

Frenkel-Kontorova model with a transversal degree of freedom: Static properties of kinks

Oleg M. Braun

Institute of Physics, Ukrainian Academy of Sciences, 252028 Kiev, Ukraine

Oksana A. Chubykalo

Departamento de Física Teórica I, Facultad de Ciencias Físicas, Universidad Complutense, E-28040 Madrid, Spain

Yuri S. Kivshar*

Institut für Theoretische Physik I, Heinrich-Heine Universität Düsseldorf, D-4000 Düsseldorf 1, Germany

Luis Vázquez

Departamento de Física Teórica I, Facultad de Ciencias Físicas, Universidad Complutense, E-28040 Madrid, Spain

(Received 8 October 1992)

We consider a generalized Frenkel-Kontorova (FK) model with a transversal degree of freedom proposed by Braun and Kivshar [Phys. Rev. B **44**, 7694 (1991)]. The model describes an atomic chain subjected to a two-dimensional (2D) substrate potential that is periodic in one direction and parabolic in the transversal direction, the interatomic interaction being exponentially repulsive. The ground state of the system undergoes a phase transition from the trivial one-dimensional (1D) to a quasi-2D state when the repulsion exceeds a certain critical value. The quasi-2D ground state admits two different types of kinks, “massive,” kinks which may be considered as a generalization of the kinks of the standard 1D FK chain, and “nonmassive,” (phase) kinks which appear to be due to dimerization of the ground state. We investigate the static characteristics of these two kinds of kinks (the kink effective mass, the kink rest energy, and the height of the Peierls-Nabarro potential) analytically as well as by means of numerical simulations when the chain with the periodic boundary conditions contains a single kink. In particular, we show that the “massive” kinks may be described in the continuum approximation by a perturbed sine-Gordon equation while properties of the “nonmassive” kinks may be analyzed within the framework of an effective ϕ^4 model derived for translational displacements. The role of the transversal degree of freedom in mass-transport properties of the generalized FK model applied to describe surface diffusion is also discussed.

I. INTRODUCTION

The well-known Frenkel-Kontorova (FK) model describes a chain of atoms interacting with harmonic forces and subject to one-dimensional sinusoidal potential. Introduced first as the simplest model for dislocations in solids,^{1,2} it was then successfully used to describe the charge-density waves in quasi-one-dimensional conductors (see, e.g., references in Ref. 3), the commensurate-incommensurate phase transitions,⁴ the “solitonic” diffusion in two-dimensional (2D) layers of atoms adsorbed on a crystal surface,⁵ the dynamics of domain walls in magnetic systems (see, e.g., Ref. 6), etc.

In applications to real physical objects, the FK model should be generalized. In particular, we would like to mention investigations of the FK model with a nonsinusoidal substrate potential^{7,8} and with an anharmonic^{8,9} or nonconvex¹⁰ interaction potential. However, one of the most serious restrictions of the standard FK model is the assumption of one-dimensional motion of atoms in the chain. Obviously, in real physical systems atoms can move in two (or three) directions, and the correspond-

ing generalization of the model to take into account the transversal degrees of freedom is of great interest. In particular, we should mention investigations of the scalar¹¹ and vector^{12,13} variants of the model, both of which describe an *isotropic* 2D layer of atoms.

However, since 2D versions of the FK model are too complicated, it is interesting to investigate a quasi-2D variant of the model where atoms in the chain are allowed to move in two directions, but the chain itself is still one dimensional. The corresponding model has been recently proposed in Ref. 14. It describes a chain of interacting atoms, subjected to the two-dimensional potential which is periodic in one direction and parabolic in the transversal direction. It was predicted that the trivial one-dimensional ground state (GS) becomes unstable and it is transferred into the dimerized GS when the repulsion between the atoms increases. Close to a certain transition point, as well as above this point, properties of the FK model are essentially changed; in particular, the kink-antikink symmetry is violated even for the harmonic interatomic interactions.¹⁴

The purpose of the present paper is to investigate the

model proposed in Ref. 14 both analytically and numerically. Here we consider only static properties of the atomic chain containing a single kink. The paper is organized as follows. In Sec. II we introduce the FK model with a transversal degree of freedom and also describe the ground state of the system and two types of the kinks (“massive” and “nonmassive”) existing for these ground states. We also introduce the main quantities (the kink mass, the kink energy, and the height of the Peierls-Nabarro potential) which characterize static properties of kinks. In Sec. III we present analytical estimations for these quantities based on the continuum approximation and the perturbation theory approach. In particular, we show that the massive kink in the continuum approximation may be described within the framework of the sine-Gordon equation while the nonmassive kink is described by a version of the ϕ^4 model. In Sec. IV we present the numerical method used and the results of simulations. Finally, Sec. V concludes the paper.

II. THE MODEL

Let us consider an atomic chain subjected to a two-dimensional potential *periodic* in one direction and *parabolic* in the transversal direction. The substrate potential energy is

$$V_{\text{sub}} = \frac{1}{2} \sum_l \left\{ \varepsilon_s \left[1 - \cos \left(\frac{2\pi x_l}{a_s} \right) \right] + m_a \omega^2 y_l^2 \right\}, \quad (1)$$

where the index l numerates atoms, $r_l = (x_l, y_l)$ is the atomic coordinate, ε_s is the amplitude and a_s is the period of the substrate potential, m_a is the atomic mass, and ω is the frequency of a single atom vibration in the transversal direction. The model (1) describes, for example, the potential energy of the atoms adsorbed on furrowed or stepped crystal surfaces (see, e.g., examples and references in Refs. 5, 8, and 15).

The limit $\omega \rightarrow \infty$ corresponds to the standard one-dimensional (1D) case. In order to have the model (1) well defined we have to assume that the frequency of the transversal vibrations, ω , exceeds the frequency of longitudinal vibrations, $\omega_0 = (\varepsilon_s/2m)^{1/2}(2\pi/a_s)$. Further it will be convenient to use the units $m_a = 1$, $a_s = 2\pi$, and $\varepsilon_s = 2$ so that $\omega_0 = 1$.

We consider the “fixed-density” FK model; i.e., we place the atomic chain of the length L consisting of N atoms into the potential (1), which has M minima on the distance L , and we assume the periodic boundary conditions

$$x_{l+N} = x_l + M a_s, \quad (2)$$

$$y_{l+N} = y_l.$$

In this paper we concentrate on the commensurate situation when $M = N$ or $M = N \pm 1$, and N is large enough ($N \gg 1$).

Let us assume that the atoms in the chain repel each other according to an exponential (Toda-like) law (the attraction branch of the interaction potential does not lead to new phenomena for static properties)

$$V(r) = V_0 \exp(-\beta r), \quad (3)$$

where V_0 is the amplitude of the potential and the parameter $1/\beta$ characterizes the length of interaction, r being the interatomic distance. The potential (3) describes, for example, the “direct” mechanism of interatomic interactions¹⁶ which is similar to the usual chemical bonding.

