Zigzag kinks in the Frenkel-Kontorova model with a transversal degree of freedom

Oleg M. Braun

Institute for Physics, Ukrainian Soviet Socialist Republic, Academy of Sciences, 46 Science Avenue, Kiev 252028, U.S.S.R.

Yuri S. Kivshar*

Institute for Low Temperature Physics and Engineering, Ukrainian Soviet Socialist Republic, Academy of Sciences,
47 Lenin Avenue, Kharkov 310164, U.S.S.R.

We consider a generalized (two-dimensional anisotropic) Frenkel-Kontorova model that takes into account a transversal degree of freedom. The model describes a chain of atoms moving in a two-dimensional substrate potential that is periodic along the chain and parabolic in the transversal direction. When the atoms interact by repulsive forces (this is valid, e.g., for adsorbed atoms), the ground state of the commensurate chain becomes zigzag above a certain threshold value. We study the zigzag kinks in such a chain and demonstrate that the transversal degree of freedom breaks the symmetry between the kink and antikink. The applicability of the model to describe surface diffusion in two-dimensional anisotropic layers adsorbed on crystal surfaces is briefly discussed.

The study of nonlinear dynamics in spin- and charge-density-wave systems, atomic monolayers adsorbed on stepped or furrowed crystal surfaces, and magnetic structures has recently been of considerable interest both for experimentalists as well as for theoreticians. Among the variety of phenomenological models proposed to describe such systems, the simple model of a chain of atoms interacting via next-neighbor harmonic forces and placed in a periodic substrate potential, due originally to Frenkel and Kontorova[1] (FK) and developed further by Frank and van der Merwe[2], has proved to be the most suitable for the theoretical description of different nonlinear phenomena: commensurate-incommensurate phase transitions,[3] charge-density-wave propagation,[4] magnetic[5] and ferroelectric[6] domain walls, dislocation dynamics,[2] and kink structures in adsorbed monolayers.[7] The model has been extended in a number of studies to nonzero temperatures,[3] anharmonic or long-range interactions between atoms (see, e.g., Ref. 8), including substrates with a more complicated structure, etc. Most of these studies have, however, been restricted to one spatial dimension. However, the physical systems mentioned above are not, in fact, one dimensional, and investigations of nonlinear phenomena in two-dimensional versions of those models are very important because the two-dimensional models have a lot of features in comparison with their one-dimensional limits and, for example, they allow new types of defects that are only possible in two dimensions (see, e.g., Refs. 9 and 10).

In particular, the study of the mobility of atoms in two-dimensional atomic layers adsorbed on crystal surfaces has a special interest in applied physics.[7,11] But the analysis of an *isotropic* two-dimensional FK model is a rather difficult problem and results may be obtained only by numerical simulations.[9,10] However, in a number of cases, two-dimensional structures may be considered as *anisotropic* ones. For example, this is the case of adsorption of atoms on "furrowed" crystal surfaces, such as the

(112) face of bcc crystals, or the (110) face of fcc crystals, when the surface potential along the furrows is much lower than that in the transversal direction. A similar situation takes place for adsorption on stepped (vicinal) surfaces when substrate atoms on the step have additional unsaturated chemical bonds and, therefore, the atoms are predominantly adsorbed on the step, where their coupling with the substrate is stronger. In such cases, it is natural to assume that the two-dimensional system is an anisotropic one, so that it consists of weakly interacting linear chains. However, these chains cannot be one dimensional because, as is well known (see, e.g., Refs. 7 and 12, and references therein), adsorbed atoms have a charge and they interact by effective repulsive forces. It means that, above a certain threshold, the linear chain may be unstable, so that one has to take into account the transversal degree of freedom.

It is our purpose in this paper to consider the generalized (anisotropic) FK model which takes account of atomic displacements in the transversal direction. We show that, above a certain threshold value, the commensurate structure of the atomic chain with repulsive interactions has a zigzag ground state, and it stipulates a number of features in the kink propagation along the chain. In particular, the transversal degree of freedom leads to an effective anharmonicity in the atomic interactions and it breaks the symmetry between kinks and antikinks which is valid for the one-dimensional FK model with harmonic interparticle interactions. We discuss the applicability of the model to describe surface diffusion in quasi-one-dimensional layers adsorbed on crystal surfaces, and describe some effects which may be explained by the creation of zigzag kinks in adsorbed atomic chains.

