Structure of kinks for a complex ground state

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We propose an approach which allows us to find the structure of elementary topologically stable excitations (kinks) for a complex ground state (GS) of an atomic chain subjected to the two-dimensional external potential periodic along the chain and bounded in the transverse direction. The approach is based on the consideration of the complex GS consisting of subchains, each being characterized by the trivial structure, so that the kink of the whole system may be considered constructed of a set of topological excitations (subkinks) of the subchains.

A number of physical systems have a degenerated ground state (GS). Such systems admit topological excitations, which ''link'' different ground states. As examples we may recall dislocations in solids,[1,2] domain walls in magnetic materials,[3] vortices in long Josephson junctions,[4] etc. These solutions (the so-called kinks) describe transitions between equivalent vacuum states.

Investigation of properties of these topological excitations is very important, because they contribute to static properties of solids (such as the spectrum of elementary excitations), as well as to dynamic ones (e.g., charge, mass, and energy transport in solids). When the degeneration of GS is ''simple,'' for example, when it is doubly degenerated as in the ϕ^4 model, or when it is generated by the Abelian group of translations as in the sine-Gordon (SG) model, the structure of topological excitations is simple too. But when GS has a complex structure, for example, when an elementary cell of the crystalline GS is non-Bravais (i.e., consists of more than one atom), the determination of the structure of topological excitations is a nontrivial problem. First, there may exist excitations of different kinds. Second, a question arises of how to find elementary excitations, which then may be used for the construction of any other topological excitation in the system under investigation.

The goal of the present work is to propose a method which allows us to find these elementary excitations. As a concrete example, we use the Frenkel-Kontorova (FK) model with a transverse degree of freedom (''zigzag-FK model'') proposed in Ref. 5. The model describes a chain of interacting atoms subjected to a two-dimensional potential which is periodic along the chain and bounded (e.g., parabolic) in the transverse direction. The Hamiltonian of the system has the form

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

where

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

describes the potential energy of interaction of the kth atom, with N^* nearest neighboring atoms ($N^*>N$), $V(r)$ is the potential energy of the pairwise atomic interaction [we took the particular case of Coulomb repulsion $V(r)=V_0/r$], ω is the frequency of a single atom transverse vibration, and

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

determines the distance between the 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. Starting with the corresponding initial configuration, we solve directly the Newton equations of motion applying a method suggested in Ref. 6.

The model (1,2) describes, for example, the adsorption of atoms on furrowed or stepped crystal surfaces (see, e.g., Refs. 7 and 8). An interesting application of the model with nonconvex transverse potential is related to the reconstruction of surface growth in crystals.[9]

When the frequency ω_y of transverse vibrations of an isolated atom tends to infinity, the zigzag-FK model reduces to the standard one-dimensional FK model,[1,2] 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 zigzag ground state (ZGS).[5,10] Further increasing of the repulsion leads to the bifurcation to the ''rhomboidal'' GS, then to the ''double zigzag'' GS, and so on.[11,12]

Topological excitations of the FK-type models are known as kinks, or topological solitons. A simple situation emerges in the standard FK model, where only two types of kinks

exist, namely, the kink, which describes the minimally possible topologically stable compression of the chain, and the antikink, which describes the analogous expansion of the atomic chain. The simplest (and most widely studied) case corresponds to the trivial ground state of the standard FK model, when the dimensionless atomic concentration θ (defined as the ratio of the number of atoms N to the number of minima of the external potential M in the limit when both N and M tend to infinity) is equal to one, so that the lattice is Bravais and each minimum of the external potential is occupied by one atom in the GS. In this case, the kink (antikink) configuration describes an extra atom (vacancy) inserted into the chain, when all other atoms are relaxed in order to adjust to the created local perturbation. However, when $\theta=r/p$ (r and p being integers) with $r\neq p$, the situation becomes nontrivial even for the standard FK model. In particular, now the kink is characterized by the fractional atomic number p^{-1}, so that one additional atom inserted into the chain produces p kinks.

