standard Map [1] which can describe the transition from regular to global chaotic motion in many physical models. However in the solid-state framework it was established, in different ways [2-5], that the ground state of this model is never chaotic and it corresponds, in the related dynamical system, to a KAM torus or to a cantorus, depending on the chaos parameter k in the Chirikov Standard Map. This transition, which was first investigated by Aubry and called transition by breaking of analyticity, leads to a drastic change in the physical properties of the model. One of the main physical results of this transition is the appearance of a gap in the spectrum of propagating waves. The appearance of this phonon gap is strictly connected with the transition from the invariant KAM curve to a cantorus in the corresponding dynamical system. However, to the best of our knowledge, up

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to now the main investigations were carried out for the 1D system corresponding to one winding number in the dynamical model.

In this paper we investigated another type of solid-state model consisting of two one-dimensional coupled solid-state chains which, from the dynamical point of view, correspond to a trajectory with two fixed winding numbers.

This model is particularly interesting since in this case the invariant set is given by two-dimensional tori instead of 1D invariant KAM curves. Due to this topological difference this invariant set does not prevent the global chaos but permits unbounded Arnol'd diffusion. The situation is qualitatively different from the case of one winding number, therefore one expects here a distinct kind of transition for the solid-state model. Another support to this expectation is given by the recent results for a 4D volume-preserving map which showed the absence of universality in the destruction of a two-frequency invariant torus [6, 7]. Oppositely to the strategy of [8] we investigate the destruction (with the change of the parameter) of one torus with fixed winding numbers, while in [8] the authors analysed the set of undestroyed tori in phase space for fixed values of the parameters.

From the solid-state point of view our model consists of two infinite arrays of harmonic oscillators (two different kinds of atoms) embedded in a periodic potential which also gives a coupling between the two chains. Another interpretation for such a model is the description of the interaction between particles with spins. In fact the cosine structure of the interaction term can be interpreted as the spin interaction between fermion particles with different spins depending on spin angles. If we let u_i^+, u_i^- be the positions of the oscillators along the two chains, we may write the potential energy as follows:

$$V\{\underline{u}^+, \underline{u}^-\} = \sum_i \frac{1}{2}(u_i^+ - u_{i-1}^+)^2 + \frac{1}{2}(u_i^- - u_{i-1}^-)^2 - K(1 - \cos u_i^-)(1 - \cos u_i^+). \quad (1)$$

By looking for the equilibrium configurations, one obtains the infinite set of coupled equations

$$\begin{cases} \dfrac{\partial V}{\partial u_i^-} = 0 = -u_{i+1}^- + 2u_i^- - u_{i-1}^- - k \sin u_i^+ (1 - \cos u_i^-), \\ \dfrac{\partial V}{\partial u_i^+} = 0 = -u_{i+1}^+ + 2u_i^+ - u_{i-1}^+ - k \sin u_i^- (1 - \cos u_i^+). \end{cases} \quad (2)$$

As in the 1D Frenkel-Kontorova case we make the identification

$$\theta_i^\pm = u_i^\pm \,(\mathrm{mod}\,(2\pi)), \qquad p_{i+1}^\pm = u_{i+1}^\pm - u_i^\pm, \quad (3)$$

and we obtain the 4D volume-preserving symplectic map:

$$\begin{cases} p_{i+1}^+ = p_i^+ - k \sin(\theta_i^+)(1 - \cos(\theta_i^-)), & \theta_{i+1}^+ = p_{i+1}^+ + \theta_i^+, \\ p_{i+1}^- = p_i^- - k \sin(\theta_i^-)(1 - \cos(\theta_i^+)), & \theta_{i+1}^- = p_{i+1}^- + \theta_i^-, \end{cases} \quad (4)$$

where now the index i plays the role of time. This map is a generalization of the well-known 2D area-preserving map called Chirikov Standard Map. As remarked before, due to Arnol'd diffusion the global spread in phase space can take place before the break-up of the last KAM torus. Moreover, it is not at all clear which type of torus will be the most robust in place of the golden-mean torus of the 1D model. In fact this system possesses three natural frequencies which are the period (2π) of the periodic potential, and the densities of the two chains

$$\omega^{\pm} = \lim_{n \to \infty} \frac{u_{n+1}^{\pm} - u_0^{\pm}}{2\pi n}.$$

According to some general beliefs [6, 9], to assure strong irrationality among them, we choose the KAM torus whose two winding numbers are the incommensurate pair

$$(\omega^+, \omega^-) = (x^{-2}, x^{-1}) = (0.56984025\ldots, 0.754877\ldots),$$

where x is the real root of the equation (spiral mean): $x^3 - x - 1 = 0$.

