Concentration dependence of the conductivity and diffusivity in one-dimensional anharmonic lattices

Oleg M. Braun
Institute of Physics, Ukrainian Academy of Sciences, 46 Science Avenue, UA-252022 Kiev, Ukraine

Yuri S. Kivshar*
Optical Sciences Centre, Australian National University, ACT 0200 Canberra, Australia
(Received 6 May 1994)

Low-temperature conductivity and diffusivity of the generalized Frenkel-Kontorova model, which takes into account realistic (*anharmonic*) interaction of particles subjected to a periodic substrate potential, are investigated analytically in the framework of a phenomenological approach which treats a system of strongly interacting atoms as a system of weakly interacting quasiparticles (kinks). Using phenomenology of the ideal kink gas, where the low-temperature ground state of the chain is described as that consisting of "residual" kinks supplemented by thermally excited kinks, we describe the ground state of the system as a hierarchy of consequently "melted" kink lattices. System dynamics is then described in terms of the kink dynamics. The motion equation for a single kink is reduced to a Langevin-type equation which is investigated with the help of the Kramers theory. In this way, we qualitatively analyze dependence of the susceptibility, conductivity, and chemical diffusivity of the chain on the concentration of atoms in the chain. The model leads to a series of effects which we expect are related to the experimentally observed phenomena in several quasi-one-dimensional systems, in particular, superionic conductors and anisotropic layers of atoms adsorbed on crystal surfaces.

I. INTRODUCTION

The study of mass and charge transport in systems with strong interatomic interactions is an important but a very difficult problem. At high temperatures transport coefficients can be found with the help of a perturbation technique starting from the case of noninteracting atoms.[1] Results already obtained may be summarized with the statement that attraction between the atoms decreases the chemical diffusivity, while the repulsion increases it compared with the noninteracting case. Besides, it was recently shown that a second-order phase transition results in a cusp peculiarity of the chemical diffusion coefficient.[2] On the other hand, experimental results show a very rich and complicated behavior of diffusion coefficients, especially as functions of the atomic concentration. The latter is the most clearly seen for diffusion in layers adsorbed on crystal surfaces, where the concentration may be varied in wide limits from zero (diffusion of isolated adsorbed atoms) to very high values (for example, in some adsorbed systems the interatomic distance in a monolayer of adatoms is lower than that in the corresponding massive crystal).[3]

Unfortunately, at low temperatures the perturbation theory breaks down, and transport characteristics may be found by computer simulations for a given choice of the system parameters.[4,5] To understand at least qualitatively the system behavior as well as to explain results of such simulations, it is useful to elaborate a phenomenological approach in which a system of strongly interacting atoms is approximately treated as a system of weakly interacting quasiparticles. In fact, in such a phenomenological approach the primary problem splits into two particular problems. First, one should introduce appropriate quasiparticles corresponding to the system of strongly interacting atoms and calculate the parameters of these quasiparticles. Second, one has to connect the parameters which characterize the system dynamics with those of the quasiparticles.

In the present paper we use such a phenomenological approach to investigate the low-temperature conductivity and diffusivity in a generalized (anharmonic) Frenkel-Kontorova (FK) model. Introduced to model the dynamics of dislocations in crystals,[6] in a rather general context a FK-type model describes a one-dimensional chain of interacting particles subjected to a periodic substrate (on-site) potential. This model may describe, for example, a closely packed row of atoms in crystals,[7] a chain of atoms adsorbed on stepped or furrowed crystal surfaces,[8] a chain of ions in a "channel" of quasi-one-dimensional conductors,[9] hydrogen atoms in hydrogen-bonded systems,[10] etc. (e.g., see the recent review paper[11] for other applications of the FK model). In all the cases mentioned above the chain of interacting particles is a part of the whole physical system under consideration, and the remainder is modeled as an external substrate potential and also as a thermal bath.

Transport properties of the FK model were a subject of intensive studies in the last decade. When the particles in the FK chain have an electric charge e, the dc conductivity σ is given by the Einstein relation

$$\sigma = \frac{ne^2}{k_B T} D_\mu. \tag{1}$$

Here n is the atomic concentration, k_B is the Boltzmann constant, T is the substrate temperature, and the *collective-diffusion* (or "jump"-diffusion) coefficient D_μ is introduced as

$$D_\mu = \lim_{\bar{\omega}\to 0+i0} \bar{\mathcal{D}}_\mu(\bar{\omega}), \quad \bar{\mathcal{D}}_\mu(\bar{\omega}) = \sum_{l=1} \bar{Q}(l;\bar{\omega}), \tag{2}$$

where $\bar{Q}(l;\bar{\omega})$ is the Laplace transform of the velocity correlation function $Q(l;t)$,

$$\bar{Q}(l;\bar{\omega}) = \int_0^\infty dt\, \exp(i\bar{\omega}t) Q(l;t), \quad \mathrm{Im}\,\bar{\omega} > 0, \tag{3}$$

$$Q(l-l';t-t') = \langle \dot{x}_l(t)\dot{x}_{l'}(t')\rangle, \tag{4}$$

$x_l(t)$ being the coordinate of the lth atom.

The chemical diffusion coefficient D_c is determined through the relation

$$D_c = D_\mu/\chi, \tag{5}$$

where χ is the dimensionless susceptibility of the system. The coefficient D_c describes the flux $J(x,t) = \sum_l \dot{x}_l(t)\delta(x - x_l(t))$ in a nonequilibrium state when the atomic density $\rho(x,t) = \sum_l \delta(x - x_l(t))$ slightly deviates from its equilibrium value. Namely, according to the second Fick law, we may write

$$\langle\langle J(x,t)\rangle\rangle \approx -D_c \frac{\partial}{\partial x} \langle\langle \rho(x,t)\rangle\rangle, \tag{6}$$

where $\langle\langle \cdots \rangle\rangle$ stands for averaging over the macroscopic distances $x \gg a_A$, and $a_A = 1/n$ is the average interatomic distance.

To our knowledge, analytical results have been obtained for two extreme cases only. First, at high temperatures the FK chain conductivity is defined by the collective-diffusion coefficient[12–14]

$$D_\mu \approx D_f \left\{ 1 + \frac{1}{8} \left[\frac{(\epsilon_s/k_BT)\sinh(k_BT/\epsilon_s g_A)}{\cosh(k_BT/\epsilon_s g_A) - \cos(2\pi a_A/a_s)} \right]^2 \right\}^{-1}. \tag{7}$$

Here $D_f \equiv k_BT/m_a\eta$, m_a is the atom's mass, η is the viscous friction coefficient which describes the coupling of the chain with the thermostat, ϵ_s and a_s are the height and period of the external potential, respectively, and the dimensionless elastic constant g_A is defined through the interatomic potential $V_{\mathrm{int}}(x)$ by the expression $g_A = a_s^2 V''_{\mathrm{int}}(a_A)/2\pi^2\epsilon_s$. The chemical diffusion coefficient D_c is determined by the analogous expression with the factor $V''_{\mathrm{int}}(a_A)a_A^2/m_a\eta$ instead of D_f in front of the right-hand side of Eq. (7). As seen, the conductivity and diffusivity are oscillating functions of the atomic concentration. Further, it is convenient to use the dimensionless atomic concentration (the so called "coverage" in surface physics) defined as $\theta = na_s = a_s/a_A$. From Eq. (7) it follows that D_μ has a local minimum at $\theta = 1$ and a local maximum at $\theta \approx 0.75$.

The second extreme case corresponds to the $T = 0$ limit, where the system behavior depends on whether the dimensionless concentration θ is a rational or irrational number. In the former case the system ground state (GS) corresponds to a commensurate structure which is locked by the substrate potential so that the conductivity is zero. Otherwise, for irrational θ the GS structure is incommensurate, and the GS may be locked (pinned) or sliding (free moving under the action of an infinitesimal external force) depending on whether the dimensionless elastic constant g_A is lower or greater than a critical threshold g_{Aubry} [where g_{Aubry} itself depends on θ, and it achieves the lowest value for the golden mean $\theta_{\mathrm{gm}} = 2/(\sqrt{5}+1)$]. Namely, at $g_A = g_{\mathrm{Aubry}}$ the Aubry transition of breaking of analyticity takes place, so that at $g_A < g_{\mathrm{Aubry}}$ the GS is pinned and the conductivity is zero, while for $g_A > g_{\mathrm{Aubry}}$ the GS is sliding and the conductivity is infinite.[15]

The aim of the present paper is to close the gap between the $T = 0$ and the high-T cases. In the low-T case, where the perturbation approach breaks down, we will use the phenomenological approach based on a kink-gas ideology introduced by Currie *et al.*[16] for the $\theta = 1$ case. Recall that at $T = 0$ the discrete FK chain for any rational θ admits the existence of topologically stable excitations (kinks) which link different ground states of the model. Within the ideal kink-gas approach the low-T $\theta = 1$ GS is considered as that consisting of the commensurate $\theta = 1$ background structure with a small number of thermally excited kinks. When $\theta \neq 1$ but the concentration is close to $\theta = 1$, the thermal kinks are additionally supplemented by residual kinks. As will be shown in the present work, for any $\theta \neq 1$ the GS may be considered as a hierarchy of consequently "melted" superkink lattices. Thus, the low-T GS of the system of strongly interacting atoms can be interpreted as a system of slowly interacting quasiparticles (kinks). Then, in the framework of the kink-gas ideology, the transport along the chain may be considered as that carried out by these quasiparticles (kinks).

In order to be applied to real physical systems, the standard FK model, where the interatomic potential $V_{\mathrm{int}}(x)$ is assumed to be harmonic, should be generalized in a way that takes into account realistic (anharmonic) interactions between atoms in the chain. The reason for such a generalization is connected with the fact that we try to describe the typical physically important situation when the mean distance between the particles in

the chain varies from a value of order of the period of the substrate potential to infinity. Clearly, in this case the harmonic approximation for the interatomic potential is not realistic, and one should use a more realistic interaction potential. In the present work for the sake of concreteness we use the exponential interatomic potential

$$V_{\rm int}(x) = V_0 \exp\left[-\beta\left(\frac{x}{a_s} - 1\right)\right], \tag{8}$$

where V_0 ($V_0 > 0$) is the interaction energy of two atoms located at the nearest minima of the substrate potential, and β is the dimensionless anharmonicity parameter of this potential. As a result, the dimensionless elastic constant g_A is determined by the expression

$$g_A(\theta) = \frac{1}{2\pi^2}\left(\frac{V_0}{\epsilon_s}\right)\beta^2 e^{\beta}\exp(-\beta/\theta). \tag{9}$$

So now g_A depends on θ, monotonically increasing with θ starting from 0. Consequently, the $T = 0$ function $D_\mu(\theta)$ has a very irregular shape: it is equal to zero for all rational θ as well as for those irrational θ whose elastic constant satisfies the inequality $g_A(\theta) < g_{\rm Aubry}(\theta)$, and D_μ is infinite for that θ where $g_A(\theta) > g_{\rm Aubry}(\theta)$. As for the function $D_c(\theta)$ at $T = 0$, it is zero for any θ, because for even infinitesimal variation of θ there are regions where θ is rational, and these regions will blockade the atomic flux. On the other hand, the high-T behavior of the generalized (anharmonic) FK model can still be approximately described by Eq. (7) if we replace the constant g_A by the effective elastic constant $g_A(\theta)$ given by Eq. (9).