Recall that the main advantage of the one-dimensional model is that atoms in it are always ordered; i.e., the atom with the number l has always two nearest neighbors with the numbers $l \pm 1$ only. However, this is not the case for two-dimensional models because in that situation any two atoms may be replaced by going through the second direction. Additionally, for a model such as that given by Eqs. (1) and (3), in general, we have to take into account the interaction between *all* the atoms in the chain. However, if the potential (3) decays quickly enough, i.e., $\beta a_A \gg 1$, where $a_A = L/N$ is the mean interatomic distance, we may restrict ourselves by the interaction of a finite number of neighboring atoms. It is clear that if $N = M$ and the ratio V_0/ω is low enough, the GS of the system is trivial: Each potential well is occupied by a single atom. When the value V_0 increases (or ω decreases) and exceeds the threshold value V_0^* (or ω^*), the trivial GS becomes unstable and it will form a dimerized GS (DGS). With a further increase of V_0 the consequences of transitions to higher-order GS structures are expected to take place. However, in this paper we restrict ourselves to the case where only trivial and dimerized GS's exist. As has been shown in Ref. 14, in this case it is enough to take into account only interactions between nearest and next-nearest neighbors.

Thus, in dimensionless units the model Hamiltonian has the form

$$H = \sum_l \left\{ \frac{1}{2} (\dot{x}_l^2 + \dot{y}_l^2) + (1 - \cos x_l) + \frac{1}{2} \omega^2 y_l^2 + V(r_{l,l+1}) + V(r_{l,l+2}) \right\}, \quad (4)$$

where $r_{l,m} = [(x_l - x_m)^2 + (y_l - y_m)^2]^{1/2}$.

The GS configuration corresponds to an absolute minimum of the potential energy of the system. When $\omega > \omega^*$ (or $V_0 < V_0^*$), where the value ω^* is determined by the expression

$$\omega^{*2} = -\frac{2}{\pi} V'(a_s) \equiv \frac{2}{\pi} V_0 \beta e^{-2\pi\beta}, \quad (5)$$

the ground-state configuration is trivial (TGS):

$$x_l = l a_s, \quad y_l = 0. \quad (6)$$

For the case of the TGS, a kink (an antikink) excitation is defined as a minimally possible topologically stable compression (expansion) of the chain when the atomic positions at the infinities are the same as in the GS. In other words, a kink (an antikink) connects two GS's: One GS, for the left part of the chain, is described by Eqs. (6), and the other GS, for the right part of the chain, is obtained by the shift $x_l \rightarrow x_l - a_s$ (or $x_l \rightarrow x_l + a_s$ for an antikink). For $\omega > \omega^*$ the antikink structure is the same as in the

standard (one-dimensional) FK model. The same is true for a kink if $\omega > \omega_k^*$, where ω_k^* ($\omega_k^* > \omega^*$) is a certain critical value (see below). As has been predicted in Ref. 14, at $\omega^* < \omega < \omega_k^*$ the kink structure becomes more complicated: In the region of the kink, where the chain is more compressed, the nearest-neighboring atoms begin to escape from the potential minima in the opposite *transversal* directions in order to increase the interatomic distances and, thus, to decrease the repulsion energy. This effect will lead to dramatic changes in properties kink and antikink.

When $\omega < \omega^*$ (or $V_0 > V_0^*$) the TGS becomes unstable, and it is transformed into a dimerized GS (DGS)

$$x_l = la_s, \quad y_l = (-1)^l b, \quad (7)$$

where the parameter b is determined by the equation¹⁴

$$\omega^2 r_0 + 4V'(r_0) = 0, \quad r_0 = (a_s^2 + 4b^2)^{1/2}. \quad (8)$$

Note that the further decrease of ω or increase of V_0 leads to an instability of the DGS, and if we take into account the interaction of more neighbors, it is transformed into more complicated GS's such as subdimerized, sub-subdimerized, etc. However, we will not discuss here transitions from the DGS to these more complicated GS's, because their correct description requires the account of interaction of all the atoms in the chain. The DGS is additionally doubly degenerated: If we designate the GS (7) as GS₁, we can also introduce GS₂ by $x_l \rightarrow x_l - a_s$, GS₃ by $x_l \rightarrow x_l + a_s$, GS₄ by $y_l \rightarrow -y_l$, etc.

The standard FK kink connects GS₁ and GS₂ (see Fig. 1), and the antikink connects GS₁ and GS₃ (see Figs. 2 and 3). We will call these types of excitations as “*massive*” kink (MK) and *antikink* (MAK), because

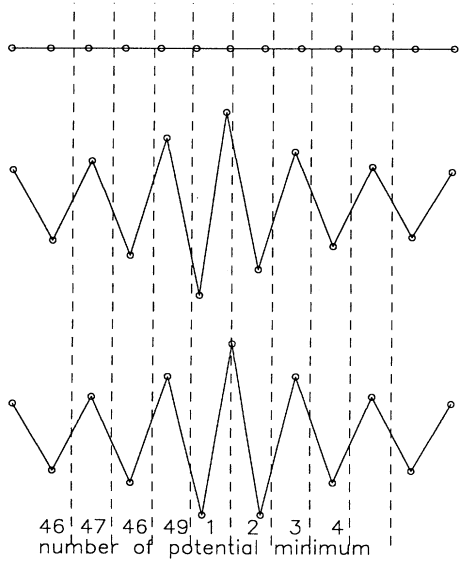


FIG. 1. Shape of the “massive” kink for (a) $\omega > \omega_k^*$, (b) $\omega < \omega^*$ ($\omega = 2.3$), the ground-state configuration, and (c) $\omega < \omega^*$ ($\omega = 2.3$), the saddle configuration. The dashed lines show the positions of substrate maxima.

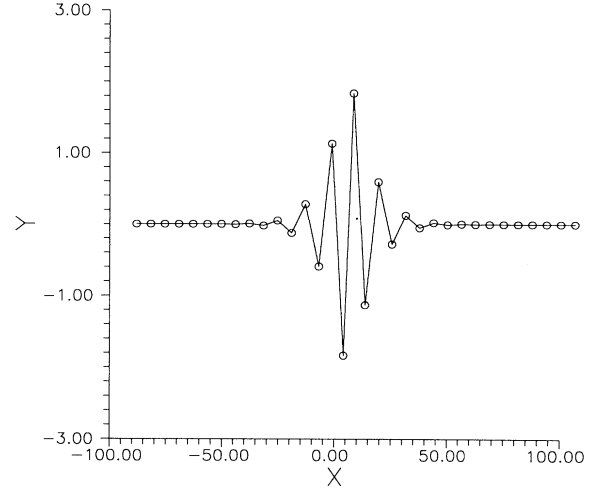


FIG. 2. Shape of the “massive” dimerized kink on the background of trivial ground state for $\omega^* < \omega < \omega_k^*$ ($\omega = 2.6$).

