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Dimerized ground states of the Frenkel–Kontorova model with a transversal degree of freedom

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Abstract

We consider the ground states of a generalized Frenkel–Kontorova model with a transversal degree of freedom. The substrate potential is taken to be sinusoidal in the longitudinal direction and parabolic in the transversal one. We assume that the atoms in the chain repel each other with a Coulomb law and that the interaction has a long-range scale. The trivial ground state in this system undergoes a phase transition to a dimerized (zigzag) ground state when the repulsion exceeds some critical value. We show that for much larger values of the interaction parameters there exists the next (zigzag-2) dimerized ground state which cannot be obtained from the previous one in a bifurcational way.

The well-known Frenkel–Kontorova (FK) model describes a one-dimensional chain of atoms interacting with harmonic forces in a periodic substrate potential [1,2]. Introduced first to describe dislocations in solids it has been later successfully used to study other similar systems [3–5]. The application of the model to real physical objects has required its modification such as introduction of an anharmonic [6,7] (including nonconvex [10]) potential of the atom interaction or a substrate potential of more realistic forms [6,9]. However, the main restriction of the model still was its one-dimensionality. In their pioneering papers [10,11] Srolovitz and Lomdahl have introduced the isotropic 2-D generalization of the simple FK model. This model has been treated numerically and it has been shown that its behaviour is much richer.

Braun and Kivshar [12] have proposed another (anisotropic) 2D generalization of the FK model in which the chain of atoms is still one-dimensional but the atoms can move in the transversal direction. In this version the substrate potential has a much larger scale in the transversal direction than in the longitudinal one and is taken to be parabolic. A similar situation takes place in the adsorption of atoms on "furrowed" or stepped surfaces [4,6,13]. The atoms form weakly interacting chains along these surfaces and the model can be applied to describe their diffusion properties. The main advantage of this version of the FK model is that being closed to a 1D model, it allows analytical treatment. In the simplest case of nearest and nearest-nearest atom interaction it has been shown [12,14] that in the case of repulsion between atoms in the chain at some values of the interaction parameters the trivial 1D ground state (GS) becomes unstable and the GS becomes dimerized. The chain is now two-dimensional and has a zigzag-like structure with opposite displacements of atoms

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in the transversal direction. The zigzag dimerized structures allow the existence of the usual "massive" kinks (a vacancy or an access atom in the chain) on its background as well as that of the "nonmassive" kink which is a pure 2D object and is called "nonmassive" because it cannot transfer mass in the system [14].

Therefore, the generalized FK model has essentially new properties: the atoms can escape from the potential minima via the transversal degree of freedom, which makes the model much more unstable. Strictly speaking, in order to have a rigorous model we have to take into account the interaction between all the atoms in the chain not restricting to nearest atoms only. The purpose of this Letter is to consider the dimerized ground states of the FK model with a transversal degree of freedom with a long-range atom interaction.

We consider an atomic chain with an anharmonic atom interaction subject to a 2D substrate potential periodic in one direction and parabolic in the transversal direction. The Hamiltonian of the system has the form

$$H=\sum_{k=1}^{N}\left[\tfrac{1}{2}\dot{x}_k^2+\tfrac{1}{2}\dot{y}_k^2+(1-\cos x_k)+\tfrac{1}{2}\omega^2 y_k^2+U_k\right], \tag{1}$$

where

$$U_k=\tfrac{1}{2}\sum_{i=1}^{N^*}\left[V(r_{k,k+i})+V(r_{k,k-i})\right] \tag{2}$$

describes the potential energy of interaction of an atom with the site k with N^* nearest atoms, V_k is the potential energy of the pairwise atom interaction, ω is the frequency of a single atom transversal vibration (we assume $\omega>1$), and

$$r_{k,j}=\left[(x_k-x_j)^2+(y_k-y_j)^2\right]^{1/2} \tag{3}$$

determines the distance between the atoms.

We consider the commensurate "fixed density" model, i.e. we place the atomic chain with N atoms in the substrate potential with M minima assuming the value $\theta=N/M$ rational and periodic boundary conditions

$$x_{l+N}=x_l+2\pi M,\quad y_{l+N}=y_l, \tag{4}$$

with N large enough and the number of neighbours with which every atoms interacts equal to $N^*=2N$. (Generally speaking N^* is chosen such that its further increase does not affect the results.) The number of atoms N must be chosen to avoid the appearance of "nonmassive" kinks, i.e. such that it may be divided by 4. We also assume that the atoms in the chain repel each other according to a Coulomb law, i.e.