Let us consider a complex GS of the FK model with $\theta=r:p$, so that the period of the GS structure is p (we take the period of the external potential as the unit of length), and each elementary cell of the GS consists of r atoms (we use here the designation $\theta=r:p$ instead of $\theta=r/p$, in order to emphasize that r and p for nontrivial GS may have a common divisor as, for example, in the ZGS of the FK model with the transverse degree of freedom, where $r=p=2$). The idea of the approach developed below is to treat a complex $\theta=r:p$ GS of the chain as consisting of r subsystems (subchains), each being characterized by the trivial stucture. In a single subchain, we may create kinks (subkinks) if we simply shift the right-hand side of the subchain for an integer number of periods of the substrate potential. In this way, we may consider any topological excitation of the whole system as constructed of subkinks. However, subchains strongly interact with each other. Consequently, many combinations of subkinks are forbidden, because the right-hand side of the chain must correspond to a true GS configuration. Thus, the problem under investigation reduces us to looking for allowed combinations of subkinks, and then to distinguishing those combinations that may be considered as elementary ones, so that any other combination can be constructed from the elementary ones.

The whole symmetry group $\mathscr{S}$ of the FK model, with $\theta=r:p$ GS, may be split to two subgroups, $\mathscr{S}=\mathscr{T}\otimes\mathscr{G}$. The first subgroup $\mathscr{T}$ is an Abelian group, $\mathscr{T}\equiv\{T^n\}$, where $n=0,\pm1,\ldots$. It is generated by the operator T, which describes translation of the chain as a whole for the distance p (i.e., for one period of the GS structure). The second subgroup $\mathscr{G}$ is a finite (''point'') group, which describes the local symmetry of the complex elementary cell. For the trivial GS, where all atoms are aligned to a line as in the standard FK model, $\mathscr{G}$ is a cyclic group consisting of p elements. $\mathscr{G}$ is generated by the operator G, $\mathscr{G}\equiv\{G^l\}$, $l=0,1,\ldots,p-1$, and $G^p=G^0=1$, where G corresponds to translation of the chain as a whole for the unit distance (i.e., for one period of the substrate potential). On the other hand, when GS is nontrivial, the point group $\mathscr{G}$ includes additionally element J ($J^2=1$), which describes the ''inversion'' of the GS. For example, in the zigzag-FK model above the first bifurcation point, when atoms in the GS are shifted from the line in the transverse direction, the action of J on the GS produces the ''mirror image'' of the state, with respect to the chain's line. Thus, for the case when r and p are not relative prime and r is even, the GS is additionally doubly degenerated.

In general, in order to create a topological excitation in the chain, we have to choose an element of the whole symmetry group and to act by this operator on the GS obtaining a new GS configuration, and then to look for the kink configuration, which links the old and new GS's, i.e., to find the minimum-energy configuration with the boundary conditions at infinities when the left-hand side of the chain is kept in the old GS, while the right-hand side is in the new GS (for the sake of concreteness, we assume that the atoms repel each other).

Although the total number of topological excitations is infinite (but countable), all of them can be constructed from few kinds of ''elementary kinks.'' To find the structure of elementary kinks, let us consider the whole system as that constructed of r subchains. Each subchain, being considered independently from other subchains, has the trivial GS configuration, i.e., an elementary cell of a subchain always contains one atom only. Analogously as it was done above, we can define translation operators G_i and T_i, $i=1,2,\ldots,r$, acting on the ith subchain only. It is evident that any element $S^{(\alpha)}$ of the whole symmetry group, $S^{(\alpha)}\in\mathscr{S}$, may be presented as a product of elements of the subchain's subgroups $\mathscr{G}_i$ and $\mathscr{T}_i$,

$$S^{(\alpha)}=\prod_{i=1}^{r} G_i^{g_i^{(\alpha)}}\otimes T_i^{t_i^{(\alpha)}}, \tag{4}$$