The main objective of our study is *to investigate the dependence of the diffusion coefficients on concentration of particles for the anharmonic FK chain in the low-temperature case.* Although the way to final expressions for diffusion coefficients is rather long, the qualitative results are sufficiently clear and may be explained in the following simple way. Let us describe first the behavior of the function $D_\mu(\theta)$. Because the mass transport within the phenomenological approach is caused by kinks, the system conductivity is to be proportional to the kink concentration. Consequently, $D_\mu(\theta)$ should have a local minimum at $\theta = 1$. Indeed, at $\theta = 1$ there exist thermal kinks only, while with small deviation of θ from the $\theta = 1$ point the thermal kinks are supplemented by residual kinks or antikinks, so that the total kink concentration increases. Analogously, $D_\mu(\theta)$ should have local minima for any other trivial GS such as $\theta = 1/2$, $\theta = 1/3$, etc. Obviously, between the local minima $D_\mu(\theta)$ should exhibit local maxima, for example, a maximum at $\theta = 2/3$ where the concentration of trivial kinks achieves the maximum. Thus such a behavior shows the function $D_\mu(\theta)$ at high temperatures as described by Eq. (7). But if we now decrease the temperature so that the thermal energy k_BT is lower than the energy of interaction of trivial kinks at the distances corresponding to, e.g., the concentration $\theta = 2/3$, the trivial kinks will form their own lattice, and the conductivity will now be carried out by superkinks (topological excitations of the kink lattice). Thus at this temperature the function $D_\mu(\theta)$ would exhibit additionally a local minimum at $\theta = 2/3$. Analogously, with further decrease of T, new local minima will emerge for more and more complicated rational θ numbers, and finally, in the limit $T \to 0$, the function $D_\mu(\theta)$ will have minima at any rational θ as was described above.

On the other hand, the behavior of the function D_c is more simple as was predicted in Ref. 17. According to Fick's law (6), the chemical diffusion coefficient is the proportionality coefficient between the (infinitesimal) gradient of the atomic concentration and the flux of atoms caused by this gradient. But the gradient of atomic concentration will automatically produce a gradient of kink concentration too. Thus, in the standard FK model, where g_A is constant and the parameters of kinks and antikinks are the same, $D_c(\theta)$ will be approximately constant, and will coincide with the kink (or antikink) diffusion coefficient. But the anharmonicity of interaction results in destroying the kink-antikink symmetry.[18] That is, effective interaction forces for the kink (in the region of a local contraction of a chain) exceed those for the antikink (in the region of a local extension of an atomic chain). As a result, at the same values of the parameters V_0 and β a kink, in comparison with an antikink, is characterized by a larger value of the rest energy and by lower values of the effective mass and the Peierls-Nabarro (PN) potential barrier which coincides with the activation energy for kink motion. Thus, when the coverage parameter θ increases passing through a commensurate value θ_0, the activation energy for the chemical diffusion should decrease in a jumplike way. Therefore, the dependence $D_c(\theta)$ will have jumps similar to the inverse devil's staircase: the value of D_c should rise sharply each time whenever the coverage parameter θ exceeds the value θ_0 that characterizes the "well-defined" commensurate structure at a given temperature T. Clearly, the abrupt (jumplike) increase of $D_c(\theta)$ will exist in the $T \to 0$ limit only; for any $T \neq 0$ these jumps will be smoothed owing to corrections from thermally excited kink-antikink pairs.

Below in the present work we put this qualitative picture on a firmer base.

The paper is organized as follows. In Sec. II we briefly describe our model and present the procedure which allows us to treat a rather complex structure of atoms at $T = 0$ as a more simple system of weakly interacting kinks. The case of $T \neq 0$ is analyzed in Sec. III using the kink-gas ideology. In Sec. IV we describe diffusion of a single kink with the help of an effective Langevin equation derived for the kink's coordinate. The main purpose of this study is to find the kink diffusion coefficient. As we show in Sec. V, the collective and chemical diffusion coefficients may be found as functions of the kink diffusion coefficient and the susceptibility of the chain. Additionally in Sec. V we discuss temperature and concentration dependences of the diffusion coefficients. At last, Sec. VI concludes the paper by discussing possible applications of the anharmonic FK model to describe recent experimental results on the surface diffusion of atoms adsorbed on anisotropic crystal surfaces as well as to predict the dependence $\sigma(\theta)$ for quasi-one-dimensional conductors at low temperature.

II. THE $T = 0$ GROUND STATE AND KINKS

Let us consider a chain of atoms subjected to a periodic substrate potential which is taken in the simplest form, $V_{\rm sub}(x) = \frac{1}{2}\epsilon_s\,[1 - \cos(2\pi x/a_s)]$. Energy exchange between the chain and substrate can be approximately described by introducing a viscous friction force together with a random force which stands for random fluctuations acting on each atom. We assume that such a fluctuation force $\delta F_l(t)$ is a local Gaussian random function,

$$\langle \delta F_l(t) \rangle = 0,$$
$$\langle \delta F_l(t)\, \delta F_{l'}(t') \rangle = 2\eta m_a k_B T \delta_{ll'} \delta(t - t'). \tag{10}$$

The motion equation of the lth atom can be written in the form

$$m_a \ddot{x}_l + m_a \eta \dot{x}_l + V'_{\rm sub}(x_l) + \sum_{l'=1}^{\infty} [V'_{\rm int}(x_l - x_{l-l'}) - V'_{\rm int}(x_{l+l'} - x_l)] = \delta F_l(t), \tag{11}$$

where $\dot{x} \equiv dx/dt$ and $V'(x) \equiv dV(x)/dx$.

In the present paper we consider the "fixed density" FK chain consisting of N atoms distributed on the length $L = Ma_s = Na_A$, where M is the number of minima of the substrate potential, so that $n = N/L$ and $\theta = N/M = a_s/a_A$. Throughout the paper we assume the limit when N, M, and $L \to \infty$ at n (or θ) fixed.

For the case $\eta = 0$, $T = 0$, and $\theta = 1/q$, q being integer, and for the strong-coupling limit when interatomic forces are much larger than the force $F_l^{\rm sub} = -V'_{\rm sub}(x_l)$ produced by the on-site potential, the motion equation (11) with the harmonic interatomic interactions reduces to the well-known sine-Gordon (SG) equation. The SG equation is exactly integrable and it admits solutions in the form of topological solitons or *kinks*. In a general case, Eq. (11) is not integrable. Nevertheless, at least at low temperatures we may describe the system dynamics in terms of kinks because the kink excitations are responsible for the mass transport along the chain and such solutions do exist as solutions of a generalized FK model.

As the first step of the phenomenological approach we have to calculate the kink parameters. For the case of weakly interacting atoms at an arbitrary value of the coverage θ, as well as for the case of strongly interacting atoms but for the trivial ground state with $\theta = 1/q$, the kink characteristics can be found analytically. Otherwise, for a general case of $\theta \neq 1/q$ when the GS at $T = 0$ has a complex unit cell, the kink parameters may be found approximately using the renormalization procedure when the complex atomic structure is treated as a more simple structure of weakly interacting kinks.

First we describe the ground state of the FK chain at zero temperature when the atoms form a regular structure. Let us denote by $G[\theta]$ the minimum-energy commensurate (C) structure with the coverage parameter $\theta = s/q$, where s and q are positive relative prime integer numbers. The C structure $G[\theta]$ has a period $a = qa_s$, and the elementary cell consists of s atoms. For any C structure we can define a kink k (antikink $\bar{k}$) with a topological charge $\sigma = +1$ ($\sigma = -1$) as a minimally possible contraction (extension) of the structure when at infinity, i.e., for $l \to \pm\infty$, the arrangement of atoms relative to the minima of the substrate potential coincides with their arrangement in the GS. Kinks are elementary excitations of the $G[\theta]$ which are spatially localized and topologically stable. The kink has the simplest structure for the trivial $G[1]$, when one kink (antikink) corresponds to one additional atom (vacancy) inserted into the chain, and the neighboring atoms are allowed to relax. In a general case, the kink structure is more complicated. In particular, for $G[s/q]$ one additional atom (vacancy) corresponds to q kinks (antikinks).

The kink is a quasiparticle with the following characteristics. First of all, the kink structure is conventionally characterized by the displacements $u_l = x_l - x_l^{(0)}$, where x_l are the atomic coordinates for the chain with a single kink and $x_l^{(0)}$ are those for the GS. Following Bergman *et al.*[19] the kink's coordinate X_k may be defined as the coordinate of the center of mass of particles,

$$X = q \sum_l x_l + C, \tag{12}$$

where the constant C is chosen in such a way that the maximum deviation from the C structure occurs at the atom with the number $l = {\rm int}(X/a)$. The kink rest energy E_k is defined as the difference between the energy of the chain with the kink and that of the GS with the same number of atoms. The amplitude of the Peierls-Nabarro (PN) barrier, $\epsilon_{\rm PN}$, is defined as the lowest energy barrier which must be overcome for a translation $\{x_l\} \to \{x_{l'}\}$, where the configuration $\{x'_l\} \equiv \{x_{l-s} + qa_s\}$ describes the kink translated by a distance $a = qa_s$, i.e., by a unit cell of the C structure. It is necessary also to introduce the adiabatic trajectory (AT) as the curve in the N-dimensional configuration space of the system, which links two minimum-energy configurations $\{x_l\}$ and $\{x_{l'}\}$, passing through the nearest saddle configuration with the lowest potential energy. Such a trajectory satisfies the set of differential equations

$$dx_l(\tau)/d\tau = -\partial V/\partial x_l, \tag{13}$$

where V is the total potential energy of the system and τ is a parameter varying along the trajectory. Thus the AT is the curve of the steepest descent. Physically, the AT describes the kink motion in the limit $\eta \to \infty$, when it moves adiabatically.

