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The Frenkel–Kontorova model with a transverse degree of freedom: kinks structures

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Abstract

By means of the crystallographic point group technique we construct elementary excitations (kinks) on complex ground states of the Frenkel–Kontorova model with a transverse degree of freedom. These complex kinks consist of elementary subkinks in each subchain of the system and correspond to the minimally possible topological charge.

Keywords: Frenkel–Kontorova model; Kinks; Elementary excitations

The Frenkel–Kontorova (FK) model with a transverse degree of freedom [1] is a quasi-2D generalization of the classical FK model [2]. It describes a chain of atoms subjected to a two-dimensional potential which is periodic in one direction and parabolic in the transverse direction. Consequently, the atoms in the chain are allowed to move in two dimensions although the chain itself is still one-dimensional. The model may be considered as the simplest approximation for an anisotropic vector 2D FK model when the interactions between nearest-neighboring rows are negligible. Among physical applications of the model one can mention the adsorption of atoms on furrowed or stepped surfaces [3], the surface reconstruction and crystal growth [4].

The introduction of an additional degree of freedom, even in its simplest version, makes the model quite rich in behavior. When the repulsion between particles increases, the trivial ground state (TGS) of the system undergoes a series of bifurcations, starting with the transition to the zigzag ground state (ZGS) [2,5]. The dynamics of the model with a transverse degree of freedom is certainly very different from the standard FK model. In particular, the bifurcations generate cusps in the variation of the effective elastic constant versus the magnitude of interatomic interaction, which results in the change of the scenario of the Aubry transitions for an incommensurate concentration of atoms [6].

Another aspect of the model is that it has a large number of metastable states for any value of the interatomic repulsion. To investigate the metastable configurations, one should first study elementary

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topological excitations in the model, i.e. kinks and antikinks. Kinks play an important role in the dynamical and thermodynamical properties of the system. They are responsible for mass and energy transport along the chain, and are related to many important characteristics such as, e.g., the conductivity or the chemical diffusion coefficient. Studying (e.g., numerically) the transport properties, one should start with the *elementary* topological excitations, because any other topologically stable excitations can be constructed of the elementary ones. The problem of construction of elementary excitations on a complex GS structure is more general and may emerge in many physical systems possessing a GS which is infinitely degenerate.

A complicated character of the GS of the FK model with a transverse degree of freedom makes the problem of determination of the number and structure of kinks non-trivial. It is clear that a "naive" approach of just inserting one additional atom into the chain is not suitable anymore, becuase instead of one kink, it will produce several kinks in the chain. The same problem arises in the standard 1D FK model when a GS is non-trivial. Aubry [7] has carried out a very extensive work to prove the minimum-energy configurations and to find the structures of elementary excitations in non-convex FK model. In this consideration, a particular emphasis has been made on the role and the value of the topological charge. Furthermore, Tang and Griffiths [8] have constructed localized defects of the FK model using the area-preserving map of the phase plane and associating a defect with a set of heteroclinic points at the intersections of expanding and contracting manifolds. Our work is totally in the spirit of these ideas and in many sense our method is the same as the symmetry considerations used before by S. Aubry in this previous works.

The present paper is aimed at the classification of possible elementary excitations in the FK model with a transverse degree of freedom. The Hamiltonian of the system has the form

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

where

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

describes the potential energy of interaction of the kth atom with N^* nearest neighboring atoms, $V(r)$ is the potential energy of the pairwise atomic interaction (which is considered to be repulsive), ω is the frequency of transverse vibration of a single atom, and

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

determines the distance between atoms. We consider the "fixed density" FK model, i.e. we place the atomic chain of length L consisting of N particles into a substrate potential which has M minima on the distance L and we assume the periodic boundary conditions. When the frequency ω of transverse vibrations of an isolated atom tends to infinity, the zigzag-FK model reduces to the standard one-dimensional FK model [1], where all atoms are aligned to a line. When the repulsion between atoms in the chain increases, the GS of the zigzag-FK model undergoes a sequence of bifurcations starting with the transition to the ZGS [6]. Further increasing of the repulsion leads to the bifurcation to the "rhomboidal" GS, then to the "double zigzag" GS and so on (see Fig. 1. Note that in order to keep the generalized form of the potential (1), in this figure and in the ones below we have drawn the forms of the solutions schematically. Readers interested in concrete parameters values for specific potential forms such as exponential or Coulomb, may find them in [5,6,9,10]).