where $g_i^{(\alpha)}$ and $t_i^{(\alpha)}$ are integers. But the opposite statement is not true, the set of all products $\Pi_i G_i^g\otimes T_i^t$ exceeds the set $\mathscr{S}$. Indeed, because the subchains are strongly interacting, a relative arrangement of the subchains in the GS must not be violated, and this leads to a constraint on the admitted values of the integers $g_i^{(\alpha)}$ in Eq. (4). Namely, the following condition must be fulfilled:

$$g_i^{(\alpha)}\bmod p=g^{(\alpha)},\quad i=1,\ldots,r \tag{5}$$

for all subchains simultaneously. If we name $g_i^{(\alpha)}\bmod p$ as the ''color'' of the ith subchain, the condition (5) means that, in the GS, all subchains must have the same color $g^{(\alpha)}$.

In the way described above, we may constuct any topological excitation of the system. Recalling that the operator G_i applied to the right-hand side of the ith subchain creates a subkink in this subchain (and, analogously, the inverse operator G_i^{-1} creates a subantikink), we see that any topological excitation may be treated as consisting of a corresponding set of subchain's subkinks. Because the GS of an isolated subchain is trivial and is characterized by the dimensionless concentration $\theta_i=1/p$, a single subkink (subantikink) has a topological charge p^{-1} (or $-p^{-1}$). Therefore, a topological excitation of the whole system can be characterized by a topogical charge $Q^{(\alpha)}=q_{\rm tot}^{(\alpha)}/p$, where

$$q_{\rm tot}^{(\alpha)}=\sum_{i=1}^{r}(g_i^{(\alpha)}+pt_i^{(\alpha)}). \tag{6}$$

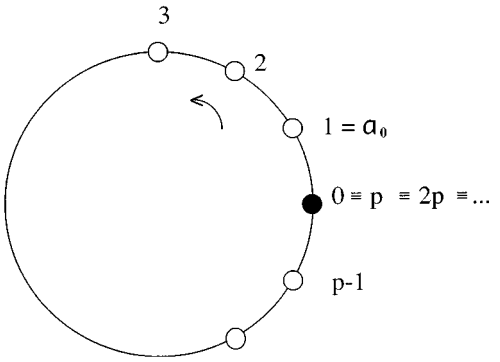

FIG. 1. Construction of elementary topological excitations.

Thus, the only question which remains still open is how to classify topological excitations, i.e., to select those excitations that may be considered as the simplest, or elementary ones. Taking into account that topological charges (6) are additive, so that the topological charge of a complex excitation always is a sum of topological charges of elementary excitations, it is not difficult to guess that elementary excitations should correspond to those with minimum topological charges, such as $q_{\rm tot}=0$ and 1 or 2.

From Eqs. (5) and (6), it follows that $q_{\rm tot}$ may be presented as

$$q_{\rm tot}=rg+ph, \tag{7}$$

where r and p are given integers determined by the concentration θ, the color g must be within the interval

$$1\leqslant g<p, \tag{8}$$

and h is an integer. So, the problem reduces to looking for such integers g [from interval (8)] and h, which minimize the absolute value of $q_{\rm tot}$ defined by Eq. (6) for given $\theta=r:p$. Let us proceed further in two steps.

Step 1. Suppose that the minimum $|q_{\rm tot}|$ is equal to one. In this case, Eq. (7) takes the form (we change here $h\rightarrow -h$ and put $q_{\rm tot}=-1$ for the sake of convenience)

$$ph=1+rg. \tag{9}$$

Suppose also that r and p are such that the integer equation

$$ph=rg \tag{10}$$

has no solutions, so that r and p are relatively simple.