Considering the generalized FK model with two degrees of freedom, we assume that the substrate potential is periodic along the chain and parabolic in the transversal direction, so that the Hamiltonian of the chain has the

form (after appropriate scaling)

$$H = \sum_k \left[\tfrac{1}{2}\dot{x}_k^2 + \tfrac{1}{2}\dot{y}_k^2 + (1 - \cos x_k) + \tfrac{1}{2}\omega^2 y_k^2 \right.$$
$$\left. + V_1(r_{k,k-1}) + V_2(r_{k,k-2}) \right] , \qquad (1)$$

where x_k and y_k are the coordinates of the kth atom,

$$r_{k,k'} = [(x_k - x_{k'})^2 + (y_k - y_{k'})^2]^{1/2} ,$$

and ω is the frequency of the transversal oscillations of an isolated atom (we assume that $\omega > 1$). The potentials V_1 and V_2 describe interactions of nearest and next-nearest neighbors in the chain.

The model (1) may be considered as an anisotropic version of the two-dimensional FK model studied numerically by Lomdahl and Srolovitz,[9,10] the transversal substrate potential $\tfrac{1}{2}\omega^2 y_k^2$ being an expansion of a more general potential $\omega^2(1 - \cos y_k)$ for small y_k. The main difference between our model and the mentioned one is the interaction interparticle potentials V_1 and V_2: the potential V_1 is repulsive and, when a zigzag structure arises, the potential V_2 also has to be taken into account.

Straightforward analysis demonstrates that the ground state of the commensurate atomic structure, when each minimum of the periodic substrate potential is occupied by an atom (at a fixed atomic concentration), is not changed in the case of attractions between atoms [Fig. 1(a)], i.e., the ground state is defined by the coordinates $x_k = ka_s = 2\pi k$, $y_k = 0$, where a_s (we assume $a_s = 2\pi$) is the period of the substrate potential. However, in the case of a repulsion, i.e., for $V_1'(a_s) < 0$, the ground state becomes zigzag [see Fig. 1(b)] provided

$$\tfrac{1}{2}\omega^2 + \frac{2}{a_s} V_1'(a_s) < 0 , \qquad (2)$$

and then the atomic coordinates are the following:

$$x_k = ka_s, \quad y_k = (-1)^k b , \qquad (3)$$

where the parameter b is determined by the equation

$$\omega^2 r_0 + 4V_1'(r_0) = 0, \quad r_0 = (a_s^2 + 4b^2)^{1/2} .$$

As a result, the chain may be considered as two subchains with opposite positions of nearest atoms [see Fig. 1 (b)].

The further increase of the repulsion between nearest neighbors leads to an instability of the ground state (3).

provided

$$1 + 4V_1''(r_0) - \left[\frac{2b}{a_s} \right]^2 (\omega^2 - 1) \leq 0 \qquad (4)$$

with respect to shifts of subchains in the opposite directions along the chain. Moreover, unlike in the one-dimensional chain, in the generalized FK model (1) with repulsive interactions between the finite number of interacting neighbors, the physically reasonable ground state corresponds to a local minimum of the potential energy because rearrangements of atoms in the chain will lead to a decrease of the energy. Besides, the repulsion of next-nearest, next-next-nearest, etc., neighbors may lead to appearance of a set of more complicated ground states: zigzag, sub zigzag, etc. As a result, to describe all of these states, the rigorous model should take into account interactions between all atoms in the chain. Here we will consider, for simplicity, the situation when only two different ground states may exist [see Figs. 1(a) and 1(b)].

Let us now investigate a topologically stable excitation of the chain in the form of a kink (antikink) that corresponds to the minimal possible compression (expansion) of the commensurate atomic structure. For the one-dimensional FK chain, the kink and antikink structures are shown in Figs. 1(c) and 1(e), respectively. It is important to note that, for the one-dimensional FK model with harmonic potentials $V_1(r)$ and $V_2(r)$, the parameters of a kink and antikink are the same. However, in the two-dimensional FK model with the zigzag ground state, the parameters of a kink and antikink [see Figs. 1(d) and 1(f)] will be drastically changed and, as it will be seen from the subsequent analysis, they are different even for harmonic interactions between atoms in the chain.