During the kink motion along the AT, the potential energy of the system oscillates with the period a and the amplitude $\epsilon_{\rm PN}$. These oscillations can be described by the function $V_{\rm PN}(X) \approx \frac{1}{2}\epsilon_{\rm PN}\,[1 - \cos(2\pi X/a)]$ which can be interpreted as the kink's potential energy. At the same time, the kinetic energy of the system moving along the AT can be presented as $K = \frac{1}{2}m_k \dot{X}^2$, where the effective mass of the kink is introduced as

$$m_k = m_a \sum_l \left(\frac{\partial u_l}{\partial X}\right)^2_{x_l \in \mathrm{AT}}. \quad (14)$$

In a general case, the kink mass m_k depends on the kink's coordinate X, but such an effect will be neglected below because oscillations of the kink's mass are usually small (e.g., see Ref. 20).

Finally, when the chain contains two kinks separated by the distance $R = |X_1 - X_2|$, the kinks interact with the energy $v_{\mathrm{int}}(R)$. Usually, a kink and antikink attract each other while two kinks as well as two antikinks repel each other. Note that there are two mechanisms of the kink interaction. First, interaction between kinks arises due to the interaction of excess atoms which effectively correspond to the kinks.[17] Besides, there always exists an interaction between kinks due to overlapping of the kinks' tails because the presence of another kink nearby perturbs the kink's shape leading to a change of the kink's energy.[21] In the chain with a small density of kinks the total interaction energy may be assumed to be pairwise.[21]

Below we restrict ourselves to the case $\theta \leq 1$ because this situation corresponds to the physical objects mentioned in the Introduction. The kink's characteristics can be simply found in the case of a weak interatomic interaction, $V_{\mathrm{int}}(a_A) \ll \epsilon_s$, when in the GS all atoms are situated at the corresponding minima of the substrate potential. Namely, for $G[\theta]$ when the reference structure is characterized by the coverage $\theta = s/q$ lying within the interval $(1+p)^{-1} < \theta < p^{-1}$, where p is integer, in the lowest approximation using a simple geometrical consideration we can find for the kinks and antikinks [including the case of a kink on the background with the coverage $\theta = (1+p)^{-1}$ and that of an antikink on the background structure with $\theta = p^{-1}$] the following results:[22,17]

$$m_k \approx m_a/q^2, \quad (15)$$

$$\epsilon_{\mathrm{pair}} = E_k + E_{\bar{k}} \approx 2\pi^2 \epsilon_s g_a (1 - 2g_a), \quad (16)$$

$$\epsilon_{\mathrm{PN}} \approx \tfrac{1}{2}\epsilon_s (2 - \pi^2 g_p), \quad (17)$$

where ϵ_{pair} is the creation energy of the $k\bar{k}$ pair, $g_a = (a_s^2/2\pi^2\epsilon_s)V''_{\mathrm{int}}(a)$, and $g_p = (a_s^2/2\pi^2\epsilon_s)V''_{\mathrm{int}}\left(pa_s + \tfrac{1}{2}a_s\right)$. Besides, the difference in the values of the PN barrier for the kink and antikink is equal to

$$\delta\epsilon_{\mathrm{PN}} = \epsilon_{\mathrm{PN}}^{\sigma=-1} - \epsilon_{\mathrm{PN}}^{\sigma=+1} \approx \tfrac{1}{2}\pi^2 \epsilon_s \tilde{\beta} g_a, \quad (18)$$

where $\tilde{\beta} = -a_s V'''_{\mathrm{int}}(a)/V''_{\mathrm{int}}(a)$. Note that for the exponential interatomic potential (8) the dimensionless elastic constant g_a and the anharmonicity parameter $\tilde{\beta}$ are equal to

$$g_a = \frac{1}{2\pi^2}\left(\frac{V_0}{\epsilon_s}\right)\beta^2 \exp[-\beta(q-1)], \quad \tilde{\beta} = \beta. \quad (19)$$

The opposite case of a strong interaction between atoms, i.e., when $V_{\mathrm{int}}(a_A) \gg \epsilon_s$, is more complicated. This case can be described analytically only for the trivial $G[\theta]$ with $\theta = 1/q$. Namely, in the strong-coupling case we can use the continuum limit approximation, $l \to x = la$, $u_l(t) \to u(x,t)$, $\sum_l \to \int(dx/a)$, which for the exponential law (8) leads to the local SG-type equation[17]

$$\tilde{u}_{\tilde{t}\tilde{t}} + \sin\tilde{u} - (1 - \alpha\tilde{u}_{\tilde{x}})\tilde{u}_{\tilde{x}\tilde{x}} = 0, \quad (20)$$

where the indices stand for the corresponding partial derivatives. In Eq. (20) we have introduced the dimensionless variables $\tilde{u}(\tilde{x},\tilde{t}) = (2\pi/a_s)u(x,t)$, $\tilde{t} = \omega_0 t$, $\tilde{x} = x/d$, where $\omega_0^2 = 2\pi^2\epsilon_s/m_a a_s^2$, $d = a\sqrt{g_{\mathrm{eff}}}$, $g_{\mathrm{eff}} = (a_s^2/2\pi^2\epsilon_s)\sum_{l=1}^{\infty} l^2 V''_{\mathrm{int}}(la) = g_a(1+s)/(1-s)^3$, $s \equiv \exp(-\beta q)$, and $\alpha = (\tilde{\beta}/2\pi\sqrt{g_a})\,(g_a/g_{\mathrm{eff}})^{3/2}$. Note that the continuum approximation is valid only if the effective elastic constant is large, $g_{\mathrm{eff}} \gg 1$, and the anharmonicity parameter is small, $\alpha \ll 1$.

The kink solution of Eq. (20) is $u_k(x,t) = u_k^{\mathrm{SG}}(x,t) + \delta u_k(x,t)$, where u_k^{SG} stands for the well-known shape of the SG kink, $u_k^{\mathrm{SG}}(x,t) = (2a_s/\pi)\tan^{-1}\exp\{-\sigma[x - X(t)]/d\}$, and $X(t)$ describes the motion of the kink's center in the case when the "relativistic" narrowing of the kink's width is neglected. The anharmonicity-induced correction δu_k to the SG kink shape was found in Ref. 17. This effect leads to a change of the effective kink width, $d \to d_{\mathrm{eff}}^{\sigma} = d + \sigma\Delta d$, of the value Δd defined as $\Delta d \approx (\pi/3)\alpha d$. Knowing the perturbed kink shape $u_k(x,t)$, we can find other characteristics of the kink, for example, the effective kink mass,

$$m_{k\sigma} \approx m_{\mathrm{SG}}\left(1 - \frac{\pi}{6}\sigma\alpha\right), \quad (21)$$

where $m_{\mathrm{SG}} = 2m_a/\pi^2 q^2\sqrt{g_{\mathrm{eff}}}$ is the SG kink mass, the energy of creation of the kink-antikink pair,

$$\epsilon_{\mathrm{pair}} \approx 8\epsilon_s\sqrt{g_{\mathrm{eff}}}, \quad (22)$$

and the amplitude of the PN relief which can be estimated as

$$\epsilon_{\mathrm{PN}}^{\sigma} \approx \epsilon_{\mathrm{PN}}^{\mathrm{SG}}(g_{\mathrm{eff}}) + \sigma\Delta g \left.\frac{\partial\epsilon_{\mathrm{PN}}^{\mathrm{SG}}}{\partial g}\right|_{g=g_{\mathrm{eff}}}, \quad (23)$$

where $\Delta g = (2\pi/3)\alpha g_{\mathrm{eff}}$, and $\epsilon_{\mathrm{PN}}^{\mathrm{SG}}$ is the barrier of the PN relief for the standard FK model, $\epsilon_{\mathrm{PN}}^{\mathrm{SG}}(g) \approx (8/3)\pi^4\epsilon_s g\exp(-\pi^2\sqrt{g})$. Finally, the interaction energy of two kinks is equal to[21]

$$v_{\mathrm{int}}(R) \approx 16\sigma_1\sigma_2\epsilon_s\sqrt{g_{\mathrm{eff}}}\exp(-R/d). \quad (24)$$

Unfortunately, the general case of $G[s/q]$ with $s \neq 1$ in the strong-coupling limit cannot be treated analytically because the continuum approximation leads to a system of s coupled differential equations. However, this case may be investigated with the help of a renormalization procedure.[23] For example, let us consider the reference $G\left[\frac{q-1}{q}\right]$ with $q \gg 1$. For definiteness, we call kinks for the trivial $G[1]$ trivial kinks (t kinks) while kinks for $G\left[\frac{q-1}{q}\right]$ are called superkinks (s kinks). According to Eqs. (21) – (24), the t antikinks are characterized by

the parameters $m_{t\bar{k}}$, $\epsilon_{\rm pair}^{tk}$, and $\epsilon_{\rm PN}^{t\bar{k}}$ which are determined by the same expressions (21) – (24), where, however, we have to use the elastic constant

$$g_t = \frac{\beta^2}{2\pi^2}\left(\frac{V_0}{\epsilon_s}\right)\frac{(1+e^{-\beta})}{(1-e^{-\beta})^3} \tag{25}$$

and the anharmonicity parameter

$$\alpha_t = \left[\frac{\epsilon_s}{2V_0}\frac{(1-e^{-\beta})^9}{(1+e^{-\beta})^3}\right]^{1/2} \tag{26}$$

instead of $g_{\rm eff}$ and α, respectively. The t antikinks may be considered as quasiparticles interacting via the exponential law $v_{\rm int}^{t\bar{k}}(\Delta X) \approx 16\epsilon_s\sqrt{g_t}\exp(-\Delta X/a_s\sqrt{g_t})$, and subjected to the external periodic potential $v_{\rm PN}^{t\bar{k}}(X) \approx \frac{1}{2}\epsilon_{\rm PN}^{t\bar{k}}[1-\cos(2\pi X/a_s)]$.