they are responsible for mass transport along the chain. Besides, the DGS admits the existence of a new type of kinks, which connect GS₁ and GS₄ (see Fig. 4). We will call these kinks as “*nonmassive*” kink and *antikink* (NMK and NMAK). Note that the parameters of NMK and NMAK are identical even for the anharmonic interaction potential. In some sense, in terms of the two-dimensional defects discussed in Refs. 12 and 13 the MK can be called *edge* and NMK *screw*. Unlike the case of the 1D FK model with the double substrate potential, where we also have two different types of kinks, we now have no topological constraints on the consequence of kinks; for example, two massive kinks may follow one another. If,

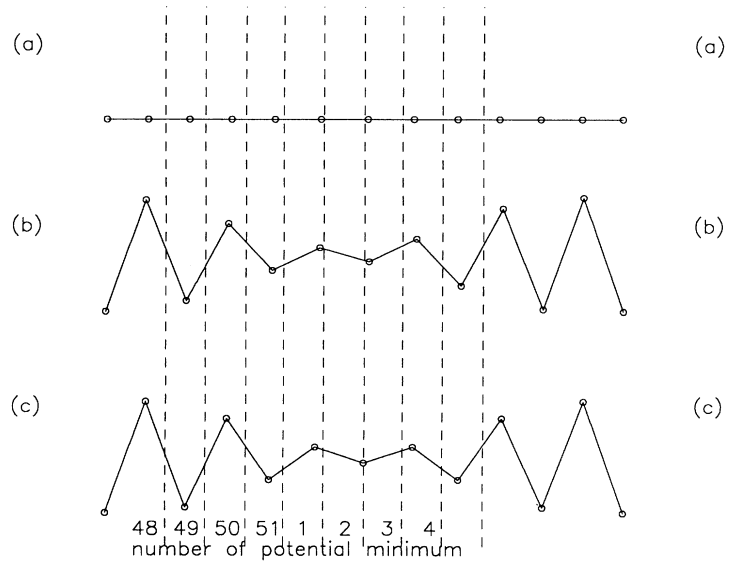


FIG. 3. Shape of “massive” antikink for (a) $\omega > \omega^*$, (b) $\omega < \omega^*$ ($\omega = 2.0$), the ground-state configuration, and (c) the saddle configuration. The dashed lines show the positions of substrate maxima.

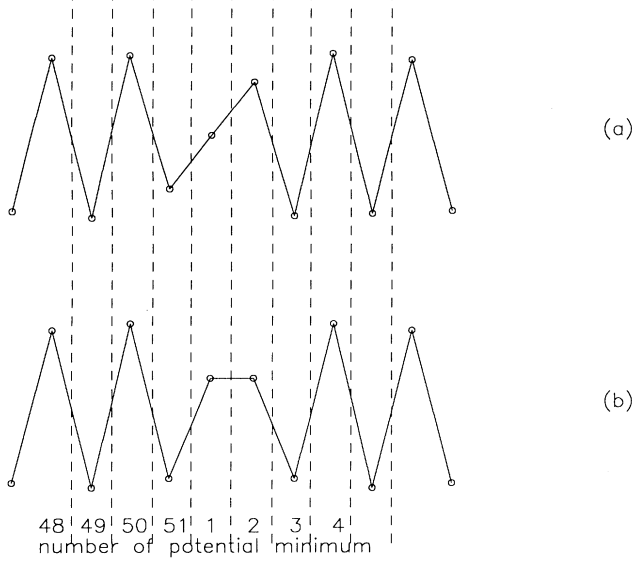


FIG. 4. Shape of “nonmassive” kinks for $\omega = 2.3$ (a) ground-state configuration, (b) saddle configuration.

however, we insert one additional atom into the DGS of the infinite chain and then allow the chain to relax, two kinks, namely, a MK and NMK, will be created simultaneously.

We will characterize the GS by the potential energy per one atom, E_0 . For the TGS we have

$$E_0(\text{TGS}) = V(a_s) + V(2a_s), \quad (9)$$

and for the DGS,

$$E_0(\text{ZGS}) = V(r_0) + V(2a_s) + \frac{1}{2}\omega^2 b^2. \quad (10)$$

As usual, a kink can be characterized by its energy E_k , by the effective mass m_{eff} , and by the amplitude of the Peierls-Nabarro (PN) potential, ε_{PN} . The rest energy of a kink can be defined as

$$E_k = E_{\text{min}}(N) - NE_0, \quad N \rightarrow \infty, \quad (11)$$

where $E_{\text{min}}(N)$ is the minimum value of the potential energy of the N atomic chain with a single kink.

Analogously to the standard FK model, a kink can be transferred along the chain. The minimum energy which is necessary to overcome in order to shift the kink on the distance a_s is known as the PN energy. It may be calculated as

$$\varepsilon_{\text{PN}} = E_{\text{saddle}}(N) - E_{\text{min}}(N), \quad N \rightarrow \infty, \quad (12)$$

where $E_{\text{saddle}}(N)$ corresponds to the potential energy of the saddle configuration of the chain with the kink. The saddle and minimum kink configurations can be connected by various trajectories; the most interesting trajectory is the adiabatic one which is defined by a set of differential equations,¹⁷

$$\frac{\partial x_l}{\partial \tau} = -\frac{\partial V_{\text{tot}}}{\partial x_l}, \quad \frac{\partial y_l}{\partial \tau} = -\frac{\partial V_{\text{tot}}}{\partial y_l}, \quad l = 1, \dots, N, \quad (13)$$

where τ is a parameter along the trajectory and V_{tot} is the total potential energy of the system. As the system moves along the adiabatic trajectory, the kinetic energy of the chain takes the form

$$\begin{aligned} K &= \frac{1}{2}m_a \sum_{l=1}^N (\dot{x}_l^2 + \dot{y}_l^2) \\ &= \frac{1}{2}m_a \sum_{l=1}^N \left[\left(\frac{\partial x_l}{\partial X} \frac{dX}{dt} \right)^2 + \left(\frac{\partial y_l}{\partial X} \frac{dX}{dt} \right)^2 \right] \\ &= \frac{1}{2}m_{\text{eff}} \left(\frac{dX}{dt} \right)^2, \end{aligned} \quad (14)$$

where we have introduced the coordinate of the kink center⁸

$$X = \sum_l x_l + \text{const}, \quad (15)$$

and the effective mass¹⁷

$$m_{\text{eff}}(X) = m_a \sum_{l=1}^N \left[\left(\frac{\partial x_l}{\partial X} \right)^2 + \left(\frac{\partial y_l}{\partial X} \right)^2 \right]. \quad (16)$$

Thus, the aim of the next sections of the paper is to calculate parameters of MK, MAK, and NMK analytically and by means of numerical simulations.