Our aim is to give a simple unique recipe to construct, and at the same time to classify, the possible kinks in the ground states of the FK model. For the trivial and zigzag ground states the procedure is trivial and known: In order to obtain a kink solution, one has to translate the chain to one period of the GS and then "link" two GS's. Therefore,

i. The trivial GS admits simple kink (an additional atom inserted into the chain) and an antikink (a vacancy). The distinguishing feature is that anharmonicity of the interatomic potential breaks the kink–antikink symmetry of the classical FK

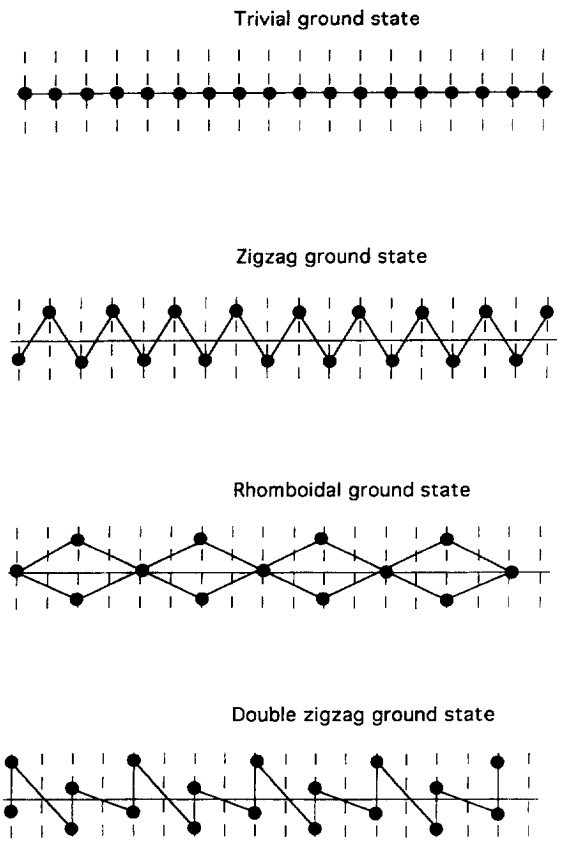

Fig. 1. Ground states structures for the Frenkel–Kontorova model with a transverse degree of freedom.

model, now they are characterized by different effective masses and energies [2,5].

ii. The zigzag GS admits two types of kinks: the "massive" kink and antikink, and the "non-massive" kink [5] (see Fig. 2). The "massive" kinks can be described in terms of the perturbed sine-Gordon (SG) equation so that they are often referred as SG kinks [2]. The "non-massive" kink appears owing to the existence of additional inverse symmetry of the chain. It represents a phase kink and can be described in terms of the perturbed Φ^4-equation [5] so that it can be also called Φ^4-kink. This kink does not participate in the mass transport along the chain, but makes contributions to the thermodynamical properties of the system.

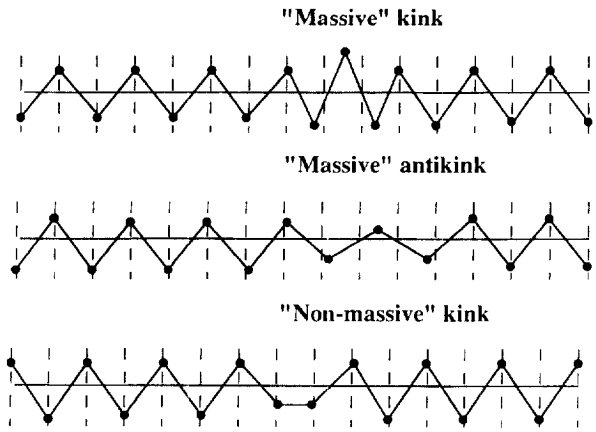

Fig. 2. Kinks structures on the zigzag ground state.