Then, let us treat $G\left[\frac{q-1}{q}\right]$ as a regular lattice of the t antikinks with the period $R = qa_s$. This lattice can be interpreted as a new ("secondary") FK model with t antikinks instead of atoms and the effective coverage $\theta_k = 1/q$. The dimensionless coupling constant g_s and the anharmonicity parameter $\tilde{\beta}_s$ of the secondary FK models are equal to $g_s \approx 3\pi^{-6}g_t^{-3/2}\exp[(\pi^2 g_t - q)/\sqrt{g_t}]$ and $\tilde{\beta}_s \approx g_t^{-1/2}$, respectively. However, it is easy to see that a kink excitation of the secondary FK model consisting of t antikinks *exactly coincides* with a kink (s kink) excitation of the primary FK chain with $\theta = (q-1)/q$. Thus in this way we can approximately calculate parameters of the s kinks and s antikinks. In particular, for $q \geq \pi^2 g_t$ the secondary FK chain is characterized by a weak coupling, i.e., $g_s \ll 1$, and Eqs. (15) – (18) give

$$m_{sk} \approx m_{t\bar{k}}/q^2, \tag{27}$$

$$\epsilon_{\rm pair}^{sk} \approx 2\pi^2\epsilon_{\rm PN}^{t\bar{k}}g_s(1-2g_s), \tag{28}$$

$$\epsilon_{\rm PN}^{sk,\sigma} \approx \tfrac{1}{2}\epsilon_{\rm PN}^{t\bar{k}}(2-\pi^2 g_s) - \tfrac{1}{2}\sigma\,\delta\epsilon_{\rm PN}^{sk},$$

$$\delta\epsilon_{\rm PN}^{sk} \approx \tfrac{1}{2}\pi^2\epsilon_{\rm PN}^{t\bar{k}}\tilde{\beta}_s g_s. \tag{29}$$

Otherwise, for $q < \pi^2 g_t$ when $g_s \gg 1$, from Eqs. (21) and (22) we obtain

$$m_{sk} \approx 2m_{t\bar{k}}/\pi^2 q^2\sqrt{g_s}, \tag{30}$$

$$\epsilon_{\rm pair}^{sk} \approx 8\epsilon_{\rm PN}^{t\bar{k}}\sqrt{g_s}. \tag{31}$$

Analogously, we can consider kinks for a more general case of $G[\theta]$, if a more simple structure with θ_0 may be found provided θ_0 is close to θ and the kink's parameters for the reference $G[\theta_0]$ are known (the corresponding technique was recently developed by Schilling[24] for a simplified version of the FK model).

Now we may describe the dependence of the kink parameters on the coverage parameter θ when the parameters V_0 and β of the interatomic interaction potential (8) are fixed. Clearly, the functions $m_k(\theta)$, $\delta m_k(\theta)$, $\epsilon_{\rm pair}(\theta)$, $\epsilon_{\rm PN}(\theta)$, and $\delta\epsilon_{\rm PN}(\theta)$ are defined only on a countable set of rational numbers θ. Besides, the functions $m_k(\theta)$ and $\epsilon_{\rm PN}(\theta)$ take two values at each rational θ, the left-side value, $\epsilon_{\rm PN}(\theta-0) = \epsilon_{\rm PN}^{\sigma=-1}(\theta)$, and the right-side value, $\epsilon_{\rm PN}(\theta+0) = \epsilon_{\rm PN}^{\sigma=+1}(\theta)$. The functions $q^2 m_k(\theta)$ and $\epsilon_{\rm PN}(\theta)$ monotonically decrease from $m_a(0) = m_a$ and $\epsilon_{\rm PN}(0) = \epsilon_s$ to zero as θ varies from $\theta = 0$ to $\theta = \infty$, undergoing a series of jumps down at each rational value of θ, so that the corresponding dependence looks like an inverse devil's staircase.

The important point is that for a given $G[\theta]$ the energies $\epsilon_{\rm pair}$ and $\delta\epsilon_{\rm PN}$ depend not on the interaction of neighboring atoms situated at the distance $x \sim a_A$, but on interaction between elementary unit cells of the reference C structure, i.e., they are determined by interatomic interactions at the distances $x \sim a = qa_s$. Therefore, the more complicated is the reference C-structure, the lower are the corresponding values of $\epsilon_{\rm pair}$ and $\delta\epsilon_{\rm PN}$. For example, if we consider two commensurate structures with the nearest values of the coverage parameter θ, e.g., $\theta_1 = \frac{1}{2}$ and $\theta_2 = \frac{100}{201}$, from Eq. (19) we obtain the ratio $g_a(\theta_2)/g_a(\theta_1) = \exp(-199\beta)$ and, according to Eqs. (16) and (18), the values $\epsilon_{\rm pair}$ and $\delta\epsilon_{\rm PN}$ for $G[\theta_2]$ will be lower than those for $G[\theta_1]$ by $\exp(199\beta)$ times. Besides, the largest jumps are expected to occur near that coverage θ_* where the dimensionless parameter g_A given by Eq. (9) is close to 1. Thus, "on average" the function $\delta\epsilon_{\rm PN}(\theta)$ has a maximum at $\theta \sim \theta_*$. The function $\epsilon_{\rm pair}(\theta)$ increases "on average" exhibiting also an irregular structure, because for two closely taken values θ_1 and θ_2 the value $\epsilon_{\rm pair}$ is lower for a higher-order structure, e.g., $\epsilon_{\rm pair}(\theta_2) \ll \epsilon_{\rm pair}(\theta_1)$.

III. THE $T \neq 0$ GROUND STATE AND SUSCEPTIBILITY

As is well known, for the one-dimensional FK model the $T = 0$ "crystalline" structure of the GS is disordered and the long-range order is destroyed at any temperature $T \neq 0$.[25] However, at low temperatures this disorder is "small," so that the short-range order still exists, allowing the existence of kinks. This is the basis for the ideal kink-gas phenomenology[16,26] when the low-temperature ground state of the system is considered as a regular lattice with a small number of thermally excited phonons and kinks. Note that thermally excited kink-antikink pairs destroy the long-range order of the "crystalline" structure.

Let us suppose that at low temperatures the equilibrium state of the chain contains N_k kinks and $N_{\bar{k}}$ antikinks. Because kinks and antikinks can be created only as $k\bar{k}$ pairs, this process may be considered as a "chemical reaction:" phonons $\leftrightarrow$ $k + \bar{k}$.[27] Therefore average numbers of kinks and antikinks are equal to $\langle N_k\rangle = \langle N_{\bar{k}}\rangle = \langle N_{\rm pair}\rangle$, where

$$\langle N_{\rm pair}\rangle = CL\exp(-\epsilon_k/k_BT), \quad \epsilon_k = \tfrac{1}{2}\epsilon_{\rm pair}. \tag{32}$$

To calculate the preexponential factor C for Eq. (32) in

a rigorous way, we should take into account kink-phonon interactions. Assuming that one kink takes away from the phonon spectrum a single degree of freedom (transforming it into the PN mode which is an analog of the Goldstone mode of a SG kink in the continuum approximation) and repeating the calculations which were done by Currie *et al.*[16] for the SG model, we obtain

$$C \approx (2\tilde{m}_k \omega_0^2/\pi k_B T)^{1/2}, \tag{33}$$

where $\tilde{m}_k = \sqrt{m_k m_{\bar{k}}}$.

Now let us consider the dimensionless susceptibility χ of the FK chain. This value is determined by the expression

$$\chi = \frac{\langle(\Delta\tilde{N})^2\rangle}{\langle\tilde{N}\rangle}, \tag{34}$$

where $\tilde{N}$ is the number of atoms on a fixed length $\tilde{L}$ ($\tilde{L} \gg a_A$ but $\tilde{L} \ll L$) and $\Delta\tilde{N}$ stands for fluctuations around $\tilde{N}$. The susceptibility χ can be easily found with the help of the ideal kink-gas approach.[28] Namely, let us assume that on the length $\tilde{L}$ there are $\tilde{N}$ atoms, $\tilde{N}_k$ kinks, and $\tilde{N}_{\bar{k}}$ antikinks with $\tilde{N}, \tilde{N}_k, \tilde{N}_{\bar{k}} \gg 1$. At low temperatures, when the concentration of kinks is small and they may be considered as noninteracting quasiparticles, the corresponding probability distributions should be Poissonian, giving the relations $\langle\tilde{N}_k^2\rangle - \langle\tilde{N}_k\rangle^2 = \langle\tilde{N}_k\rangle$, $\langle\tilde{N}_{\bar{k}}^2\rangle - \langle\tilde{N}_{\bar{k}}\rangle^2 = \langle\tilde{N}_{\bar{k}}\rangle$, and $\langle\tilde{N}_k\tilde{N}_{\bar{k}}\rangle = \langle\tilde{N}_k\rangle\langle\tilde{N}_{\bar{k}}\rangle$. Recalling that each kink corresponds to $1/q$ excess atoms, and each antikink to the same quantity of vacancies, we can write the number of atoms on the length $\tilde{L}$ as

$$\tilde{N} = \tilde{N}_0 + \frac{1}{q}(\tilde{N}_k - \tilde{N}_{\bar{k}}), \tag{35}$$

where $\tilde{N}_0 = n\tilde{L}$ is the number of atoms at $T = 0$. Substituting Eq. (35) into Eq. (34), we obtain the result

$$\chi = \frac{\langle N_{\rm tot}\rangle}{q^2\langle N\rangle}, \tag{36}$$

where $\langle N_{\rm tot}\rangle = \langle N_k\rangle + \langle N_{\bar{k}}\rangle$, and all the tildes are finally omitted. Thus, at low temperatures the susceptibility behaves as

$$\chi \approx \frac{2\omega_0}{q^2 n}\left(\frac{2\tilde{m}_k}{\pi k_B T}\right)^{1/2} \exp\left(-\frac{\epsilon_{\rm pair}}{2k_B T}\right). \tag{37}$$

The results (36) and (37) are valid provided $k_B T \ll \epsilon_k$.