$$V(r)=V_0/r. \tag{5}$$

According to the results of Ref. [14] we may assume that for small values of V_0 at fixed ω (or for large ω at fixed V_0) the ground state of the system (1) is trivial, i.e. coincides with that of the 1D FK model:

$$x_k=2\pi k,\quad y_k=0, \tag{6}$$

and then with the further increase of V_0 (decrease of ω) it is dimerized,

$$x_k=2\pi k,\quad y_k=(-1)^k b, \tag{7}$$

where the value of b in the case of long-range atom interaction is determined by the equation

$$\tfrac{1}{4}\omega^2+\sum_{k=1}^{N^*/2}\frac{V'(r_k(b))}{r_k(b)}=0, \tag{8}$$

and

$$r_k(b)=2\left[b^2+\pi^2(2k-1)^2\right]^{1/2}. \tag{9}$$

To investigate the stability properties of these ground states we use two methods. First, we investigate numerically the linear stability of the chain with N particles with given ground state calculating the eigenvalues of the corresponding elastic matrix. The resulting diagram of linear stability is shown in Fig. 1. It is clear that for large values of V_0 the zigzag structure (7) also becomes unstable.

In order to study the ground state of the system in the region where the configuration (7) is linearly unstable we use the global integration of the Newton equations of motion of the system (1). To avoid metastable configurations, during the first 100 steps in the associated equations of motion we introduce a small random force with normal distribution and after that allow the atoms to relax with the additional friction force $F_{\mathrm{fr}}^{l}=-\eta\dot{x}_l$. The obtained structure is just the stable static configuration which corresponds to the case $\dot{x}_l=0$. In the region where the structure (7)

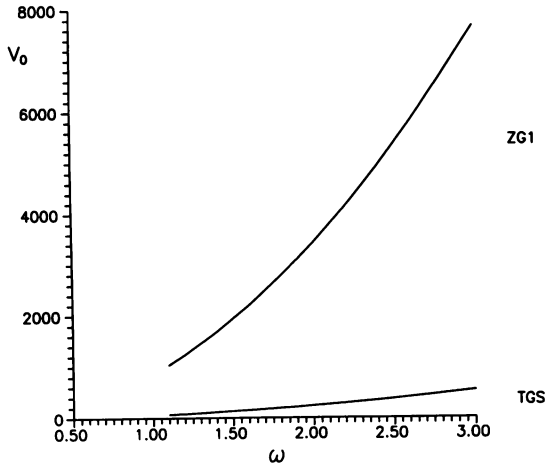

Fig. 1. The diagram of the linear stability of the system. In the region TGS the trivial ground state (6) is linearly stable and ZG1 indicates the region for linear stability of the zigzag ground state (7).

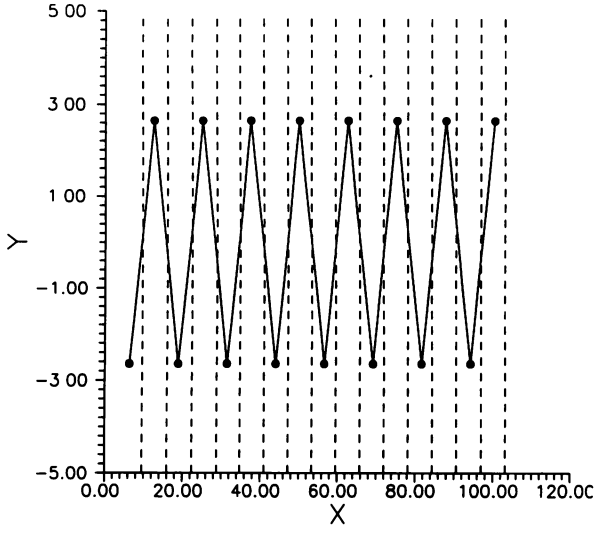

Fig. 2. The zigzag ground state (7) of the system for $V_0=500.0$, $\omega=2.0$ obtained by direct numerical simulations of the Newton equations of motion. The dashed vertical lines indicate the positions of the substrate potential minima.

is linearly stable the results of the two methods coincide. The obtained zigzag structure is shown in Fig. 2.

Similar numerical simulations (with ground state (7) as initial configuration) are applied in the region of parameters where zigzag state (7) is linearly unstable. The obtained structure may be called zigzag-2 since the absolute displacements of atoms in the transversal direction have two values b_1 and b_2. This structure cannot be considered as the ground state of the system since the resulting configuration is the following: two atoms with opposite displacements in the transversal direction have the same x-coordinate, i.e. occupy the same minimum of the substrate potential, and the next minimum is empty, etc. This gives us the idea how to obtain the next dimerized GS: to place the chain of $2M$ atoms in the M minima, where M is even. The resulting structure (ZG2) has the following form,

$$x_k=2\pi[k/2]\,,$$
$$y_k=(-1)^{[k/2]}b_1,\quad k\,\text{odd}\,,$$
$$=(-1)^{[k/2]}b_2,\quad k\,\text{even}\,. \tag{10}$$