III. ANALYTICAL APPROACH

A. One-dimensional “massive” kinks

As is well known, in the case of a strong interatomic interaction, i.e., when $g \equiv \sqrt{V''(a_s)} \gg 1$, the continuum limit may be used to reduce the motion equations describing the 1D FK model to the sine-Gordon (SG) equation with a correction term due to anharmonicity of the interparticle interaction,^{8,9}

$$u_{tt} - D_0^2 u_{xx} (1 - \alpha_0 u_x) + \sin u = 0, \quad (17)$$

where

$$D_0 = 2\pi[V''(a_s) + 4V''(2a_s)]^{1/2}, \quad (18)$$

$$\alpha_0 = -\left(\frac{2\pi}{D_0}\right)^3 [V'''(a_s) + 8V'''(2a_s)] \quad (19)$$

(for 1D kinks we use the subindex “zero”). For the potential (3) these formulas are reduced to the following expressions:

$$D_0 = \sqrt{2\pi V_0 \beta} e^{-\pi\beta} (1 + 4e^{-2\pi\beta})^{1/2} \quad (20)$$

and

$$\alpha_0 = \left(\frac{2\pi\beta}{D_0}\right)^3 V_0 e^{-2\pi\beta} [1 + 8e^{-2\pi\beta}]. \quad (21)$$

As has been shown in Ref. 8, anharmonicity of the interatomic potential breaks the symmetry between a kink and antikink. Namely, we have (see Ref. 8)

$$m_{\text{eff}} = \frac{4}{\pi D_0} \left(1 - \frac{1}{6} \sigma \pi \alpha_0 \right), \quad (22)$$

where $\sigma = +1$ for the MK or $\sigma = -1$ for the MAK, and

$$E_k \simeq \frac{1}{2\pi} \{ 8D_0 - 2\sigma\pi^2 [2V'(a_s) + V'(2a_s)] - \frac{1}{3} \alpha_0 \sigma \pi D_0 \}. \quad (23)$$

It is clear that the results (18)–(23) remain valid for the model (1) as long as it is one dimensional, namely, for the MK, if $\omega > \omega_k^*$, and for the MAK, if $\omega > \omega^*$.

B. Dimerized “massive” kinks

When $\omega < \omega^*$ the calculation of the kink parameters for the DGS is more complicated than for the 1D FK

chain, because now we have two strongly coupled subchains. But in the case $b \simeq a_s$ the interatomic interactions are strong, and we can again try to use an approximation of slowly varying envelopes.

To calculate the kink parameters in the case of the DGS we will use the approach proposed in Refs. 14 and 18 introducing two new variables u_l and v_l as

$$x_l = la_s + u_l, \quad y_l = (-1)^l (b + v_l). \quad (24)$$

When the displacements u_l and v_l vary slowly, i.e., when $|u_l - u_{l-1}| \ll a_s$, $|v_l - v_{l-1}| \ll a_s$, and $|v_l| \ll a_s$, we may expand the potential $V(r)$ in a Taylor series up to terms of third order in the differences to obtain a system Hamiltonian in the form¹⁴

$$\begin{aligned} H = \sum_l \left[\frac{1}{2} \dot{u}_l^2 + \frac{1}{2} \dot{v}_l^2 + (1 - \cos u_l) + \frac{1}{2} \omega^2 v_l^2 + \omega^2 b v_l - \frac{\pi \omega^2}{2} (u_l - u_{l-1}) - \frac{b \omega^2}{2} (v_l + v_{l-1}) - \pi \omega_1^2 (u_l - u_{l-2}) \right. \\ \left. + \frac{1}{2} A_1 (u_l - u_{l-1})^2 + \frac{1}{2} A_2 (v_l + v_{l-1})^2 + \frac{\pi b}{r_0^2} (\omega^2 + 4g) (u_l - u_{l-1}) (v_l + v_{l-1}) - \frac{\omega_1^2}{8} (v_l - v_{l-2})^2 \right. \\ \left. + \frac{1}{2} g_1 (u_l - u_{l-2})^2 + A_3 (u_l - u_{l-1})^3 + A_4 (u_l - u_{l-2})^3 + A_5 (v_l + v_{l-1})^3 + A_6 (u_l - u_{l-1})^2 (v_l + v_{l-1}) \right. \\ \left. + A_7 (u_l - u_{l-1}) (v_l + v_{l-1})^2 + \frac{1}{32\pi} (\omega_1 + 4g_1) (u_l - u_{l-2}) (v_l - v_{l-2})^2 \right], \quad (25) \end{aligned}$$

where

$$g_1 = V''(2a_s), \quad g = V''(r_0),$$

$$\omega_1^2 = -\frac{2}{a_s} V'(2a_s),$$

$$A_1 = \frac{1}{r_0^2} (4\pi^2 g - \omega^2 b^2),$$

$$A_2 = \frac{1}{r_0^2} (4b^2 g - \omega^2 \pi^2),$$

$$A_3 = \frac{\pi b^2}{r_0^4} (\omega^2 + 4g) + \frac{1}{6} \left(\frac{2\pi}{r_0} \right)^3 V'''(r_0), \quad (26)$$

$$A_4 = \frac{1}{6} V'''(2a_s),$$

$$A_5 = \frac{\pi^2 b}{r_0^4} (\omega^2 + 4g) + \frac{1}{6} \left(\frac{2b}{r_0} \right)^3 V'''(r_0),$$

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

$$A_7 = \frac{\pi}{4r_0^2} \left[1 - 3 \left(\frac{2b}{r_0} \right)^2 \right] (\omega^2 + 4g) + \frac{4b^2 \pi}{r_0^3} V'''(r_0).$$

In the continuum limit, the Hamiltonian (25) gives two coupled equations of motion,

$$u_{tt} - (2\pi)^2 (A_1 + 4g_1) u_{xx} + \sin u$$

$$- \frac{4\pi^2 b}{r_0^2} (\omega^2 + 4g) v_x - 6(2\pi)^3 (A_3 + 8A_4) u_x u_{xx}$$

$$- 16\pi A_7 v v_x - 16\pi^2 A_6 (u_{xx} v + u_x v_x) = 0, \quad (27)$$

$$v_{tt} + \frac{4b^2}{r_0^2} (\omega^2 + 4g) v + 24A_5 v^2 + \frac{4\pi^2 b}{r_0^2} (\omega^2 + 4g) u_x$$

$$+ 8\pi^2 A_6 u_x^2 + 16\pi A_7 v u_x = 0. \quad (28)$$

Since we study the stationary characteristics of kinks, we omit the term v_{tt} . Then, from Eq. (28) the following approximate expression follows:

$$v \simeq -\frac{\pi^2}{b} u_x - \frac{2\pi^2 r_0^2}{b^2 (\omega^2 + 4g)} \left[\frac{3\pi^2}{b^2} A_5 + A_6 - \frac{2\pi}{b} A_7 \right] u_x^2. \quad (29)$$