For $k_B T \geq \epsilon_k$ the concentration of thermally excited $k\bar{k}$ pairs becomes so large that they "melt" the reference C structure and the approach based on the ideal kink gas breaks down. However, if $\theta \neq 1/q$, i.e., the $T = 0$ $G[\theta]$ is nontrivial, the kink-gas ideology remains useful up to temperatures $k_B T \leq \epsilon_{tk}$. For example, let us consider again the case $\theta = (q-1)/q$ with $q \gg 1$ when the $T = 0$ $G[\theta]$ may be treated as a regular structure of t antikinks with the number N_w (these t antikinks are known as the "residual" t antikinks). Analogously to Eq. (32) we can introduce the energies $\epsilon_{sk} = \frac{1}{2}\epsilon_{\rm pair}^{sk}$ and $\epsilon_{tk} = \frac{1}{2}\epsilon_{\rm pair}^{tk}$. From Eq. (28) or (31) we see that $\epsilon_{sk} \ll \epsilon_{tk}$ provided $q \geq \sqrt{g_t}$. Thus there may exist a wide temperature interval,

$$\epsilon_{sk} < k_B T < \epsilon_{tk}, \tag{38}$$

where the trivial $\theta = 1$ structure of atoms still exists while the original $\theta = (q-1)/q$ atomic superstructure is disordered. Thus in the temperature interval (38) the lattice of t antikinks is "melted" and, therefore, the t antikinks can be considered as a gas of weakly interacting quasiparticles. Now, repeating the calculations similar to those we have done above, we obtain for the interval (38) the expression $\chi \approx \langle N_{\rm tot}\rangle/\langle N\rangle$, where now $N_{\rm tot}$ is the total number of trivial kinks and antikinks. As was shown by Currie *et al.*,[27] the average number $N_{\rm tot}$ is given by the formula

$$\langle N_{\rm tot}\rangle = \left[\langle N_w\rangle^2 + \langle 2N_{\rm pair}\rangle^2\right]^{1/2}, \tag{39}$$

where $\langle N_w\rangle = N_w$ is the number of residual t antikinks and $\langle N_{\rm pair}\rangle$ is the average number of thermally created trivial $k\bar{k}$ pairs determined by Eqs. (32) and (33) with ϵ_{tk} instead of ϵ_k and $\tilde{m}_{tk} = \sqrt{m_{tk} m_{\bar{t}\bar{k}}}$ instead of $\tilde{m}_k$. From Eqs. (39), (32), and (33) it follows that on the left-hand side of the interval (38) the function $\chi(T)$ has a plateau $\chi \approx w \equiv N_w/N$, and on the right-hand side $\chi(T)$ increases exponentially due to thermal excitation of the $k\bar{k}$ pairs, which join those already present from the "melted" t antikink lattice.

With the help of the renormalization arguments presented in the previous section, we may describe in a similar way the temperature dependence of $\chi(T)$ for more complicated structures with $\theta = s/q$ where $s \neq 1$ and $s \neq (q-1)$. Considering the system as a hierarchy of the consequently melted superkink lattices, we can divide the whole temperature interval $0 < k_B T < \epsilon_{tk}$ into subintervals; in each of them a more complex superkink structure is already melted, but more simple structure still exists and it allows strong definition of the corresponding s kinks and s antikinks which are approximately noninteracting in this temperature subinterval. Within each subinterval the susceptibility is defined by Eqs. (36), (39), (32), and (33), where the parameters q and N_w characterize the more simple structure, and $\epsilon_{\rm pair}$ and $m_k, m_{\bar{k}}$ correspond to kinks defined on the basis of this reference structure. Thus the function $\chi(T)$ has to display a series of plateaus at the low-temperature sides of these subintervals, and it changes exponentially between the plateaus. Note that computer simulations of Gillan and Halloway[4] for the standard FK model as well as the analytical results of Schilling[24] obtained for a simplified FK model, are in good agreement with the results of our phenomenological approach.

At last, here we will estimate also the "melting" temperatures of the hierarchy of superkink lattices. Let us consider a regular lattice of interacting quasiparticles (atoms, trivial kinks, superkinks, etc; below we will call them "atoms") interpreted as the reference structure which is characterized by an effective value of the coverage $\tilde{\theta} = \tilde{s}/\tilde{q}$ and by an effective external potential with the period $\tilde{a}_s$. We assume that the system has a small quantity of approximately noninteracting

topological excitations (trivial kinks, superkinks, super-superkinks, etc.; below we will call them "kinks") which are characterized by the width $\tilde{d}$ and the mean rest energy $\tilde{\epsilon}_k$. Note that the "kinks" may be residual as well as thermally excited. According to the definition of the susceptibility χ, this value describes the mean square fluctuations of the relative atomic displacements $x_{l'+l} - x_{l'}$,[28]

$$\Lambda_l \equiv \frac{1}{N}\sum_{l'} \langle [(x_{l'+l} - x_{l'}) - \langle x_{l'+l} - x_{l'}\rangle]^2\rangle = \chi a_A^2 |l|. \tag{40}$$

Thus, the mutual positions of two "atoms" separated by the distance x ($x = la_A$) fluctuate with the amplitude $\delta(x) = \sqrt{\Lambda_l} = \sqrt{\chi a_A x}$. In order to construct "kinks" for the reference structure with $\tilde{\theta} = \tilde{s}/\tilde{q}$, the mutual fluctuations must be small, $\delta(x) \leq \tilde{a}_s/\tilde{s}$, at least on distances of order of the "kink" width, $\tilde{x} \geq \tilde{d}$. In this way we obtain the upper limit when a given reference structure may be considered as a regular one; the corresponding equation is $\delta(\tilde{d}) = \tilde{a}_s/\tilde{s}$, or

$$\chi(T) a_A \tilde{s}^2 \tilde{d} = \tilde{a}_s^2. \tag{41}$$

A solution of Eq. (41) defines the temperature $\tilde{T}_{\rm melt}$, above which the short-range order in the given reference structure is completely destroyed by thermal fluctuations. Using the expression (36) for $\chi(T)$, we can see that at $T = \tilde{T}_{\rm melt}$ the average distance $\tilde{R}$ between "kinks" is equal to $\tilde{d}$, so that at $T > \tilde{T}_{\rm melt}$ the total concentration of such "kinks" becomes so large that they begin to overlap.

When the reference structure has no residual "kinks" (i.e., for the lowest temperature interval in the kink-lattice hierarchy), Eq. (41) leads to the result $k_B \tilde{T}_{\rm melt} \approx \tilde{\epsilon}_k$. However, when the quantity of residual "kinks" is nonzero, it follows that $k_B \tilde{T}_{\rm melt} < \tilde{\epsilon}_k$ because the residual "kinks" supplement thermally excited "kink-antikink" pairs and, therefore, the criterion $\tilde{R} = \tilde{d}$ will be achieved at lower temperatures.

Thus the more complex (higher-order) is the reference structure, the lower is the energy $\tilde{\epsilon}_k$ of its topological excitations and, therefore, the lower is its "melting" temperature $\tilde{T}_{\rm melt}$.

IV. KINK DIFFUSION

In this section we study the system dynamics when the FK chain contains a single kink only. Using a phenomenological approach we may consider a kink as a quasiparticle of the mass m_k which is characterized by the coordinate $X_k(t)$ and has the kinetic energy $\frac{1}{2} m_k \dot{X}_k^2$ moving in the potential relief $V_{\rm PN}(X_k)$. Thus it is reasonable to suppose that the kink's coordinate $X_k(t)$ satisfies the Langevin-type equation

$$m_k \ddot{X}_k + m_k \eta_k \dot{X}_k + V'_{\rm PN}(X_k) = \delta F_k(t). \tag{42}$$

It is clear that Eq. (42) is an approximate one and, therefore, it cannot be rigorously derived from the primary motion equation (11). However, in order to find the kink friction coefficient η_k and the fluctuation force $\delta F_k(t)$, below we briefly outline a way to reduce Eq. (11) to the form given by Eq. (42).

In Sec. II we introduced the adiabatic trajectory $x_l(\tau)$ as a solution of the system of equations (13). When the FK chain contains a single kink only, we can set each value $X(\tau)$ from Eq. (12) to correspond uniquely to each point of the AT. Thus, we can introduce the functions $u_l^{\rm kink}(X_k)$ according to the equation $u_l^{\rm kink}(X_k) = x_l(\tau)\big|_{X(\tau)=X_k} - x_l^{(0)}$. The functions $u_l^{\rm kink}(X_k)$ describe atomic displacements in the FK chain with a single (adiabatically slowly moving) kink. Then, let us suppose that the system moves strictly along the AT only, looking for a solution of the motion equation (11) in the form $u_l(t) = u_l^{\rm kink}[X_k(t)]$. Suppose now that, during a short time interval Δt, the fluctuation forces $\delta F_l(t)$ and $\delta F_k(t)$ are constant, while the atoms and the kink are shifted by small distances Δx_l and ΔX_k, respectively. The displacements Δx_l and ΔX_k are coupled by the relation

$$\Delta x_l = \frac{du_l^{\rm kink}(X_k)}{dX_k} \Delta X_k. \tag{43}$$

The work done by the fluctuation forces can be written as

$$\delta F_k \Delta X_k = \sum_l \delta F_l \Delta x_l. \tag{44}$$

Substituting Eq. (43) into Eq. (44), we obtain

$$\delta F_k(t) = \sum_l \frac{du_l^{\rm kink}(X_k)}{dX_k} \delta F_l(t). \tag{45}$$

Now, using Eq. (10) for $\delta F_l(t)$ and taking into account the definition (14) for the kink's mass, we find correlation functions for the kink fluctuation force,

$$\langle \delta F_k(t)\rangle = 0,$$

$$\langle \delta F_k(t) \delta F_k(t')\rangle = 2\eta_k m_k k_B T \delta(t - t'), \tag{46}$$

where $\eta_k = \eta$.

To find the friction force acting on the kink, let us take the sum over l for the first two terms in the motion equation (11),

$$(q m_k/m_a) \sum_l (m_a \ddot{x}_l + m_a \eta \dot{x}_l) = m_k \ddot{X}_k + m_k \eta \dot{X}_k, \tag{47}$$

where we have used Eq. (12) to introduce $X \equiv X_k$. Comparing Eqs. (42) and (47), we see that the friction coefficient η_k in Eq. (42) exactly coincides with the atomic friction coefficient η.

It should be emphasized that the parameters m_k, η_k, and the function $V_{\rm PN}(X)$ in Eqs. (42) and (46) coincide with those calculated for the kink only if the atoms move strictly along the AT. As a matter of fact, a real trajectory deviates from the AT. For example, even at $T = 0$ a

moving kink radiates phonons, and this leads to an additional damping of the kink's velocity. Besides, at $T \neq 0$ the system contains a certain number of thermally excited phonons. Collisions of a kink with the phonons as well as with other kinks lead to energy and momentum exchange between them; the rate of this exchange may be approximately described by introducing an additional "intrinsic" viscous friction $\eta_{\rm int}$. Besides, kink-phonon interactions may increase the effective kink mass (due to a phonon "dressing") and decrease the height of the effective PN barrier (analogously to the Debye-Waller effect). Thus the parameters $m_k, \eta_k = \eta + \eta_{\rm int}$, and $\epsilon_{\rm PN}$ used in Eqs. (42) and (46) are effective parameters which in the general case depend on T. However, these effects can be neglected when the kink-phonon interaction is small in comparison with interaction with the substrate, i.e., if $\eta_{\rm int} \ll \eta$. In real physical objects, when the FK chain is only a part of the whole three-dimensional system, the latter inequality is usually fulfilled.