Let us put p points on a circumference and numerate them from 0 to $p-1$, as shown in Fig. 1. Then, let us begin from the point number 1, $a_0=1$, and make an anticlockwise rotation moving by ''large'' steps, each of r unit steps. After the first turn by several ''large'' steps, we come to a point a_1', which is the closest to the initial point a_0. Calculate the integer

$$s_1=(p-a_0)\,{\rm mod}\,r. \tag{11}$$

If $s_1=0$, then $a_1'=0$ (recall that the points with numbers p and 0 coincide), and Eq. (9) has a solution with $h=1$, while the color g is determined by the number of ''large'' steps during the first turn.

Otherwise, $a_1'=p-s_1$, and the next point in the anticlockwise direction is $a_1=r-s_1\neq a_0$. To prove that $a_1\neq a_0$, let us suppose that $a_1=a_0$. Then we get $r-s_1=1$, $(p-1)\,{\rm mod}\,r=r-1$, $p-1=jr+r-1$ (j is an integer), and finally $p=(j+1)r$, which contradicts the assumption that Eq. (10) has no solutions.

Then, starting from the point a_1, after the second rotation, we come to a point a_2'. We calculate

$$s_2=(p-a_1)\,{\rm mod}\,r. \tag{12}$$

If $s_2=0$, we have $a_2'=0$, so that $h=2$ in Eq. (9). Otherwise, the next point is $a_2=r-s_2$. Again, in the same way, we can prove that $a_2\neq a_1$ and also $a_2\neq a_0$. Thus, after each turn, we come to a new point in the circumference. But because the number of these points is finite ($=p$), after a finite number of steps, we finally come to the point with the number 0, and the number of turns just gives the value of h in Eq. (9). So, we have proved that Eq. (9) always has a solution provided Eq. (10) has no solutions, and have shown how to find it.

Step 2. Now let us suppose that Eq. (10) has a solution. It is easy to see that it is true, if and only if p and r have a common divisor $j_0>1$, i.e., if

$$p=p_0j_0 \quad \text{and} \quad r=r_0j_0. \tag{13}$$

Indeed, represent the product $\Pi=ph=rg$ as

$$\Pi=\underbrace{i_1\ldots i_m}_{r}\,\overbrace{Ri_{m+1}\ldots i_n}^{p}, \tag{14}$$

where $i_1,\ldots,i_n$ are simple integers. From (14), we see that if r and p have no common divisors, it should be $g=Rp$ with $R>1$, but this is forbidden by the restriction (8).

Let j_0 correspond to the greatest common divisor. If we now put $g=p_0$ and $h=-r_0$ in Eq. (7), we obtain $q_{\rm tot}=0$, i.e., we have found one kind of kink with zero total topological charge. Putting $q_{\rm tot}=0$ in Eq. (6) and taking into account Eq. (5), one can see that the elementary excitations should correspond to the integers $g=p/2$ and $h=r/2$.

Besides, in the present case there exist also solutions with a nonzero topological charge equal to $Q=j_0/p$. Their structure can be found from the solution of the equation

$$p_0h=1+r_0g, \tag{15}$$

similarly as it was done above in step 1, because now the integer equation $p_0h=r_0g$ has no solutions.

To summarize, when the point group $\mathscr{G}$ does not include the inversion operator J, so that r and p are relatively simple, $\theta=r:p$ GS admits the existence of a single kind of elementary topological excitation, the SG-type kink with to-

pological charge $Q=1/p$. The kink structure, in this case, may be found from the solution of the integer equation (9).

Otherwise, when r and p are not relative prime and have the greatest common divisor j_0, $\theta=r:p$, GS supports the existence of two kinds of kinks. The first kind is the ϕ^4-type kink, it has the topological charge $Q=0$, and its structure is characterized by the color $g=p/2$. The second kind of kink is the SG-type kink with topological charge $Q=j_0/p$, and its structure is determined by Eq. (15). These two kinds of kinks were named in Ref. 10 as ''massive'' kink and ''nonmassive'' kink, respectively, because mass (charge) transport along the chain may be carried out only by kinks with nonzero topological charge, i.e., by ''massive'' kinks. It is important to note that, in the model under investigation, there is no constraint on a sequence of kinks of different kinds.