To calculate the kink parameters in the generalized FK model (1), let us introduce the new variables u_k and v_k defined as

$$x_k = ka_s + u_k, \quad y_k = (-1)^k (b + v_k) . \qquad (5)$$

When the displacements u_k and v_k slowly depend on k, i.e., when $|u_{k+1} - u_k| \ll a_s$, $|v_{k+1} - v_k| \ll a_s$, and $|v_k| \ll a_s$, we can expand the potentials $V_1(r)$ and $V_2(r)$ in the Taylor series up to the third-order terms in the differences $r^2 - r_0^2$ and $r^2 - r_1^2$, respectively, where $r_0 \equiv (a_s^2 + 4b^2)^{1/2}$ and $r_1 = 2a_s$. Taking into account those expansions, we may reduce the Hamiltonian (1) to the following form (we take here $a_s = 2\pi$):
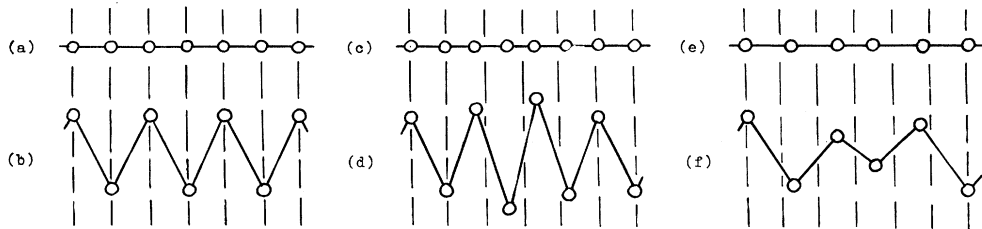

FIG. 1. Comparison of the ground states [(a) and (b)], kinks [(c) and (d)], and antikinks [(e) and (f)] for the one-dimensional [(a), (c), and (e)] and generalized [(b), (d), and (f)] Frenkel-Kontorova models. Dashed lines show minima of the substrate periodic potential.

$$H = \sum_k \left[\tfrac{1}{2}\dot{u}_k^2 + \tfrac{1}{2}\dot{v}_k^2 + (1-\cos u_k) + \tfrac{1}{2}A_1(u_{k+1}-u_k)^2 + \tfrac{1}{2}g_1(u_{k+2}-u_k)^2 + \tfrac{1}{2}(\omega^2+4g)(2b/r_0)^2 v_k^2 \right.$$

$$+ \tfrac{1}{2}A_2(v_{k+1}-v_k)^2 + 2A_2 v_k(v_{k+1}-v_k) - \tfrac{1}{8}\omega_1^2(v_{k+2}-v_k)^2 + A_3(u_{k+1}-u_k)^3$$

$$+ \tfrac{1}{4}(\omega^2+4g)(4\pi b/r_0^2)(u_{k+1}-u_k)(v_{k+1}+v_k) + A_4(u_{k+2}-u_k)^3 + A_5(v_{k+1}+v_k)^3$$

$$+ A_6(u_{k+1}-u_k)^2(v_{k+1}+v_k) + A_7(u_{k+1}-u_k)(v_{k+1}+v_k)^2$$

$$\left. + (1/32\pi)(\omega_1^2+4g_1)(u_{k+2}-u_k)(v_{k+2}-v_k)^2 \right] , \tag{6}$$

where we have introduced the notations

$$g = V_1''(r_0), \quad g_1 = V_2''(r_1) , \quad \omega_1^2 = -4V_2'(r_1)/r_1, \quad A_1 = g(2\pi/r_0)^2 - \tfrac{1}{4}\omega^2(2b/r_0)^2 ,$$

$$A_2 = g(2b/r_0)^2 - \tfrac{1}{4}\omega^2(2\pi/r_0)^2, \quad A_3 = \frac{1}{8r_0}(2b/r_0)^2(2\pi/r_0)(\omega^2+4g) + \tfrac{1}{6}(2\pi/r_0)^3 V_1'''(r_0) ,$$

$$A_4 = \tfrac{1}{6}V_2'''(r_1) , \quad A_5 = \frac{1}{8r_0}(2\pi/r_0)^2(2b/r_0)(\omega^2+4g) + \tfrac{1}{6}\left[\frac{2b}{r_0}\right]^3 V_1'''(r_0) , \tag{7}$$

$$A_6 = \frac{1}{8r_0}(2b/r_0)[1-3(2\pi/r_0)^2](\omega^2+4g) + [b(2\pi)^2/r_0^3]V_1'''(r_0) ,$$

$$A_7 = (\pi/4r_0^2)[1-3(2b/r_0)^2](\omega^2+4g) + [\pi(2b)^2/r_0^3]V_1'''(r_0) .$$