When the parameters of Eq. (42) are known, the kink diffusion coefficient can be found as

$$D_k = \int_0^\infty dt\, e^{i\bar{\omega}t} \langle \dot{X}_k(t) \dot{X}_k(0) \rangle. \tag{48}$$

According to the Kramers theory,[29] at low temperatures, i.e., when $k_B T < \epsilon_{\rm PN}$, the kink diffusion coefficient should have the Arrhenius form,

$$D_k = D_{k0} \exp(-\epsilon_{\rm PN}/k_B T), \tag{49}$$

where

$$D_{k0} \approx \begin{cases} a^2 \omega_{\rm PN}/2\pi & \text{if } \eta_{lk} < \eta < \omega^*_{\rm PN}, \\ a^2 \omega_{\rm PN} \omega^*_{\rm PN}/2\pi\eta_k & \text{if } \eta > \omega^*_{\rm PN}. \end{cases} \tag{50}$$

Here $\omega_{\rm PN} = \sqrt{V''_{\rm PN}(0)/m_k}$, $\omega^*_{\rm PN} = \sqrt{-V''_{\rm PN}(a/2)/m_k}$, and $\eta_{lk} = \omega_{\rm PN} k_B T/2\pi\epsilon_{\rm PN}$. For the trivial GS the activated kink diffusion was predicted by Pietronero and Strässler[30] (see also Refs. 31 and 32) and observed in molecular-dynamics simulation by Combs and Yip.[33]

In the FK chain with strong coupling, for a $G[\theta]$ with a simple elementary cell the inequality $\epsilon_{\rm PN} < \epsilon_k$ may be easily fulfilled. In the temperature interval $\epsilon_{\rm PN} < k_B T \ll \epsilon_k$ the kink diffusion coefficient may be found in the form (see, e.g., Refs. 34, 19, and 35)

$$D_k \approx \frac{k_B T}{m_k \eta_k} \left[1 - \frac{1}{8} \left(\frac{\epsilon_{\rm PN}}{k_B T} \right)^2 \right]. \tag{51}$$

When the $G[\theta]$ of the system is nontrivial, i.e., $\theta \neq 1/q$, the phenomenological approach is useful not only to be applied for the lowest temperature subinterval in the hierarchy of the kink lattices, but also at the left-hand side of any of these subintervals. For example, for $\theta = (q-1)/q$ with $q \gg 1$ for temperature $\epsilon_{sk} \leq k_B T \ll \epsilon_{tk}$ the GS may be considered as a system consisting of N_w weakly interacting residual t antikinks. If collisions of these kinks are approximately elastic (as they are in the SG model), the kink collective-diffusion coefficient

$$D_{\mu k} \equiv \int_0^\infty dt\, N_w^{-1} \sum_{kk'}^{N_w} \langle \dot{X}_k(t) \dot{X}_{k'}(0) \rangle$$

coincides with the diffusion coefficient of a single kink for the same reference structure (namely, with the diffusion coefficient of a single t antikink). On the other hand, the chemical diffusion coefficient of the kink is equal to $D_{ck} = D_{\mu k}/\chi_k$, where χ_k is the dimensionless susceptibility of the t antikink system. When the PN barrier for the t antikinks may be neglected, which is valid for $\epsilon^{\bar{t}k}_{\rm PN} \ll k_B T$, the susceptibility χ_k is calculated with the help of perturbation theory[1] and the result is given by the integral $\chi_k \approx \left[1 + (n_w/k_B T) \int_{-\infty}^{\infty} dX\, v_{\rm int}(X) \right]^{-1}$, where $n_w = N_w/L$ is the concentration of the residual t antikinks. Otherwise, for $k_B T \ll \epsilon^{\bar{t}k}_{\rm PN}$ the system Hamiltonian reduces to that for an effective lattice-gas model, and χ_k is equal to $\chi_k \approx 1 - \theta_w$, where $\theta_w = N_w/M$.

V. CONDUCTIVITY AND DIFFUSIVITY OF THE MODEL

In order to find the system diffusion coefficients in the framework of the phenomenological approach, let us suppose that at low temperatures the GS of the FK chain contains a certain number of phonon modes, kinks, and antikinks, neglecting the mutual influence of one excitation on others. In this case the atomic displacements can be represented as the sum

$$u_l(t) = u^{\rm ph}_l(t) + \sum_{j=1}^{N_{\rm tot}} u^{\rm kink}_l[\sigma_j, X_j(t)], \tag{52}$$

where $u^{\rm kink}_l(\sigma, X)$ stands for the shape of a slowly moving kink with the coordinate X and the topological charge σ, and $u^{\rm ph}$ describes phonons adjusted to the kinks. From Eq. (52) we obtain for the atomic velocities the expression

$$\dot{u}_l(t) = \dot{u}^{\rm ph}_l(t) + \sum_{j=1}^{N_{\rm tot}} \dot{X}_j(t) w_l[\sigma_j, X_j(t)], \tag{53}$$

where $w(\sigma, X) = \frac{\partial}{\partial X} u^{\rm kink}(\sigma, X)$.

Substituting Eq. (53) into Eqs. (2) – (4) for $\mathcal{D}_\mu(t)$, we obtain three types of terms. The contribution from the phonon correlation function $\langle \dot{u}^{\rm ph}(t) \dot{u}^{\rm ph}(0) \rangle$ is $\Delta\bar{\mathcal{D}}^{\rm ph}_\mu(\bar{\omega}) = D_f \sum_\kappa i\bar{\omega}\eta/[i\bar{\omega}\eta + \bar{\omega}^2 - \omega^2_{\rm ph}(\kappa)]$, where κ stands for the phonon modes with the frequencies $\omega_{\rm ph}(\kappa)$. Because the phonon spectrum of the FK chain is optical, i.e., $\omega_{\rm ph}(\kappa) \geq \omega_0$, this contribution tends to zero in the limit $\bar{\omega} \to 0$. The mixed correlation functions $\langle \dot{u}^{\rm ph}(t) \dot{X}_j(0) \rangle$ describe kink-phonon interactions. Although a rigorous calculation of these functions is too complicated, in the phenomenological approach we may assume that these interactions are already taken into account if the kink concentration and the kink friction coefficient η_k are calculated in a way which includes the kink-phonon interactions. Finally, in order to find the last contribution, let us assume that the kink concentration is small, $n_{\rm tot} \ll n$, so that kinks can be considered as independent quasiparticles. This assumption yields

$$\int_0^\infty dt\langle \dot{X}_j(t)\dot{X}_{j'}(0)\rangle = \delta_{jj'}D_{k(\bar{k})}, \tag{54}$$

where $D_{k(\bar{k})}$ is the diffusion coefficient for a single kink (antikink). Then, using Eq. (54) and the equality

$$\sum_l w_l(X) = \frac{d}{dX}\sum_l u_l^{\rm kink}(X) = \frac{d}{dX}\left(\frac{X}{q}\right) = \frac{1}{q}, \tag{55}$$

which follows from Eq. (12), we obtain the approximate expression for the collective diffusion coefficient D_μ,

$$D_\mu \approx \frac{1}{q^2 N}\left(\langle N_k\rangle D_k + \langle N_{\bar{k}}\rangle D_{\bar{k}}\right). \tag{56}$$

Thus, the conductivity of the FK chain is directly proportional to the total kink concentration (see also Refs. 30, 34, and 36).

For the standard FK model with the trivial GS at $\theta = 1$, in the strong-coupling limit when the SG equation is valid, we can take $D_k = D_{\bar{k}} = k_BT/m_k\eta$, $\langle N_k\rangle = \langle N_{\bar{k}}\rangle = Na_s\omega_0\sqrt{2m_k/\pi k_BT}\exp(-\epsilon_k/k_BT)$, $m_k = 2m_a/\pi^2\sqrt{g_a}$, and $\epsilon_k = 4\epsilon_s\sqrt{g_a}$, thus obtaining from Eq. (56) the expression

$$D_\mu^{(\rm SG)} \approx D_f(\pi m_a\omega_0^2 a_s^2/\epsilon_s)^{1/2}(\epsilon_k/k_BT)^{1/2} \times \exp(-\epsilon_k/k_BT). \tag{57}$$

This result was obtained by Landauer and Büttiker[37] with the help of the generalized rate theory (see also Ref. 38).

While the collective-diffusion coefficient is known, the chemical diffusion coefficient can be obtained as $D_c = D_\mu/\chi$. Using Eq. (36) for χ, we can find from Eq. (56) that

$$D_c \approx \frac{\langle N_k\rangle D_k + \langle N_{\bar{k}}\rangle D_{\bar{k}}}{\langle N_k\rangle + \langle N_{\bar{k}}\rangle}. \tag{58}$$

We should note that by kinks (antikinks) in Eqs. (56) and (58) we must understand those "kinks" (trivial kinks, superkinks, super-superkinks, etc.) which are well defined as quasiparticles at a given temperature interval for a given coverage θ.

For the lowest temperature interval of the kink-lattice hierarchy, Eq. (58) leads to

$$D_c \approx \tfrac{1}{2}(D_k + D_{\bar{k}}). \tag{59}$$

When the $G[\theta]$ is nontrivial, i.e., $\theta \neq 1/q$, Eq. (58) allows us to find the chemical diffusion coefficient at the left-hand side of each temperature subinterval of the hierarchy. Indeed, in this case the number of residual kinks (or antikinks) exceeds the number of thermally excited kink-antikink pairs, $\langle N_w\rangle \gg \langle N_{\rm pair}\rangle$, and, therefore, using the condition $\langle N_k\rangle \gg \langle N_{\bar{k}}\rangle$ (or $\langle N_k\rangle \ll \langle N_{\bar{k}}\rangle$) in Eq. (58), we obtain

$$D_c \approx D_k \ (\text{or } D_{\bar{k}}). \tag{60}$$

For example, let us consider the coverages $\theta_\pm$ defined by $\theta_\pm = (q \pm 1)/q$ with $q \gg 1$, which are close to the trivial coverage $\theta_0 = 1$. According to Eq. (60), we would have $D_c(\theta_+) \approx D_{tk}$ and $D_c(\theta_-) \approx D_{t\bar{k}}$ at the temperature interval $\epsilon_{sk} < k_BT \ll \epsilon_{tk}$.