In practice we study the periodic approximants to the KAM torus (p_n^+/q_n, p_n^-/q_n), where $p_n^{\pm}$, q_n obey the recursion relation

$$F_n = F_{n-2} + F_{n-3}$$

with $F_{-3} = 0$, $F_{-2} = 0$, $F_{-1} = 1$ and $p_n^+ = F_{n-2}$, $p_n^- = F_{n-1}$, $q_n = F_n$.

From the dynamical point of view this corresponds to approximating an orbit with irrational winding number with periodic orbits having longer and longer period. From the solid-state point of view one can visualize two situations. First, we can consider the q_n oscillators (u^+) disposed along the chain of length $L^+ = 2\pi p_n^+$. In the same way the q_n oscillators (u^-) should be disposed along the other chain of length $L^- = 2\pi p_n^-$ which is of course different from L^+. The system can be thought of as two concentric rings with a periodic potential acting along the radius. On the other hand, we may safely rescale the length L^- by considering a potential with a different period in the u^- chain (*e.g.*, of period $2\pi p_n^-/p_n^+$).

One of the main features of the 1D FK model was the Transition by Breaking of the Analyticity (TBA). This means that the positions along the chain could be parametrized by a «hull function» f such that

$$u_i = f((il + \alpha)(\mathrm{mod}\, 2\pi)),$$

where l is the unperturbed distance between two oscillators and α is an initial phase. That function shows an analytical character for a perturbation strength less than some value k_c; while it becomes an infinite sum of step functions for $k > k_c$. For the same value of the parameter the KAM torus corresponding to that winding number undergoes a transition to a cantorus [10].

Many other characteristics accomplish this transition, for example the appearance of a phonon gap. We remind that such a name is devoted to the smallest allowable frequency of the linearized motion. The presence of a gap in the spectrum of the linearized motion can be associated with the existence of a cantorus in the related dynamical model, or, in general, with the presence of uniform hyperbolicity [11].

To find the equilibrium position, we use the gradient method [12]. This means to transform the system (2) into a set of coupled differential equations depending on a fictitious time τ (integration time):

$$\frac{\mathrm{d}u_i^{\pm}}{\mathrm{d}\tau} = \frac{\partial V}{\partial u_i^{\pm}}.$$

The integration procedure was acted on until the equilibrium configuration was obtained ($\|u^{\pm}\| < 10^{-25}$ or less). To do that, one has to use a good starting configuration. We started from $k = 0$ and we slowly increase k by δk, each time using the previously obtained configuration. Basing on the analogy with the case of one winding number, we suppose that this method gives the ground state of the solid-state model. Perhaps, the rigorous proof of that can be obtained on the basis of the same strategy as in [2-4].

From the equilibrium positions we obtained the «hull functions» $f_i^{\pm}$ (at least formally, we do not know if they really correspond to a well-defined mathematical object), such that

$$u_i^{\pm} = f_i^{\pm}, \qquad (u_i^{0+} \bmod (2\pi),\ u_i^{0-} \bmod (2\pi)), \tag{5}$$

where $u_i^{0\pm}$ are the unperturbed equilibrium positions (*i.e.* for $k = 0$). From the equilibrium positions we can also investigate the spectrum of the linearized motion.

In our numerical simulations we analysed the two main properties of the model: the hull functions and the spectrum of excitations near the ground state. The hull functions are here dependent on two phases: the unperturbed positions $\theta_i^{0\pm} = u_i^{0\pm} \bmod (2\pi)$ (see (5)). For small coupling constant k these functions form a smooth surface in the cube $[0, 2\pi)^3$ as is shown in fig. 1*a*)-*c*). However, with the increase of the perturbation the invariant torus is destroyed leaving place to a 2D invariant Cantor set. This transition is reflected in the hull function as the destruction of the smooth surface in many disconnected two-dimensional pieces (devil's fragmentation): fig. 2*a*)-*c*). It is interesting to note that this surface is formed by one line in the infinite volume of $u^{\pm}$, u^{0+}, u^{0-} and only after taking modulus 2π this line forms a smooth surface or a devil's fragmentation. This transition also leads to a change of the spectrum of excitations near the ground state. For small coupling constant the invariant torus is smooth and this permits the propagation of small-frequency phonons. On the other side, above the transition the cantor structure of the invariant set leads to the appearance of a gap in the phonon spectrum (see fig. 3). In this picture we present the smallest phonon frequency as a function of the perturbation strength for different rational approximants to the spiral mean. While for small k the phonon gap is going to zero, with the increase of the approximant it remains the same for high values of k. From that picture we roughly estimate the transition