If we denote by k ($\overline{k}$) the subkink (subantikink) in a subchain, then an elementary topological excitation K of the whole system may be represented as a set of r elements, such as $K=\{g_1k,g_2k,\ldots,g_rk\}$. For example, Fig. 2 shows the structure of elementary kinks for the trivial $\theta=3:5$ GS. Because 3 and 5 are relatively simple, in this case, we have only one kind of kink, the SG-type kink with the topological charge $Q=1/5$. Indeed, Eq. (9) has the solution for $g=2$ and $h=1$, so that the kink structure is characterized by $g_1=2$, $g_2=2$, and $g_3=-3$, or $K=\{2k,2k,3\overline{k}\}$. It is interesting that this structure essentially differs from what might be expected from a naive approach. Indeed, if we, following the kink definition as the minimally possible compression of the chain, simply compress the chain by shifting its right-hand side for one period of the substrate potential to the left, we create a topological excitation with topological charge $Q=3/5$ and structure $\{k,k,k\}$, which then has to be split into three elementary excitations, $\{k,k,k\}\rightarrow\{2k,2k,3\overline{k}\}+\{2k,3\overline{k},2k\}+\{3\overline{k},2k,2k\}=3K$.

To illustrate the conclusions made above, we have per-

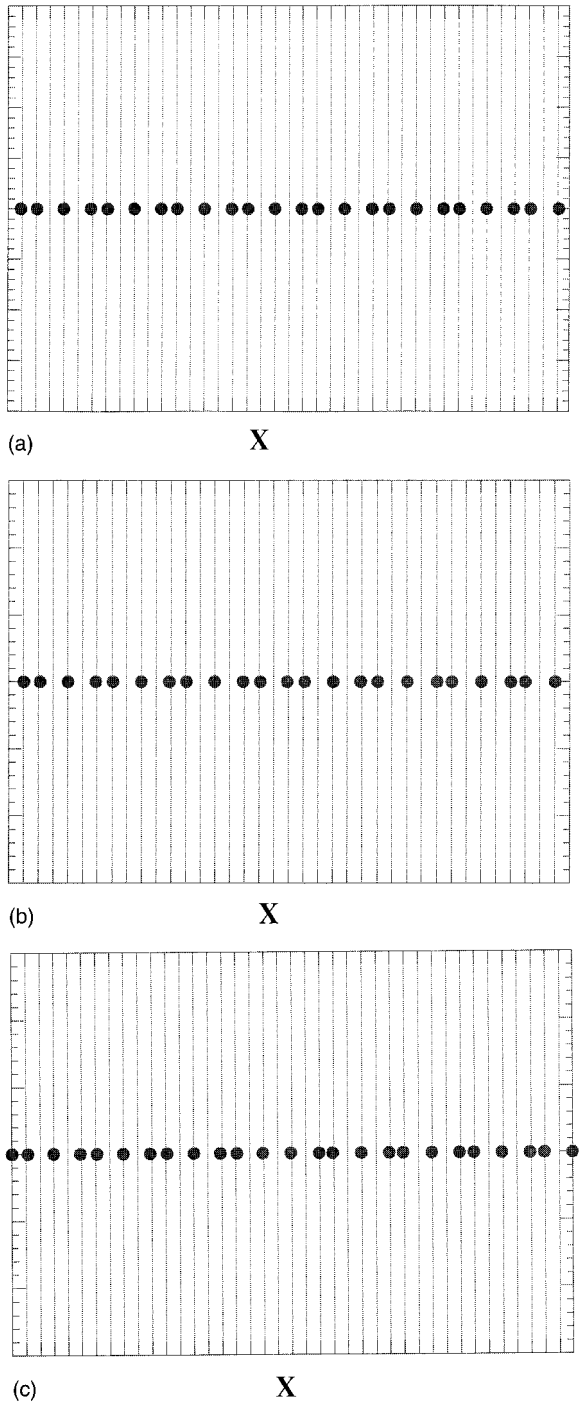

FIG. 2. Structure of trivial $\theta=3:5$ configurations ($\omega=2.0$, $V_0=40$). (a) Ground state, (b) kink, and (c) antikink structures. The vertical dashed lines show the positions of the minima of the substrate potential $X_i=2\pi i$, $i=1,\ldots,M$.