The result (60) has a simple physical interpretation. Indeed, for $k_BT \leq \epsilon_k$ the mass transport along the chain is carried out by kinks. Because the concentration of kinks is proportional to the concentration of atoms, the ratio of the flux of kinks to the gradient of the kink concentration (which determines the coefficient D_{ck}) is exactly equal to the ratio of the atomic flux to the atomic gradient [which defines the coefficient D_c according to Fick's law (6)]. Moreover, this explanation shows that, in order to take into account kink-kink interactions, we should use, instead of Eq. (60), the equation $D_c \approx D_{ck}$ (or $D_{c\bar{k}}$), where D_{ck} is the chemical diffusion coefficient for kinks determined in the previous section.

Now we can qualitatively describe dependences of the diffusion coefficients D_c and D_μ on temperature T and the atomic concentration n. Let us begin from the temperature dependence. For definiteness, we consider a physically important case when $\theta \leq 1$, namely, $\theta = (q-1)/q$ with $q \gg 1$. Recall that the $T = 0$ GS of the chain is the commensurate structure with the period $a = qa_s$, and topologically stable excitations are s kinks (s antikinks) which are characterized by the effective mass m_{sk} and the half-pair creation energy ϵ_{sk}. The adiabatically slow motion of the s kinks is carried out in the PN periodic relief described by $V_{\rm PN}^{sk}(X) \approx \frac{1}{2}\epsilon_{\rm PN}^{sk}[1-\cos(2\pi X/a)]$ with the height $\epsilon_{\rm PN}^{sk}$, and small vibrations of the kink at the bottom of the PN potential are characterized by the PN frequency $\omega_{\rm PN}^{sk} \approx \sqrt{\epsilon_{\rm PN}^{sk}/2q^2m_{sk}}$. The effective friction for a moving s kink we denote by η_{sk}. According to Sec. II, the described $T = 0$ GS can be treated as a regular lattice of trivial ($\theta = 1$) antikinks.

At the lowest temperature interval, $0 < k_BT < \epsilon_{sk}$, mass transport along the chain is carried out by s kinks, and the chemical diffusion coefficient is equal to

$$D_c \approx \mathcal{K}_{sk}(qa_s)^2\exp(-\epsilon_{\rm PN}^{sk}/k_BT), \tag{61}$$

where

$$\mathcal{K}_{sk} \approx \begin{cases} \omega_{\rm PN}^{sk}/2\pi & \text{if } \eta_{sk} < \omega_{\rm PN}^{sk}, \\ \left(\omega_{\rm PN}^{sk}\right)^2/2\pi\eta_{sk} & \text{if } \eta_{sk} > \omega_{\rm PN}^{sk}, \end{cases} \tag{62}$$

while the collective-diffusion coefficient is determined by the expression

$$D_\mu \approx D_c\frac{(\langle N_{sk}\rangle + \langle N_{\bar{sk}}\rangle)}{q^2\langle N\rangle} \propto \exp[-(\epsilon_{\rm PN}^{sk} + \epsilon_{sk})/k_BT]. \tag{63}$$

Notice that both D_c and D_μ have the Arrhenius form but they are determined by different activation energies. When temperature increases, $k_BT \to \epsilon_{sk}$, the number of thermally excited sk-$\bar{sk}$ pairs also increases, and their mutual attraction should decrease the values of D_c and D_μ in comparison with those given by Eqs. (61) – (63).

When the temperature increases to be above the "melting" temperature $T_{sk} \approx \epsilon_{sk}/k_B$, the lattice of t antikinks becomes disordered due to thermal creation of a large quantity of sk-$\bar{sk}$ pairs. According to the kink-lattice-

hierarchy ideology of Sec. III, within the temperature interval $\epsilon_{sk} < k_BT < \epsilon_{tk}$ the equilibrium state of the FK chain can be considered as a commensurate structure with the period a_s where, however, there exist $N_w = N/q$ residual t antikinks and $N_{\rm pair}$ thermally created tk-$\bar{tk}$ pairs. Let ϵ_{tk} denote the half-pair creation energy of the $\theta = 1$ kinks, m_{tk} denote their effective mass, and $V_{\rm PN}^{tk}(X) \approx \frac{1}{2}\epsilon_{\rm PN}^{tk}[1 - \cos(2\pi X/a_s)]$ denote the shape of the PN relief, so that $\omega_{\rm PN}^{tk} \approx \sqrt{\epsilon_{\rm PN}^{tk}/2m_{tk}}$ is the PN frequency, and η_{tk} stands for the corresponding friction coefficient. Notice that the parameters of s kinks and t kinks satisfy two inequalities, $\epsilon_{\rm PN}^{sk} < \epsilon_{\rm PN}^{tk} < \epsilon_s$ and $\epsilon_{sk} < \epsilon_{tk}$.

At low temperatures, $\epsilon_{sk} < k_BT < \min(\epsilon_{\rm PN}^{tk}, \epsilon_{tk})$, the superkinks are likely destroyed by thermal fluctuations, but the trivial kinks still exist, and this time they are responsible for the mass transport. Neglecting interactions of t kinks, we obtain

$$D_c \approx \mathcal{K}_{tk} a_s^2 \exp(-\epsilon_{\rm PN}^{tk}/k_BT), \tag{64}$$

$$\mathcal{K}_{tk} \approx \begin{cases} \omega_{\rm PN}^{tk}/2\pi & \text{if } \eta_{tk} < \omega_{\rm PN}^{tk}, \\ \left(\omega_{\rm PN}^{tk}\right)^2/2\pi\eta_{tk} & \text{if } \eta_{tk} > \omega_{\rm PN}^{tk}, \end{cases} \tag{65}$$

$$D_\mu \approx \frac{D_c}{q}\left(1 + \frac{4q^2 m_{tk}\omega_0^2 a_s^2}{\pi k_BT} e^{-\epsilon_{tk}/k_BT}\right). \tag{66}$$

The mutual repulsion of the residual t antikinks increases the values of D_c and D_μ in comparison with those defined by Eqs. (64) – (66).

Analogously, we may describe the case of the $G[s/q]$ with $2 \le s \le q-2$, when the kink-lattice hierarchy consists of more than two temperature intervals.

The limits of the intermediate temperature interval depend on the model parameter g_s; namely, when $g_s \ge 1$, there exists the temperature interval $\epsilon_{\rm PN}^{tk} < k_BT < \epsilon_{tk}$, within which t kinks still exist, but their motion is not thermally activated. In this case we have

$$D_c \approx \frac{k_BT}{m_{tk}\eta_{tk}}\left[1 - \frac{1}{8}\left(\frac{\epsilon_{\rm PN}^{tk}}{k_BT}\right)^2\right] \tag{67}$$

and

$$D_\mu \approx D_c \frac{\langle n_{\rm tot}\rangle}{\langle n\rangle} \propto \exp(-\epsilon_{tk}/k_BT). \tag{68}$$

The described analytical predictions are in good agreement with molecular-dynamics simulations of Holloway and Gillan[4] carried out for the standard undamped FK chain, if we put in Eq. (67) $\eta_{tk} = \eta_{\rm int} \approx 0.028\omega_0$.

If $g_s \ll 1$, the intermediate temperature interval is determined as $\epsilon_{tk} < k_BT < \epsilon_{\rm PN}^{tk}$. Within this interval the diffusion coefficient can be found only numerically. It may be expected, however, that D_c and D_μ will have the Arrhenius behavior with the activation energy $\epsilon_s^{\rm eff}$ where $\epsilon_{\rm PN}^{tk} < \epsilon_s^{\rm eff} < \epsilon_s$.[12]

Finally, at high temperatures, $k_BT > \max(\epsilon_s, \epsilon_{tk})$, a perturbation theory approach may be used which leads to the expression (7).

Let us describe now the behavior of the diffusion coefficients as functions of the coverage $\theta \equiv a_s/a_A$. As can be seen from Eq. (7), at high temperature within the interval $k_BT > \max(\epsilon_s, \epsilon_{tk})$, the collective diffusion coefficient $D_\mu(\theta)$ shows oscillations as a function of θ, achieving minima for the trivial ground states when $\theta = 1/q$, where the atoms in the GS are situated at the bottoms of the substrate potential wells. On the other hand, local maxima of $D_\mu(\theta)$ occur at $\theta = 2/(2q-1)$. Maxima and minima of $D_\mu(\theta)$ become more pronounced with increase of the interatomic interaction and decrease of temperature. Because for the exponential interaction (8) the parameter g_A defined by Eq. (9) increases with θ, the amplitude of the oscillations of the diffusion coefficient $D_\mu(\theta)$ will also increase with θ. Thus, the dc conductivity of the FK chain as a function of θ, $\sigma(\theta) \propto \theta D_\mu(\theta)$, would have an absolute maximum within the interval $0 \le \theta \le 1$ at the concentration value θ between 0.75 and 0.80 (cf. Ref. 13).

At low temperatures, the phenomenological approach developed above leads to similar behavior of the function $D_\mu(\theta)$. Indeed, let us consider the FK chain within the temperature interval $\epsilon_{sk} < k_BT < \min(\epsilon_{\rm PN}^{tk}, \epsilon_{tk})$ for coverage θ which is close to the value $\theta_0 = 1$, i.e. $|\theta - \theta_0| \ll 1$, when interaction between the residual t kinks is small enough so that they do not form a kink lattice. In this case the chemical diffusion coefficient D_c is equal to D_{tk} for $\theta > \theta_0$ and $D_{\bar{tk}}$ for $\theta < \theta_0$, and it is approximately independent of θ. Because the quantity of thermally excited kinks $\langle N_{\rm pair}\rangle$ is approximately independent of θ while the quantity of the residual kinks $|N_w|$ linearly increases with $|\theta - \theta_0|$, the susceptibility $\chi \approx \langle N_{\rm tot}\rangle/N$ as a function of θ should have a local minimum at $\theta = \theta_0$. Therefore the function $D_\mu(\theta)$ will have a local minimum at $\theta = \theta_0$ too. Analogously, the function $D_\mu(\theta)$ will have local minima at each of those commensurate coverages θ_0 whose "melting" temperature $T_{\rm melt}(\theta_0)$ is larger than T. It is clear that between the neighboring local minima the function $D_\mu(\theta)$ has local maxima. At high temperatures this criterion is fulfilled only for the trivial coverages $\theta_0 = 1/q$. But with decrease of T, new local minima of the function $D_\mu(\theta)$ will arise and they correspond to higher-order commensurate structures, and in the limit $T \to 0$ the function $D_\mu(\theta)$ should have minima at each rational value of the coverage parameter θ. It is clear that the values of $D_\mu(\theta)$ at those minima will tend to zero according to the Arrhenius law, provided $T \to 0$. Otherwise, local maxima of $D_\mu(\theta)$ at irrational θ will tend to infinity when $T \to 0$ provided the dimensionless elastic constant $g_A(\theta)$ of the model is larger than the Aubry threshold $g_{\rm Aubry}(\theta)$ where the $T = 0$ GS exhibits the existence of the "sliding mode." In the opposite case, i.e., when $g_A(\theta) < g_{\rm Aubry}(\theta)$, the value of $D_\mu(\theta)$ at local minima will tend to zero for $T \to 0$ according to the Arrhenius law, too.