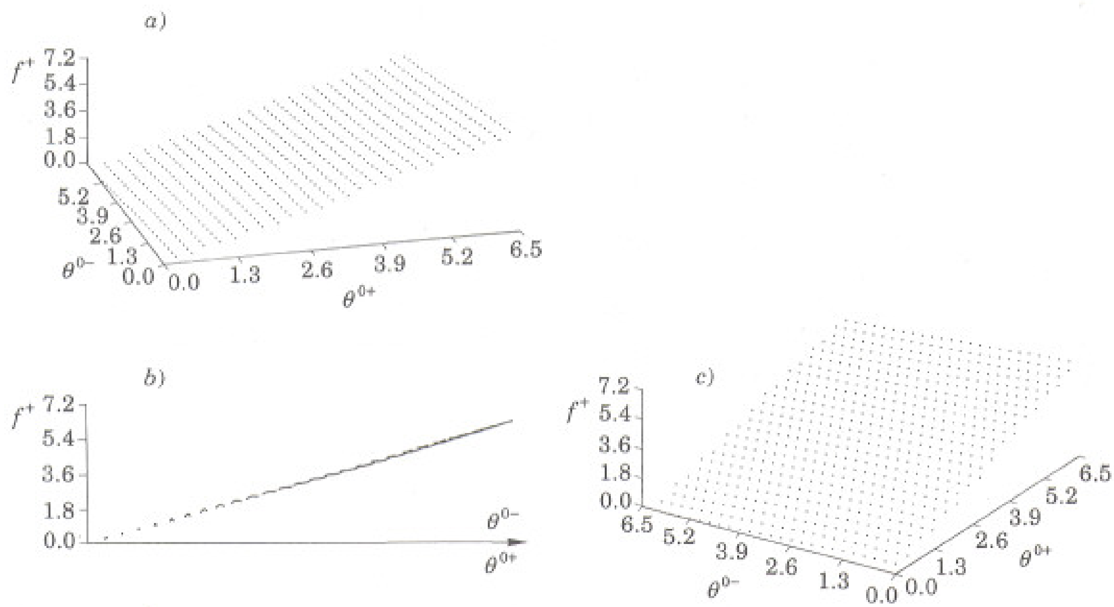

Fig. 1. – Hull function f^+ in the undercritical regime $k = 0.1$ (below the critical point). The periodic approximants for the spiral mean rotation numbers are $\omega^+ = 351/616$ and $\omega^- = 465/616$; *a*), *b*) and *c*) show different orientations.