Note that the ansatz (29) differs from that used in Ref. 14 by the presence of the second term which makes the approximation better. The relation (29) remains valid until $b \simeq 1$. Substituting the expression (29) into Eq. (27) we obtain the *perturbed* SG equation (17) but now with the parameters

$$D = 2\pi (4g_1 - \frac{1}{4}\omega^2)^{1/2} \quad (30)$$

and

$$\alpha = -\frac{64\pi^3}{D^3} V'''(2a_s) \quad (31)$$

instead of D_0 and α_0 , respectively. The parameters of the expansions in Eqs. (27) and (28) is now of the order of D^{-1} : $u_x \sim u/D \ll u$ (for $D \gg 1$). When α is small, the perturbation theory for the kink of the SG equation can be applied (see, e.g., Ref. 19 for a review). This way the approximate kink solution of Eq. (17) can be written as

$$u(x) = 4 \tan^{-1} \exp(-\sigma x/D) + \frac{4}{3} \alpha \frac{\tan^{-1}[\sinh(x/D)]}{\cosh(x/D)}. \quad (32)$$

Using the definition of the kink mass, given by Eq. (16), we obtain the effective mass with the same accuracy as has been mentioned above,

$$m_{\text{eff}} = \frac{4}{\pi D} \left(1 + \frac{\pi^4}{3D^2 b^3} - \frac{1}{6} \sigma \alpha \pi \right). \quad (33)$$

It is important to note that this expression differs from Eq. (22) by a second term which appears due to the *transversal degree of freedom* and it gives the main contribution to the kink mass after the leading term, and *increases* the effective masses of both the kink and antikink.

In order to calculate the rest energy of MK according to Eq. (11), we use the continuum version of the discrete Hamiltonian (25) which, using the results given by Eqs. (29)–(32), can be rewritten in the following form:

$$E_k = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx \left[(1 - \cos u) - \pi^2 (\omega^2 + 4\omega_1^2) u_x + \frac{D^2}{2} u_x^2 - \frac{1}{6} D^3 \alpha u_x^3 \right]. \quad (34)$$

Equation (34) includes a term linear in u_x . Although this term does not produce any change in the motion equa-

tion, it is important for the energy of kinks defined by Eq. (11). Unlike the case of the standard Hamiltonian of the SG model where the energies of the kink and antikink are equal, this new term leads to their crucial difference. It is not difficult to obtain the following expansion:

$$E_k = \frac{1}{2\pi} \left[8D + 2\sigma\pi^3(\omega^2 + 4\omega_1^2) - \frac{1}{3}\alpha\sigma\pi D \right]. \quad (35)$$

Although the most crucial difference in the energies of the kink and antikink is produced by the second term in the expansion (35), the effective anharmonicity parameter α also lowers the kink energy. The latter is in agreement with the conclusions of Ref. 9.

C. “Nonmassive” kinks

The expansions presented above cannot be used to estimate the parameters of nonmassive kinks which connect GS₁ and GS₄. To do this in a proper way, in this subsection we use the ansatz

$$\begin{aligned} x_l &= l a_s + u_l, \\ y_l &= (-1)^l w_l, \end{aligned} \quad (36)$$

to derive equations for the functions u_l and w_l . We will assume that the values of the functions w_l slightly differ from b so that the parameter

$$z = (w_l + w_{l-1})^2 - 4b^2 \quad (37)$$

may be considered as a small one. The expansions we are going to do now are more general in comparison with those in the case considered above. Additionally, we assume $|u_l - u_{l-1}| \sim z \ll a_s$ and lead our expansions up to second order in the small parameter z . The reduced Hamiltonian (4) may be written now in the following form:

$$\begin{aligned} H = \sum_l \left\{ \frac{\dot{x}_l^2}{2} + \frac{\dot{y}_l^2}{2} + \frac{1}{2} \omega^2 w_l^2 + (1 - \cos u_l) - \frac{\pi \omega^2}{2} (u_l - u_{l-1}) - \pi \omega_1^2 (u_l - u_{l-2}) - \frac{\omega^2}{8} (w_l + w_{l-1})^2 + B_1 (u_l - u_{l-1})^2 \right. \\ \left. + B_2 [(w_l + w_{l-1})^2 - 4b^2] (u_l - u_{l-1}) + \frac{B_2}{8\pi} [(w_l + w_{l-1})^2 - 4b^2]^2 - \frac{\omega_1^2}{8} (w_l - w_{l-2})^2 + \frac{1}{2} g_1 (u_l - u_{l-2})^2 \right\}, \end{aligned} \quad (38)$$

where the values ω_1 and g_1 are given in Eq. (25) and

$$B_1 = \frac{1}{r_0^2} (4\pi^2 g - \omega^2 b^2), \quad B_2 = \frac{\pi}{4r_0^2} (\omega^2 + 4g). \quad (39)$$

In the continuous limit equations of motion corresponding to the Hamiltonian (38) may be written in the following form ($\tilde{w} = w/b$):

$$-\delta_1^2 u_{xx} + \sin u = 16\pi B_2 b^2 \tilde{w} \tilde{w}_x, \quad (40)$$

$$-\delta^2 \tilde{w}_{xx} - \tilde{w} + \tilde{w}^3 = -\frac{2\pi^2}{b^2} \tilde{w} u_x - 3\pi^2 (\tilde{w}^2 \tilde{w}_{xx} + \tilde{w} \tilde{w}_x^2) \quad (41)$$

(we dropped here the corresponding time derivatives since we again are interested in static properties only),

where

$$\delta_1^2 = 8\pi^2 (B_1 + 2g_1), \quad (42)$$

$$\delta^2 = \pi^2 \left[1 + \frac{\pi}{8b^2 B_2} (\omega^2 - 4\omega_1^2) \right]. \quad (43)$$

The latter gives us the condition for the NMK's stability: $\delta^2 > 0$.

Therefore, for the *longitudinal* displacements the kink shape is described again by a perturbed version of the SG equation while the *transversal* displacements are described by the perturbed ϕ^4 model. The more general case is realized when there are two “massive” and “non-massive” kinks in the system (e.g., in the situation when $M = N \pm 1$ and N is odd). A detailed analysis of this

case will be presented elsewhere. Since here we are interested in the case of a single kink in the chain, let us suppose that in one direction the kink is absent. This may be reached if we demand a corresponding boundary condition in this direction and assume that one of the parameters δ_1 or δ is small (while the other one is large, which is necessary for the continuum approximation). For example, for a “massive” kink we should take $\delta_1 \ll \delta$ and $\lim_{x \rightarrow \pm\infty} u = 0$; then from Eq. (41) we have the expansion

$$w = b - \frac{\pi^2}{b} u_x, \quad (44)$$

which exactly corresponds to the previous case [see Eq. (29)].