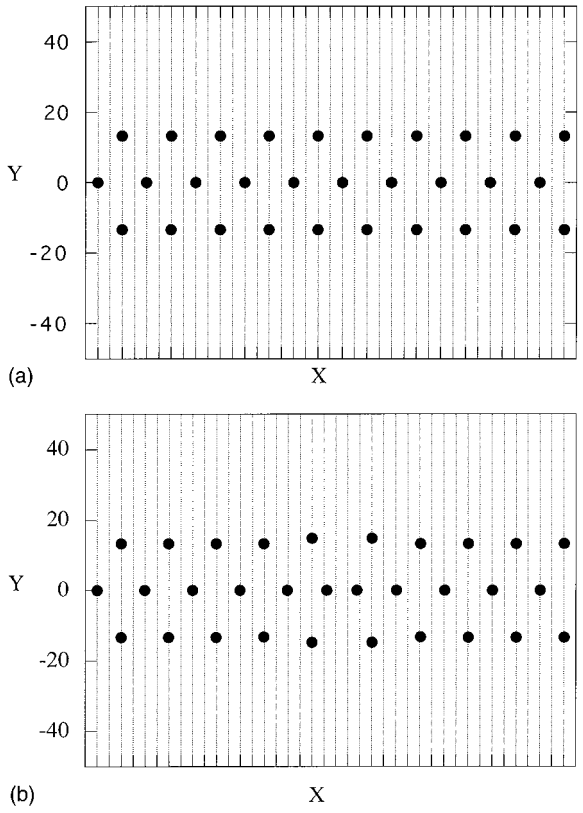

FIG. 3. ''Rhomboidal'' $\theta=3:4$ configurations ($\omega=2.0$, $V_0=4000$). (a) Ground state, (b) kink configuration ($r=3$, $p=4$, $g=1$, $h=1$, $Q=1/4$). The vertical dashed lines show the positions of the minima of the substrate potential $X_i=2\pi i$, $i=1,\ldots,M$.