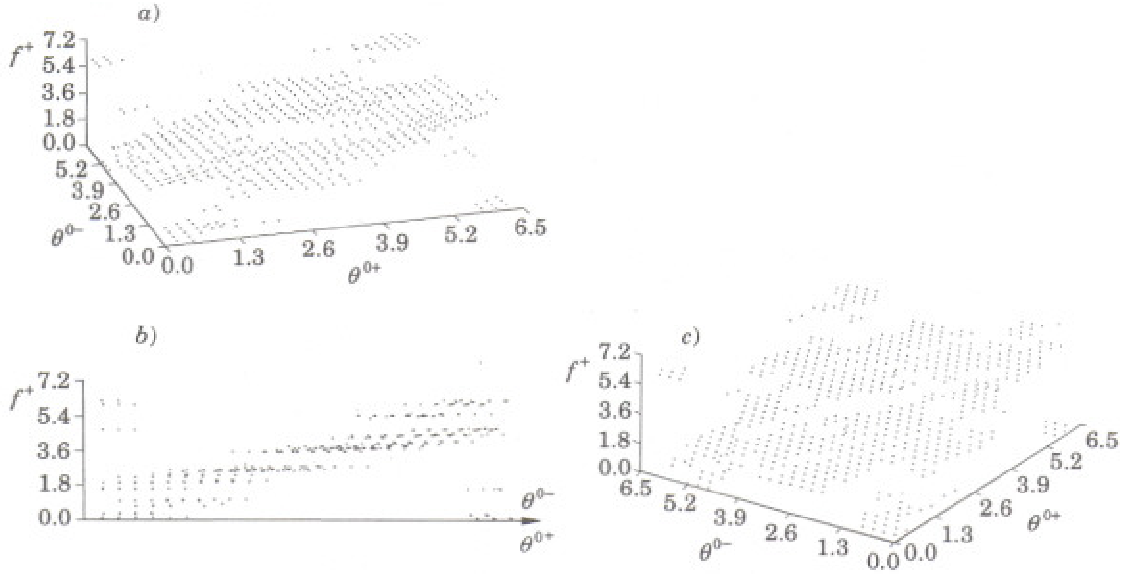

Fig. 2. – The same as fig. 1 for $k = 1$ (above the critical point).

to occur at $k = k_c \simeq 0.2$. This behaviour is in agreement with the KAM theory which provides the existence of an invariant torus for a sufficiently small perturbation.

The phonon spectrum of excitations is presented in fig. 4 as a function of the wave number. For small k it is going linearly to zero, while above the critical point k_c it does not go to zero. The other interesting feature of such a spectrum consists in its flat step structure which looks like the devil's staircase one. The existence of flat steps for small values of the wave number

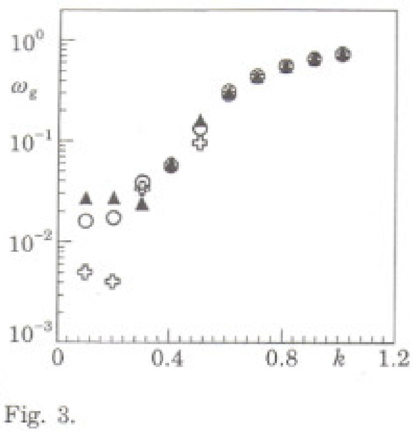

Fig. 3.

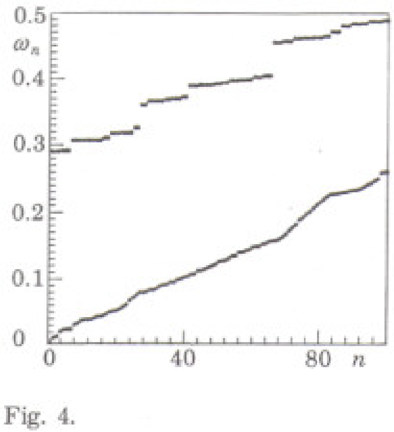

Fig. 4.

Fig. 3. – Phonon gap as a function of the strength k for different rational approximants (triangles are for $q_n = 114$, circles for $q_n = 200$, crosses for $q_n = 616$).

Fig. 4. – Phonon spectrum, for small wave numbers, for two different k values and rotation numbers: $\omega^+ = 351/616$ and $\omega^- = 465/616$. The upper curve is for $k = 0.6$, while the lower one is for $k = 0.2$.

n qualitatively corresponds to the presence of quasi-particle excitations with a very big mass.

We also used Green's residue method [13] to identify the transition between a smooth invariant torus and a 2D cantorus. This method gives approximately the same parameter value for the transition. However, we were not able to apply it for the analysis of the renormalization group dynamics at the critical point due to a very large CPU time required for that.

In this letter we investigated the destruction of a two-frequency torus and the influence of this transition on the solid-state properties of two 1D interacting chains in a periodic potential. We found the existence of a critical value of the perturbation strength above which a two-dimensional invariant Cantor set is formed instead of a smooth 2D invariant surface. The hull functions above the transition remind a devil's fragmentation and they are formed by small separate surfaces. It will be interesting to analyse the fractal properties of this fragmentation. The transition to devil's fragmentation is accomplished by the presence of a gap in the phonon spectrum of the excitations. The spectrum of excitations, above the critical point, shows a devil's staircase character. The existence of flat steps in the phonon spectrum can lead to a sharp change of the properties of the ground state. Indeed, the degeneracy in phonon spectrum makes the theorem KAM unapplicable and due to that even negligibly small nonlinearity in phonon excitations can give chaotic exchange between modes. Such phenomenon of degenerate weak chaos is well known for few degrees of freedom [14] and it will be interesting to analyse its properties in the case of many freedoms.

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