In the opposite case, when only a “nonmassive” kink is present in the chain, we have the result

$$u \simeq 16\pi B_2 b^2 \tilde{w} \tilde{w}_x, \quad (45)$$

and after a change of variables, $x \rightarrow \delta \tilde{x}$, Eq. (41) is reduced to the perturbed ϕ^4 equation

$$-\tilde{w}_{\tilde{x}\tilde{x}} - \tilde{w} + \tilde{w}^3 = -\gamma(\tilde{w}^2 \tilde{w}_{\tilde{x}\tilde{x}} + \tilde{w} \tilde{w}_{\tilde{x}}^2), \quad (46)$$

where the parameter γ ,

$$\gamma = \frac{\pi^2}{\delta^2} (32\pi B_2 + 3), \quad (47)$$

is assumed to be small (for $\delta \gg 1$). Therefore, similar to the previous case, we may apply the perturbation theory for the kink of the ϕ^4 equation⁹ to obtain the approximate kink's form as

$$\tilde{w} = \sigma \left[\tanh \chi + \frac{\gamma}{2 \cosh^2 \chi} (\chi - \tanh \chi) \right], \quad (48)$$

where $\chi = x/\sqrt{2}\delta$.

Unlike the previous case, the transversal degree of freedom gives the same contribution to the kink mass as the correction term to its form, since $\gamma \sim 1/\delta^2$. Using the formulas (45) and (48) and the definition (16), we obtain the kink's mass as

$$m_{\text{eff}} \simeq \frac{\sqrt{2}b^2}{3\pi\delta} \left[1 + \frac{\gamma}{10} + \frac{2}{7} \left(\frac{16\pi B_2 b}{\delta} \right)^2 \right]. \quad (49)$$

If we take into consideration the property

$$\int_{-\infty}^{+\infty} dx u_x = 16\pi B_2 b^2 \tilde{w} \tilde{w}_x|_{-\infty}^{+\infty} = 0,$$

then in the continuum approximation the Hamiltonian (38) may be written in the form

$$E \simeq \frac{4b^4 B_2}{\pi^2} \int_{-\infty}^{\infty} dx \left[\frac{\delta^2}{2} \tilde{w}_x^2 + \frac{1}{4} (1 - \tilde{w}^2)^2 - \frac{\gamma \delta^2}{2} \tilde{w}^2 \tilde{w}_x^2 \right]; \quad (50)$$

i.e., the energy of a single NMK is

$$E_k \simeq \frac{16b^4 B_2 \sqrt{2}\delta}{3} \left(1 - \frac{3}{10} \gamma \right). \quad (51)$$

As has been pointed out above, all the characteristics of NMK and NMAK are *identical*. For $\omega \rightarrow \omega^*$ (i.e., for $b \rightarrow 0$) we naturally get $E_k \rightarrow 0$; i.e., this kind of excitation does not exist in the 1D case.

IV. NUMERICAL SIMULATION RESULTS

The perturbation theory approach developed above gives good estimations for the kink parameters only in a restricted region of the system parameters, e.g., for $D \gg 1$ and $\alpha \ll 1$ (MK) or for $\delta \gg 1$ and $\gamma \ll 1$ (NMK). In a real situation, a kink is localized at several (or even a few) atomic sites so that the continuum approximation is not valid to describe such types of structures. Besides that, the very interesting, from the physical point of view, cases of $g \sim 1$ or $\omega \sim \omega^*$ cannot be treated analytically. Therefore, we investigate these cases with the help of numerical simulations.

In numerical simulations we use the method proposed in Ref. 20 and then used in Ref. 8. Namely, we start from an appropriate configuration $(\{x_l\}, \{y_l\})$ at $t = 0$ and then allow the atoms to relax to the configuration corresponding to a minimum potential energy, solving the Newton equations of motion which follow from the Hamiltonian (3) with the additional friction force acting on each atom, $F_{\text{friction}}^l = -\eta \dot{x}_l$. To obtain the saddle configuration, we artificially keep the X coordinate of the kink at the maximum of the PN potential. Namely, we take the following configurations as initial ones.

(a) For the MK ($M = N - 1$, N is even) (see Fig. 1),

$$x_1 = \begin{cases} 2\pi - 2\pi/5, & \text{ground-state configuration,} \\ 2\pi, & \text{saddle configuration,} \end{cases} \quad (52)$$

$$x_2 = \begin{cases} 2\pi + 2\pi/5, & \text{ground-state configuration,} \\ 3\pi, & \text{saddle configuration,} \end{cases}$$

$$x_l = 2\pi(l - 1), \quad l = 3, 4, \dots, N,$$

$$y_l = (-1)^l b, \quad l = 1, 2, \dots, N.$$

(b) For the MAK ($M = N + 1$, N is even) (see Fig. 3),

$$x_1 = 2\pi,$$

$$x_2 = \begin{cases} 6\pi, & \text{ground-state configuration,} \\ 5\pi, & \text{saddle configuration,} \end{cases} \quad (53)$$

$$x_l = 2\pi(l + 1), \quad l = 3, \dots, N,$$

$$y_l = (-1)^l b, \quad l = 1, \dots, N.$$

(c) For the NMK ($M = N$ and M, N are odd) (see Fig. 4),

$$x_l = 2\pi l, \quad l = 1, \dots, N,$$

$$y_1 = \begin{cases} 0, & \text{ground-state configuration,} \\ b, & \text{saddle configuration,} \end{cases}$$

$$y_2 = \begin{cases} -b, & \text{ground-state configuration,} \\ b, & \text{saddle configuration,} \end{cases} \quad (54)$$

$$y_l = (-1)^l b, \quad l = 3, 4, \dots, N.$$

For the saddle configuration, we solve the Newton equations of motion artificially keeping $x_2 = \text{const}$ for cases (a) and (b), and $y_1 = y_2$ for case (c).

In our numerical simulations we take $N = 50$ for MK, $N = 51$ for NMK, and $\eta = 1$. The Newton equations of motion are solved up to the time when all atomic velocities are smaller than 10^{-6} , and so we expect that the static configurations are finally realized in the chain. For the interatomic interaction we take $V_0 = 200$, $\beta = 0.3$, so that the width of 1D FK kink is $D_0 \simeq 13.17$, the anharmonicity parameter $\alpha_0 \simeq 0.197$, and $\omega^* \simeq 2.41$. The results of our simulations are presented in Figs. 5 and 6.

In Fig. 5 we present the results of numerical and analytical calculations for the kink energies. The continuum approximation (solid curves in Fig. 5) gives rather good estimations for MK (circles) when $\omega < \omega^*$ and $\omega > \omega_k^*$ and for MAK (squares) when ω is not close to ω^* , since in that region the conditions $D \gg 1$ and $\alpha \ll 1$ are not satisfied. Unfortunately, for NMK good analytical estimations are available only in a very small region near ω^* , because our analytical approach assumes the smallness of b [see (43)], but this latter condition is valid only in a small region (when $\gamma \ll 1$).