In the continuum limit, the Hamiltonian (7) yields the following equations of motion:

$$u_{tt} - (2\pi)^2(A_1+4g_1)u_{xx} + \sin u - (4\pi^2 b/r_0^2)(\omega^2+4g)v_x$$

$$-6(2\pi)^3(A_3+8A_4)u_x u_{xx} - 16\pi A_7 vv_x - 16\pi^2 A_6(u_{xx}v+u_x v_x) = 0 , \tag{8a}$$

$$v_{tt} + (2b/r_0)^2(\omega^2+4g)v + 24A_5 v^2 + (4\pi^2 b/r_0^2)(\omega^2+4g)u_x + 8\pi^2 A_6 u_x^2 + 16\pi A_7 vu_x = 0 . \tag{8b}$$

In the lowest approximation from Eq. (8b) it follows that

$$v(x,t) \approx -(\pi^2/b)u_x(x,t) , \tag{9}$$

the relation being valid for $b \simeq 1$. Then, substituting Eq. (9) into Eq. (8a), we obtain the perturbed sine-Gordon (SG) equation

$$u_{tt} + \sin u - D^2 u_{xx}(1-\alpha D u_x) = 0 , \tag{10}$$

where $D \equiv 2\pi(4g_1 - \tfrac{1}{4}\omega^2)^{1/2}$ (11a)

and $\alpha \equiv -D^{-3}[(4\pi)^3 V_2'''(r_1) + (\pi^2/b)^2(\omega^2+4g)]$. (11b)

The perturbed SG equation has the kink solution which, for $\alpha \ll 1$, may be found, e.g., by the perturbation theory (see, e.g., Ref. 13)

$$u_k(x) = 4\tan^{-1}\exp(-\sigma x/D)$$

$$+ \tfrac{4}{3}\alpha\frac{\tan^{-1}[\sinh(x/D)]}{\cosh(x/D)} , \tag{12}$$

The effective width of the kink $(\sigma = +1)$ or antikink $(\sigma = -1)$ in that case is

$$D_{\text{eff}} = D(1 + \tfrac{1}{3}\alpha\pi\sigma) , \tag{13}$$

and it depends sufficiently on the anharmonicity parameter α. As is seen from Eq. (13), the values D_{eff} for the kink and antikink are different. The similar dependences are valid for the effective mass of the kink

$$m_{\text{eff}} = (4/\pi D)(1 - \tfrac{1}{6}\sigma\pi\alpha) , \tag{14}$$

and the effective periodic potential stipulated by the discretenesses effects (the so-called Peierls-Nabarro potential)

$$(\epsilon_p)_{\text{eff}} \simeq \epsilon_p(D) + \tfrac{1}{3}\sigma\pi\alpha D\frac{d\epsilon_p(D)}{dD} , \tag{15}$$

where (see, e.g., Ref. 8, and references therein)

$$\epsilon_p(D) \simeq \tfrac{2}{3}\frac{(\pi D)^2}{\sinh(\pi D/2)}(1+2/D^2) . \tag{16}$$

It is important to compare the obtained results with those for the one-dimensional FK model. In that case, the FK model is described (in the continuum limit) by the same SG equation (10) but with the parameters D_0 and α_0 (instead of D and α),

$$D_0 = 2\pi(g+4g_1)^{1/2} , \tag{17a}$$

$$\alpha_0 = -(2\pi/D_0)^3[V_1'''(r_0) + 8V_2'''(r_1)] . \tag{17b}$$

As can be seen from (17b), the asymmetry of the kink and antikink in that case is caused by the anharmonicity of the interactions between atoms ($\sim V'''$). Unlike that case, the zigzag chain stipulates the asymmetry for any type of interactions [cf. Eqs. (17b) and (11b)]. To demonstrate the differences, we present our results in two physically important cases.

Harmonic interactions. In the simplest case we put $V_1(r) = \tfrac{1}{2}g(r-a)^2$, $V_2(r) = \tfrac{1}{2}g_1(r-a_1)^2$, $a_1 = 2a_s$. The one-dimensional kinks are characterized by the parameters $D_0 = 2\pi(g+4g_1)^{1/2}$ and $\alpha_0 = 0$. These kinks exist provided $a < a_{\text{cr}} \equiv 2\pi(1+\omega^2/4g)$. The zigzag ground state arises in the region ($\omega^2 > 1$)

$$a_{\text{cr}} < a < \tilde{a}_{\text{cr}} \equiv a_{\text{cr}}\left[\frac{\omega^2+4g}{\omega^2-1}\right]^{1/2} ,$$

and, in this case, the kink parameters are

$$D = 2\pi(4g_1 - \tfrac{1}{4}\omega^2)^{1/2} \ ,$$

$$\alpha = -\frac{ga_{\mathrm{cr}}^3}{(2\pi)^2(a^2 - a_{\mathrm{cr}}^2)(4g_1 - \tfrac{1}{4}\omega^2)^{3/2}} \ .$$

As a result, the zigzag structure of the kink leads to an effective anharmonicity ($\alpha \neq 0$) unlike to the one-dimensional chain.