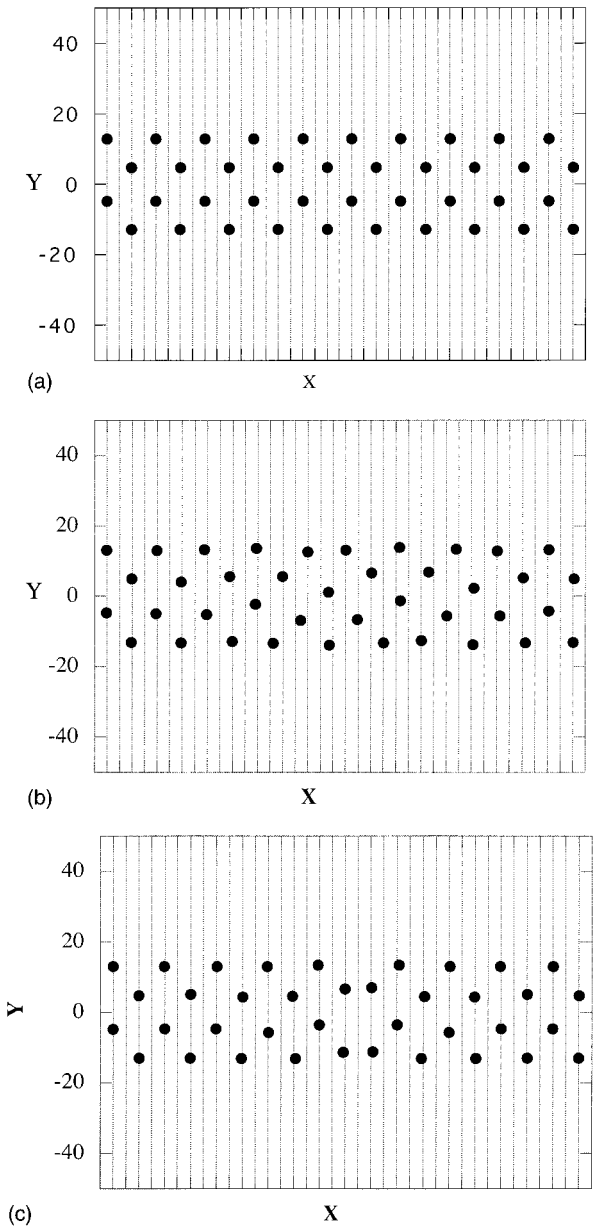

FIG. 4. Structure of ''double zigzag'' $\theta=4:4$ configurations ($\omega=2.0$, $V_0=6660$). (a) Ground state, (b) ''massive'' kink $\{k,k,k,k\}$ ($r=p=4$, $Q=1$, $g=2$), and (c) ''nonmassive'' kink $\{2k,2k,2k,2k\}$ ($r=p=4$, $Q=0$, $g=2$). The vertical dashed lines show the positions of the minima of the substrate potential $X_i=2\pi i$, $i=1,\ldots,M$.

formed numerical simulations for a Frenkel-Kontorova model with a transverse degree of freedom (1,2). Kinks for the ZGS were studied in detail in Ref. 10. In this case, the GS state is additionally doubly degenerated, $j_0=2$, and we have two kinds of kinks, the ''massive'' kink $=\{k,k\}$ with $Q=2/p$ and the ''nonmassive'' kink $=\{k,k\}$ with $Q=0$.

A more complicated case of ''rhomboidal'' $\theta=3:4$ GS, which arises after the second bifurcation in the zigzag-FK model,[12] is shown in Fig. 3. The solution of Eq. (9) is $h=g=1$ in this case, so that the kink structure may be represented as $K=\{k,3k,k\}$.

Finally, Fig. 4 demonstrates configurations for the ''massive'' and ''nonmassive'' kinks for the ''double-zigzag'' $\theta=4:4$ GS, where the point group $\mathscr{G}$ includes the inversion operator J. In this case, we have $j_0=4$ and $g=2$, so that the ''massive'' kink has topological charge $Q=1$ and is characterized by the structure $=\{k,k,k,k\}$, while the ''nonmassive'' kink has the configuration $=\{2k,2k,2k,2k\}$.

In the model under investigation, the atoms may be shifted not only along a given subchain, but also they may be transferred from one subchain to another one. However, the subkinks which form the kink are to be spatially bounded in a localized region, because a displacement of a single subkink from the region of the kink localization leads to an increase of the system energy linearly with this displacement. Thus, in this sense the subkinks are like quarks of the field theory, while the kink, an elementary particle constructed from the quarks.

Note that all topological excitations with the same total topological charge are identical from the topological point of view. For example, the ''massive'' kink shown in Fig. 4(b) has the structure $K=\{k,k,k,k\}$. But the configurations $K=\{k,5k,3k,k\}$ and $K=\{3k,5k,3k,5k\}$ describe the same topological excitation as well. Besides, any subchain may contain additionally any number of k-k pairs. All these configurations are different from the physical viewpoint, in particular, they may be characterized by different potential energies. One of them corresponds to a minimum of the system potential energy, others may correspond to local minima or saddle configurations. Because the configurations with the same topological charge may be transformed to each other in a continuous way, the strategy developed in the present work helps to look for possible trajectories of motion of a kink along the chain. Besides, owing to the intrinsic structure of kinks for a complex GS, the kinks have to have intrinsic (''shape'') modes, which describe oscillations of the subkinks with respect to each other.

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