In Figs. 6(a) and 6(b) we show the height of Peierls-Nabarro potential. We should note that although in this picture the value of ε_{PN} seems go to zero when $\omega > \omega^*$ for MAK and, when $\omega > \omega_k^*$, for MK, in fact these values for

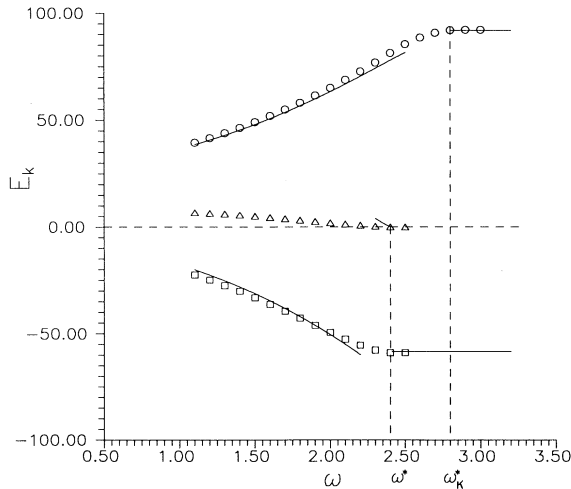


FIG. 5. Kink energies vs the transversal frequency ω for “massive” kink (circles) and antikink (squares), and for “non-massive” kink and antikink (triangles). The solid lines show the analytical estimations for these values.

1D kinks are only small but not zeros: $\varepsilon_{\text{PN}} \simeq 2 \times 10^{-4}$ for MAK and $\varepsilon_{\text{PN}} \simeq 5 \times 10^{-5}$ for MK so that $\varepsilon_{\text{PN}}(\text{MAK}) > \varepsilon_{\text{PN}}(\text{MK})$. For the dimerized structure the values of the PN potential for MK is larger than for MAK in a wide range of the parameter ω . The function $\varepsilon_{\text{PN}}(\omega)$ has an additional maximum associated with the appearance of the dimerized MK created on the TGS.

The results of the numerical simulations for NMK are shown in Fig. 6(b) by triangles. Recall that NMK’s exist provided $\omega < \omega^*$, i.e., for the DGS only. It is interesting that ε_{PN} as a function of ω has a local minimum at $\omega \simeq 1.31$. This effect is analogous to that is known for a nonsinusoidal substrate potential.^{7,8} Namely, for $1.31 < \omega < \omega^*$ the minimum of the potential energy is realized for the configuration shown in Fig. 4(a), while the configuration of Fig. 4(b) corresponds to the saddle one. However, at $1 < \omega < 1.31$ the situation is just opposite: The configuration shown in Fig. 4(a)

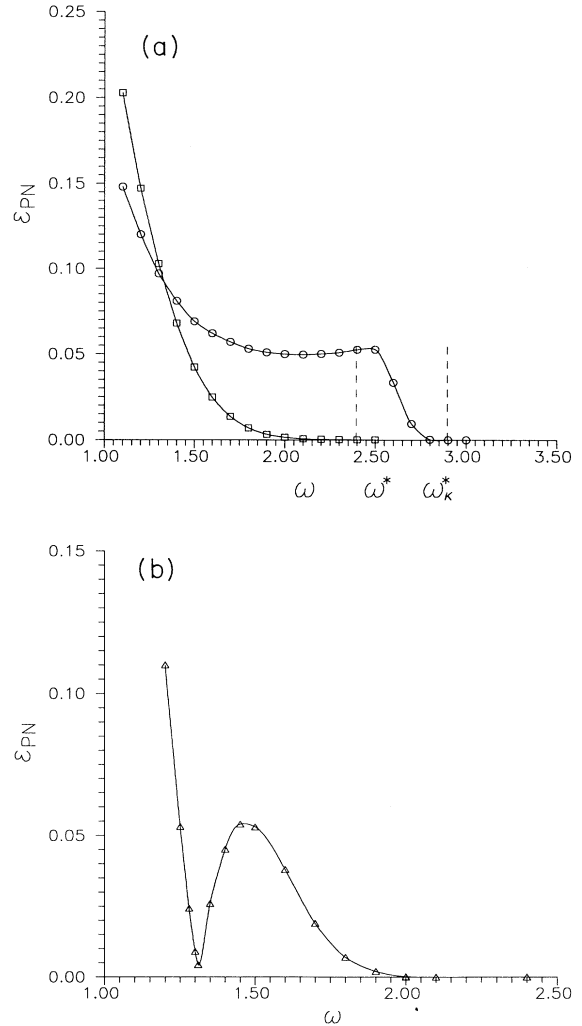


FIG. 6. Peierls-Nabarro potential vs the parameter ω for (a) “massive” kink (circles) and antikink (squares), and (b) for “nonmassive” kink and antikink (triangles). The points are joined with a solid line by means of a cubic spline.

corresponds to the saddle state, while the configuration shown in Fig. 4(b) to the minimum. Moreover, close to the value $\omega = 1.41$ both the configurations of Figs. 4(a) and 4(b) correspond to local *maxima* of the energy, while the minimum configuration is realized at an intermediate state.

V. DISCUSSION

As we have shown, in the generalized FK model for the case $\omega > \omega_k^*$ (as well as in the 1D FK model with anharmonic interatomic interactions), a kink has a lower effective mass m and a PN barrier ε_{PN} , in comparison with an antikink. If we suppose that the FK chain is subjected to a thermostat with temperature T , and the rate of the energy exchange between the chain and the thermostat may be described by an effective friction coefficient η , then the diffusion coefficient of a kink may be estimated as^{8,21}

$$D_k \simeq \begin{cases} \frac{\omega_{PN} \alpha_s^2}{2\pi} \exp(-\varepsilon_{PN}/k_B T), & \text{if } \eta < \omega_{PN}, \\ \frac{\omega_{PN}^2 \alpha_s^2}{2\pi \eta} \exp(-\varepsilon_{PN}/k_B T), & \text{if } \eta > \omega_{PN}, \end{cases} \quad (55)$$

where $\omega_{PN} \simeq (\varepsilon_{PN}/2m)^{1/2}$, and k_B is the Boltzmann constant. Therefore, the kink (i.e., an extra atom in the chain) should have a larger diffusion coefficient than that for the antikink (a vacancy in the chain). The chemical diffusion coefficient D_c (according to Fick's first law, D_c describes the atomic flux in a nonequilibrium state where the gradient of atomic concentration is small but nonzero) coincides with the antikink diffusion coefficient if the concentration of atoms, $\theta = N/M$, is slightly lower than the value $\theta = 1$, because in this case the mass transport along the chain is carried out by antikinks

$$D_c(\theta) |_{\theta=1-0} \equiv D_c^- = D_k(\text{MAK}). \quad (56)$$

Otherwise, when $\theta = 1 + 0$, the mass transport is carried out by kinks, and

$$D_c(\theta) |_{\theta=1+0} \equiv D_c^+ = D_k(\text{MK}). \quad (57)$$

As long as the FK chain is exactly one dimensional, the anharmonicity parameter α_0 is positive, and $\varepsilon_{PN}(\text{MAK}) > \varepsilon_{PN}(\text{MK})$, thus leading to the relation

$$D_c^- < D_c^+. \quad (58)$$

Therefore, the diffusion coefficient D_c as a function of θ should jump like the increase at $\theta = 1$.