Long-range power interactions. As is well known,[8,12] in many cases the interaction between atoms chemisorbed on a crystal surface may be described by the power law $V_1(r) = V_2(r) = V_0(a_s/r)^n$, where $n = 1$ or 3, V_0 being a constant parameter. In such a case, the one-dimensional kink has the parameters[8] $D_0 = [V_0 n(n+1)(1+2^{-n})]^{1/2}$, $\alpha_0 = (n+2)/D_0$. In the extended model, the zigzag ground state arises provided $V_0 > (\pi\omega)^2/n$ and the zigzag kinks are characterized by the parameters

$$D = (\pi\omega)[\gamma(n+1)/2^n - 1]^{1/2} \ ,$$

$$\alpha = (n+2)(\pi\omega)^2[2^{-n}\gamma(n+1) - (\gamma^{2/(n+2)} - 1)^{-1}]/D^3 \ ,$$

where $\gamma \equiv nV_0/(\pi\omega)^2 > 1$. It is important to note that the anharmonicity parameter α may change its sign. (Strictly speaking, to have a rigorous model in the latter case, the interactions between all atoms of the chain should be taken into account; see, e.g., Ref. 8.)

Thus, the creation of the zigzag ground state in the chain leads to a drastic decreasing of the kink width and, moreover, to changing of the sign of the anharmonicity parameter. The effects are especially important near the critical conditions when the one-dimensional ground state becomes unstable. In this case, the ground state corresponds to the one-dimensional chain [Fig. 1(a)], but the kink has the zigzag structure shown in Fig. 2. Unfortunately, such a case cannot be investigated analytically in the lowest approximation used above because the parameter b in this case is small.

Finally, we briefly discuss the applicability of the model to describe surface diffusion of atoms adsorbed on stepped or furrowed crystal surfaces when a monolayer of atoms may be considered as a system of weakly interacting FK chains. When the concentration θ of the adatoms is slightly lower than the value θ_0 corresponding to a commensurate structure, the mass transport along the chains may be treated as propagation of antikinks (or
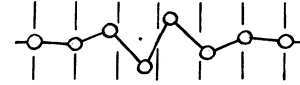

FIG. 2. Structure of the zigzag kink near the critical value of the interatomic repulsion. That shown is the same as in Fig. 1.

kinks when $\theta \gtrsim \theta_0$). While the FK chains of adatoms are exactly one dimensional, the anharmonicity parameter α_0 is positive and the activation energy for the surface diffusion, ϵ_p, decreases jump-likely with increasing of the parameter θ when it passes the values $\theta_0^{(n)}$ corresponding to a set of commensurate structures of the chain, n being the ratio of the periods of the chain and substrate. As a result, the dependence $\epsilon_p(\theta)$ has to be of a form which is similar to the reverse devil's staircase (see the discussions of such a dependence in Ref. 8). However, increasing the concentration θ leads to increasing repulsion forces between adatoms and, therefore, at some critical value θ_{cr} (which has to be a function of the parameter ω), the kink structure is changed from that shown in Fig. 1(c) to that shown in Fig. 2, and then to that shown in Fig. 1(d). At $\theta \gtrsim \theta_{\mathrm{cr}}$, jumps of the function $\epsilon_p(\theta)$ corresponding to the commensurate structures will decrease or they may change their signs so that the activation energy will increase jump-likely when θ is changing through the values $\theta_0^{(n)}$ ($\theta_0^{(n)} > \theta_{\mathrm{cr}}$). We believe that the experimental observations of these effects could directly prove the soliton mechanism of the surface diffusion of adsorbed atoms.

In conclusion, we have considered the generalized FK model, which includes a transversal degree of freedom. The most interesting result is the threshold creation of the zigzag ground state of the commensurate chain and propagation of zigzag kinks in this structure. We have studied properties of the zigzag kink (antikink) in the continuum limit and have demonstrated that the parameters of the kink and antikink are different for any type of interatomic interactions due to effective anharmonicity stipulated by an effective coupling of two degrees of freedom. The obtained results may be useful to directly prove a solitonic mechanism of surface diffusion of atoms adsorbed on stepped or furrowed crystal surfaces.

*Present address: Departamento de Física Teórica I, Facultad de Ciencias Físicas, Universidad Complutense 28040 Madrid, Spain.

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