The behavior of the function $D_c(\theta)$ becomes clear if we recall that the mass transport along the chain is carried out by kinks at $\theta = \theta_0 + \delta$ and by antikinks at $\theta = \theta_0 - \delta$ (where $\delta \to 0$), provided the temperature T of the system is lower than the "melting" temperature

$T_{\rm melt}(\theta_0)$ for the structure with a given value of $\theta = \theta_0$. For anharmonic interatomic interactions such as the exponential law (8), the PN barriers for the kinks are lower than those for antikinks. Therefore, when the coverage parameter θ increases passing through the value θ_0, the activation energy for the chemical diffusion decreases in a jumplike way. Consequently, the dependence given by $D_c(\theta)$ should behave similarly to the inverse devil's staircase: the value of D_c will rise sharply each time whenever the coverage parameter θ exceeds the value θ_0 that characterizes the structure which is commensurate with the substrate and has a "melting" temperature larger than T. It may be predicted also that both the diffusion activation energy and (owing to decrease of the free path length of kinks) the preexponential factor in the formula for $D_c(\theta)$ decrease simultaneously with increasing θ (the so called compensation effect). It is clear that the jump in $D_c(\theta)$ at a given $\theta = \theta_0$, as well as a local minimum for $D_\mu(\theta)$, exists only if $T < T_{\rm melt}(\theta_0)$; when the temperature increases to be above $T_{\rm melt}(\theta_0)$, the singularities disappear. Thus the structure of the inverse devil's staircase for $D_c(\theta)$ [and an irregular structure for $D_\mu(\theta)$] will be smoothed with increasing temperature, since only those singularities which correspond to the simple commensurate structures ($\theta_0 = 1, \frac{1}{2}$, etc.) will "survive."

VI. CONCLUSIONS

In conclusion, using a phenomenological approach based on the ideal kink-gas ideology and the hierarchy of "melted" kink lattices, we have analyzed the diffusion coefficients of the anharmonic FK chain as functions of the dimensionless concentration θ and temperature T. We have shown that the chemical diffusion coefficient $D_c(\theta)$ as a function of θ has a form similar to the inverse devil's staircase, i.e., the function $D_c(\theta)$ should exhibit jumps at those rational values of θ where, at a given value of T, the corresponding commensurate structure has a short-range order that allows one to describe the system dynamics in terms of the well-defined kink excitations. At the same time, the chain conductivity $\sigma(\theta) \propto \theta D_\mu(\theta)$ will display local minima at the same rational values of the coverage θ. The quantity of such singularities, i.e., the quantity of the jumps for $D_c(\theta)$ and the minima for $D_\mu(\theta)$, should increase with decreasing T.

The predicted behavior of the diffusion coefficients D_c and D_μ is expected to be observed in those physical objects which may be described with the help of the anharmonic FK model, such as one-dimensional conductors and adsorbed layers. For example, the experimentally measured dc conductivity of one-dimensional conductors exhibits a local maximum between $\theta = 0.75$ and $\theta = 0.80$,[13] i.e., $D_\mu(\theta)$ has local minima at $\theta_1 = \frac{1}{2}$ and $\theta_2 = 1$, and a local maximum between those values. According to our predictions, at lower temperatures the function $D_\mu(\theta)$ would have, additionally to the minima at θ_1 and θ_2, a local minimum at $\theta_3 = \frac{2}{3}$. Then, with further decrease of temperature, an additional minimum would appear at $\theta_4 = \frac{3}{4}$, and so on.

Referring to adsorbed layers, we should mention the sharp increase of the chemical diffusion coefficient for Ag atoms adsorbed on a stepped (vicinal) Ge surface when the concentration of atoms increases to be above the value corresponding to the commensurate (4×2) structure of adsorbed atoms.[39] Unfortunately, we do not know at the moment the detailed results of investigations for surface diffusion on furrowed surfaces, although preliminary results of Vedula and Paliy[40] are in good qualitative agreement with the predictions of the present analysis.

Finally, we would like to mention briefly possible generalizations of the model. First, in more realistic physical models the periodic substrate potential may have a more complicated than sinusoidal shape. If the shape of the potential $V_{\rm sub}(x)$ allows the existence of different types of kinks, the low-temperature activation energy which determines the diffusion coefficients will be given by the contribution of the kinks corresponding to the largest value of the PN barrier. Second, in real physical objects we have not a single isolated chain but, instead, a system of weakly coupled parallel FK chains. The interaction between the chains leads to interaction between kinks in the chains and, therefore, to a modification of the diffusion coefficients. Third, in the model we have investigated in the present work, atoms were allowed to move along one-dimensional "channels" only. But with increasing of interatomic repulsion, for example, by means of increasing θ, compression forces in the atomic chain may become so strong that the atoms may escape from the channel, and the atoms will also move in the transversal direction. In such a case, we should use the FK model with a transversal degree of freedom.[41] Finally, it would also be important to investigate two- (and three-) dimensional FK models as well as to take into account a possible role of impurities in the effects described above.

ACKNOWLEDGMENTS

O. Braun was partially supported by a Soros grant awarded by the American Physical Society. Yu. Kivshar and O. Braun are indebted to K. H. Spatschek for hospitality at Institut für Theoretische Physik I (Düsseldorf) where a part of the work in this paper was done.

* Also at Institute for Low Temperature Physics and Engineering, Ukrainian Academy of Sciences, UA-310164 Kharkov, Ukraine.

[1] W. Dieterich and I. Peschel, Physica A **95**, 208 (1979).

[2] A. A. Tarasenko and A. A. Chumak, Poverkhnost' No. 11, 98 (1989); V. P. Zhdanov, Phys. Lett. A **161**, 556 (1992).

[3] A. G. Naumovets and Yu. S. Vedula, Surf. Sci. Rep. **4**, 365 (1985); R. Gomer, Rep. Prog. Phys. **53**, 917 (1990).

[4] R. W. Holloway and M. J. Gillan, Solid State Commun. **52**, 705 (1984); M. J. Gillan and R. W. Holloway, J. Phys. C **18**, 4903 (1985).
[5] M. J. Gillan and R. W. Holloway, J. Phys. C **18**, 5705 (1985).
[6] Ya. Frenkel and T. Kontorova, Phys. Z. Sowjetunion **13**, 1 (1938).
[7] H. R. Paneth, Phys. Rev. **80**, 708 (1950).
[8] I. F. Lyuksyutov, A. G. Naumovets, and V. L. Pokrovsky, *Two-Dimensional Crystals* (Naukova Dumka, Kiev, 1983) (in Russian; English translation: Academic, Boston, 1992).
[9] J. B. Boyce and B. A. Huberman, Phys. Rep. **51**, 189 (1979).
[10] St. Pnevmatikos, A. V. Savin, A. V. Zolotaryuk, Yu. S. Kivshar, and M. J. Velgakis, Phys. Rev. A **43**, 5518 (1991).
[11] O. M. Braun and Yu. S. Kivshar, Phys. Rep. (to be published).
[12] T. Munakata and A. Tsurui, Z. Phys. B **34**, 203 (1979).
[13] T. Geisel, Phys. Rev. B **20**, 4294 (1979).
[14] A. R. Bishop, W. Dieterich, and I. Peschel, Z. Phys. B **33**, 187 (1979).
[15] S. Aubry, Physica D **7**, 240 (1983).
[16] J. F. Currie, J. A. Krumhansl, A. R. Bishop, and S. E. Trullinger, Phys. Rev. B **22**, 477 (1980).
[17] O. M. Braun, Yu. S. Kivshar, and I. I. Zelenskaya, Phys. Rev. B **41**, 7118 (1990).
[18] A. Milchev and I. Markov, Surf. Sci. **136**, 503 (1984); **136**, 519 (1984); **145**, 313 (1984); **156**, 392 (1985).
[19] D. J. Bergman *et al.*, Phys. Rev. A **27**, 3345 (1983).
[20] C. R. Willis, M. El-Batanouny, and P. Stancioff, Phys. Rev. B **33**, 1904 (1986).
[21] Y. Hsu, Phys. Rev. D **22**, 1394 (1980).
[22] B. Joos, Solid State Commun. **42**, 709 (1982).
[23] B. Joos, B. Bergersen, R. J. Gooding, and M. Plischke, Phys. Rev. B **27**, 467 (1983).
[24] R. Schilling, *Phase Transitions and Relaxation in Systems with Competing Energy Scales* (Kluwer Academic Publishers, Dordrecht, 1993), p. 285.
[25] R. E. Peierls, Helv. Phys. Acta **7**, 81 (1934).
[26] S. E. Trullinger, Phys. Rev. B **22**, 418 (1980).
[27] J. F. Currie, M. B. Fogel, and F. L. Palmer, Phys. Rev. A **16**, 796 (1977).
[28] M. J. Gillan, J. Phys. C **18**, 4885 (1985).
[29] H. A. Kramers, Physica **7**, 284 (1940).
[30] L. Pietronero and S. Strässler, Solid State Commun. **27**, 1041 (1978).
[31] J. A. Combs and S. Yip, Phys. Rev. B **28**, 6873 (1983).
[32] C. Kunz and J. A. Combs, Phys. Rev. B **31**, 527 (1985).
[33] J. A. Combs and S. Yip, Phys. Rev. B **29**, 438 (1984).
[34] M. Remoissenet, Solid State Commun. **27**, 681 (1978).
[35] F. Marchesoni, Phys. Lett. A **115**, 29 (1986).
[36] A. R. Bishop, J. Phys. C **11**, L329 (1978).
[37] M. Büttiker and R. Landauer, J. Phys. C **13**, L325 (1980).
[38] H. U. Beyeler, L. Pietronero, and S. Strässler, Phys. Rev. B **22**, 2988 (1980).
[39] E. Suliga and M. Henzler, J. Phys. C **16**, 1543 (1983).
[40] Yu. S. Vedula and M. V. Paliy (private communication).
[41] O. M. Braun and Yu. S. Kivshar, Phys. Rev. B **44**, 7694 (1991); O. M. Braun, O. A. Chubykalo, Yu. S. Kivshar, and L. Vázquez, *ibid.* **48**, 3734 (1993).