The existence of a transversal degree of freedom changes drastically this picture. Namely, when $\omega^* < \omega < \omega_k^*$ the repulsion forces between the neighboring atoms in the region of a kink exceed the forces which hold the atoms within the 1D line, the atoms begin to escape out of the line, and the kink becomes less mobile than the antikink, $D_c^- > D_c^+$, so that the jump in the function $D_c(\theta)$ at $\theta = 1$ changes its sign. In the case of $\omega < \omega^*$ the system GS becomes dimerized, and now we have two different types of kinks, "massive" and "nonmassive." If $T \neq 0$, concentration of thermally created kinks is determined mainly by their creation energy, $n_k \propto \exp(-\tilde{E}_k/k_B T)$,

where $\tilde{E}_k = \frac{1}{2}[E_k(\text{kink}) + E_k(\text{antikink})]$. From Fig. 5 it follows that $\tilde{E}_k(\text{NMK}) < \tilde{E}_k(\text{MK})$, so that the following inequality should be valid: $n_k(\text{NMK}) \gg n_k(\text{MK})$. Therefore, "nonmassive" kinks will give the main contribution to *thermodynamic* properties of the quasi-2D system such as heat capacity, free energy, etc. On the contrary, *dynamical* properties of the chain (such as conductivity, diffusional properties, etc.) will be mainly determined by "massive" kinks. As can be seen from Eq. (33) and Fig. 5 for a wide range of values of ω , a dimerized "massive" antikink (a vacancy) is more mobile compared with a dimerized "massive" kink (an additional atom in the chain).

The proposed generalized FK model which describes a chain with a transversal degree of freedom can be directly applied to describe surface diffusion of atoms adsorbed on *anisotropic* (furrowed or stepped) crystal surfaces when the adsorbed atoms form a 2D system of parallel chains (along furrows or steps). In such a case, the model (1) and (3) corresponds to the situation when the interaction between the neighboring chains is weak and it can be neglected. This may be valid, for example, when the distance between the steps is large enough as it is at high-order vicinal surfaces. So our model may be used to predict the value of the diffusion coefficient D_c in that case. However, in a general case we have to take into account the interaction between the chains, thus coming to a more realistic 2D FK model. The situation when the 2D structure is formed by a system of coupled standard FK chains was considered in Refs. 22 and 23. Analogously to that study, we may consider a 2D structure composed of weakly interacting FK chains with transversal degrees of freedom. Such a model will correspond to an *anisotropic* 2D FK model. In the case $\omega = 1$ we come close to the isotropic FK model studied by Lomdahl and Srolovitz,^{12,13} where the substrate potential is periodic in both directions.

Another interesting generalization of the model (1) and (3) is to consider a situation when the number of atoms, N , is not equal to the number of wells, M . Recall that the standard FK model with a variation of $\theta = N/M$ displays a number of interesting physical phenomena such as commensurate-incommensurate phase transitions, devil's staircase structures, etc. We may naturally expect that the behavior of the generalized FK model will be more rich due to the existence of nontrivial GS's and the possibility of phase transitions between them. Besides the diffusion properties, this model may be very useful to describe crystal-growth processes.

ACKNOWLEDGMENTS

O.M. Braun thanks Universidad Complutense de Madrid for hospitality during his short visit when a part of this work has been done. O.A. Chubykalo is grateful to the Ministry of Education and Science of Spain for financial support. Two of the authors (O.C. and L.V.) also thank Professor N. de Diego and Professor V.V. Kono-top for useful discussions. The work by Yu. Kivshar has been supported by the Alexander von Humboldt-Stiftung. This work has been also partially supported by the Comunidad de Madrid under the grant C174/91.

- *On leave from Institute for Low Temperature Physics and Engineering, 310164 Kharkov, Ukraine.
- ¹J. Frenkel and T. Kontorova Phys. Z. Sowjetunion **13**, 1 (1938).
 - ²F.C. Frank and J.H. van der Merwe, Proc. R. Soc. London A **198**, 205 (1949).
 - ³R.K. Dodd, J.C. Eilbeck, J.D. Gibbon, and H.C. Morris, *Solitons and Nonlinear Wave Equations* (Academic, London, 1984).
 - ⁴For a review see, e.g., P. Bak, Rep. Prog. Phys. **45**, 587 (1982).
 - ⁵A.G. Naumovets and Yu.S. Vedula, Surf. Sci. Rep. **4** 365 (1984).
 - ⁶V.G. Bar'yakhtar, B.A. Ivanov, and A.L. Sukstanskii, Zh. Eksp. Teor. Fiz. **78**, 1509 (1980) [Sov. Phys. JETP **51**, 757 (1980)].
 - ⁷M. Peyrard and M. Remoissenet, Phys. Rev. B **26**, 2886 (1982).
 - ⁸O.M. Braun, Yu.S. Kivshar, and I.I. Zelenskaya, Phys. Rev. B **41**, 7118 (1990).
 - ⁹O.M. Braun, Z. Fei, Yu.S. Kivshar, and L. Vázquez, Phys. Lett. A **157**, 241 (1991).
 - ¹⁰C.S.O. Yokoi, L.-H. Tang, and W. Chon, Phys. Rev. B **37**, 2173 (1988).
 - ¹¹J. Pouget, S. Aubry, A.R. Bishop, and P.S. Lomdahl, Phys. Rev. B **39**, 9500 (1989).
 - ¹²P.S. Lomdahl and D.J. Srolovitz, Phys. Rev. Lett. **57**, 2702 (1986).
 - ¹³D.J. Srolovitz and P.S. Lomdahl, Physica D **23**, 402 (1986).
 - ¹⁴O.M. Braun and Yu.S. Kivshar, Phys. Rev. B **44**, 7694 (1991).
 - ¹⁵I.F. Lyuksyutov *et al.*, *Two-Dimensional Crystals* (Naukova Dumka, Kiev, 1988).
 - ¹⁶O.M. Braun and V.K. Medvedev, Usp. Fiz. Nauk **157**, 631 (1989) [Sov. Phys. Usp. **32**, 328 (1989)].
 - ¹⁷O.M. Braun, Surf. Sci. **230**, 262 (1990).
 - ¹⁸A.S. Kovalev (private communication).
 - ¹⁹Yu.S. Kivshar and B.A. Malomed, Rev. Mod. Phys. **61**, 763 (1989).
 - ²⁰M. Peyrard and S. Aubry, J. Phys. C **16**, 1593 (1983).
 - ²¹M.J. Gillan and R.W. Holloway, J. Phys. C **18**, 4903 (1985).
 - ²²O.M. Braun, Yu.S. Kivshar, and A.M. Kosevich, J. Phys. C **21**, 3881 (1988).
 - ²³O.M. Braun and Yu. S. Kivshar, J. Phys. Condens. Matter **2**, 5961 (1990).