In order to find elementary excitations in a complex GS, we use the technique of crystallographic point groups presented in [9] which we briefly review here. Consider a complex GS of the FK model with $\theta = r : p$ coverage so that the period of the GS is p and each elementary cell of the GS consists of r atoms. First of all we represent a complex GS by a set of r subchains each one having a trivial GS structure. The quantity which plays the central role in the approach is a total topological charge of the excitation $Q = q_{\text{tot}}/p$, where

$$q_{\text{tot}} = \sum_{i=1}^{r} (g_i + pt_i). \tag{4}$$

In this expression g_i is the so-called "color" of the ith subchain which is equal to the number of translations of the right-hand side of the subchain within an elementary cell, and t_i is the number of periods of GS structure for which the subchain is translated. Because the subchains are strongly interacting, the following condition must be fulfilled:

$$g_i \bmod p = g. \tag{5}$$

Furthermore, since topological charges are additive, the elementary excitation should correspond to a minimum topological charge. Then the

solution of the problem reduces to the solution of the following equation:

$$ph = q_{\text{tot}} + rg. \tag{6}$$

i.e. we have to find such integers g and h ($1 < g < p$) which minimize the value q_{tot} for the given structure. The answer is the following:

(1) When r and p are relatively simple, the GS admits the existence of a single kind of elementary topological excitation, the SG kink with $|q_{\text{tot}}| = 1$.

(2) When r and p have a common divisor $j_0 > 1$ (this case corresponds to the situation when the point group includes the "inversion" symmetry), two kinds of kinks cam exist:

(a) The SG kink with $|q_{\text{tot}}| = j_0$ and the structure determined by Eqs. (6) and (5),

(b) The Φ^4, or phase kink with $q_{\text{tot}} = 0$ and the structure characterized by the color $g = p/2$.

Based on this method we complete the consideration of possible elementary excitations on the complex GS structure in the FK model with a transverse degree of freedom:

iii. The "rhomboidal" ground state has the configuration $\theta = 3 : 4$. The solution of Eq. (6) gives $g = 1$ and $q_{\text{tot}} = 1$. If we denote k ($\bar{k}$) the subkink (subantikink) in a subchain, then from Eq. (5) we can obtain the kink structure as $K = \{\bar{k}, 3k, \bar{k}\}$ and for an antikink $\bar{K} = \{k, 3\bar{k}, k\}$. The kink and antikink structures are presented in Fig. 3.

iv. The "double zigzag" GS $\theta = 4 : 4$ has additionally the "inversion" symmetry and thus it has two types of kinks, the "massive" kink with $q_{\text{tot}} = 4(Q = 1)$ and $g = 2$, and the "non-massive" kink with $q_{\text{tot}} = 0$ and $g = 2$ (see Fig. 4). The "massive" kink is characterized by the structure $\{k, k, k, k\}$, while the non-massive kink has the configuration $\{2k, 2\bar{k}, 2k, 2\bar{k}\}$.

Starting with these elementary excitations as initial conditions one can perform numerical calculations and find how the system adjusts to produce the actual structure.

To conclude, we have presented the structure of elementary excitations in the FK model with a transverse degree of freedom. These excitations correspond to a minimally possible topological charge in the system and consist of subkinks in every subchain. The subkinks are spatially bounded in a localizes region so that a kink for a complex GS should have a shape mode usually. During kink motion along the chain, the subkinks structure may rearrange, give birth to additional subkinks and subantikinks, but the total number of elementary excitations should correspond to a single kink (antikink) in the whole chain.

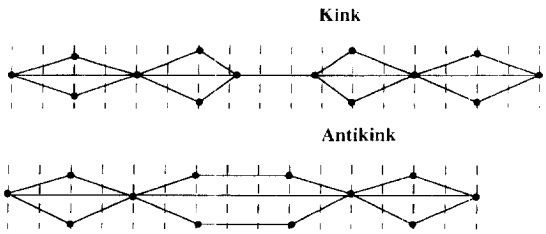

Fig. 3. Kinks structures on the rhomboidal ground state.

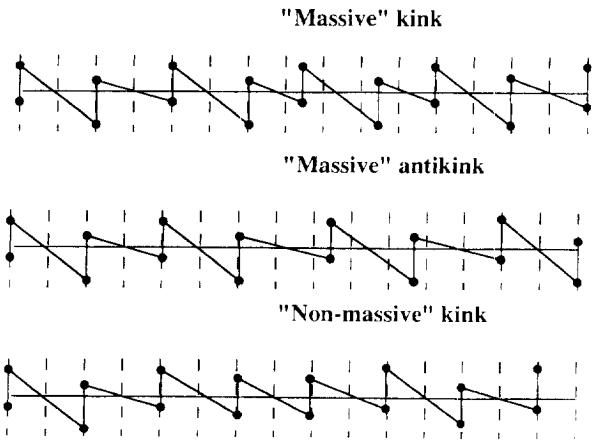

Fig. 4. Kinks structures on the double zigzag ground state.

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