The values b_1 and b_2 are determined by the system of equations

$$\tfrac{1}{2}\omega^2 b_1+(b_1+b_2)S_1(b_1+b_2)+(b_1-b_2)S_1(b_1-b_2)+b_1S_2(2b_1)=0\,, \tag{11}$$

$$\tfrac{1}{2}\omega^2 b_2+(b_1+b-2)S_1(b_1+b_2)+(b_2-b_1)S_1(b_2-b_1)+b_2S_2(2b_2)=0\,, \tag{12}$$

where

$$S_1(b)=\sum_{k=1}^{N^*/2}\frac{V'(r_k^{(1)}(b))}{r_k^{(1)}(b)}\,, \tag{13}$$

$$S_2(b)=\sum_{k=1}^{N^*/2}\frac{V'(r_k^{(2)}(b))}{r_k^{(2)}(b)}\,, \tag{14}$$

$$r_k^{(1)}(b)=[(2\pi(2k-1))^2+b^2]^{1/2}\,,$$
$$r_k^{(2)}(b)=[(4\pi(k-1))^2+b^2]^{1/2}\,. \tag{15}$$

The direct numerical simulations with the values (10) as initial configuration and the method described above shows that this GS is really stable (see Fig. 3).

The dimerized GS (10) cannot be obtained from GS (7) in a simple bifurcational way since it has a different coverage $\theta=N/M$. The kinks existing with it as a background must have more complicated structure. For instance, in Fig. 4 we placed $N=2M-2=24$ particles in $M=13$ minima of the substrate potential which can be called a simple antikink. The structure looks very much as if we had

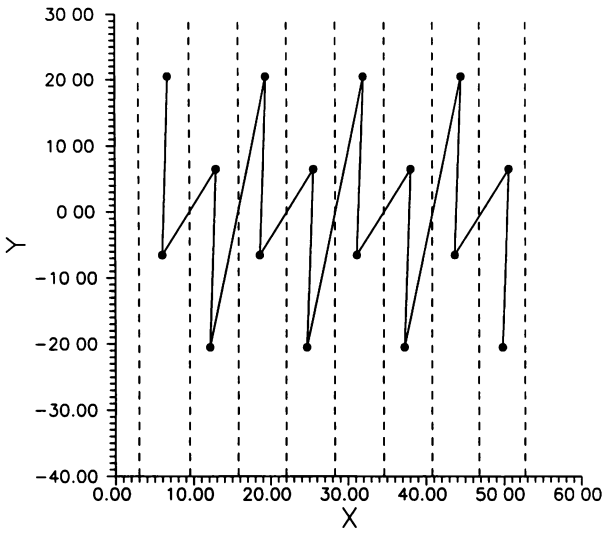

Fig. 3. The zigzag-2 ground state of the system for $V_0=4000.0$, $\omega=2.0$ obtained by the direct numerical integration of the Newton equations of motion with the initial conditions (10). The dashed vertical lines indicate the positions of the substrate potential minima.

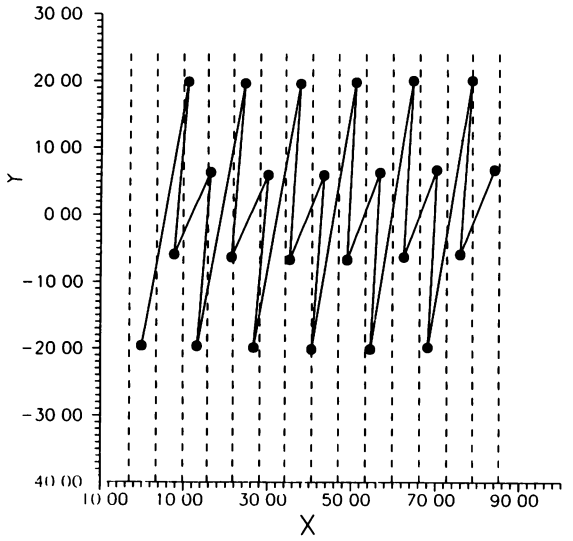

Fig. 4. The shape of a "nonmassive" antikink ($N=24$ particles placed in $M=13$ minima) with the zigzag-2 ground state as a background for $V_0=4000$, $\omega=2.0$. The dashed vertical lines indicate the positions of the substrate potential minima.

four subchains with a simple 1D kink in every one. Other structures have not such simple forms. Unfortunately, the introduction of the transversal degree of freedom leads to the mixing of atoms in the chain and as a result the appearance of instabilities, which is clearer for the strong atom interaction in the system, i.e. in the region of dimerized structure (10).

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