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The Frenkel-Kontorova Model With Nonconvex Interparticle Interactions

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We present an analytical and numerical study of a chain of atoms moving in a periodic potential with nonlinear, nonconvex interparticle interactions, described by the Hamiltonian

$$H = \sum_n \frac{1}{2}\dot{u}_n^2 + A(u_{n+1} - u_n)^4 - B(u_{n+1} - u_n)^2 - \cos(u_n)$$

The ground state is shown to be homogeneous for B < 1/8 and dimerized for B > 1/8. The nonconvexity is shown to also play an important role when excitations are considered. In the dimerized phase, we define the staggered order parameter $v_n = (-1)^n u_n$ and map the model to the on-site ϕ^4 problem. In particular we find a localized kink solution, v = tgh(x/d), with a width d varying form infinity at B = 1/8 to zero at B = 3/16, where the interparticle interactions in the ground state crossover from the nonconvex region to the convex one. We also show that at this point the kinks are pinned to the lattice. These results are verified by a direct numerical simulation of the discrete model. Finite temperature effects are discussed in terms of a displacive phase transition at B = 1/8 becoming order disorder transition at B = 3/16. When coupling between the springs is introduced by adding a strain gradient term $G(u_{n-1} - 2u_n + u_{n+1})^2$ to the Hamiltonian, we observe a crossover from an infinite kink width at B = 1/8 to a finite width for B > 3/16, determined by the competition between the effective double well and the interspring coupling.

Physical systems with competing interactions that include incommensurate length scales have become a subject of intense interest because they can lead both to modulated ground states and to unusual dynamics and excitations. Most of the theoretical studies to date have been limited to cases where the interparticle interactions are convex and where there are two competing length scales. For these cases it was shown [1] that the ground states are always periodic or quasi-periodic and that the phase transitions are continuous. Those results are valid only for convex interparticle interactions and it was shown by Aubry, Fesser and Bishop [2] that first order phase transitions might occur when nonconvexity is introduced. See also Griffiths et al. [3] and Marchand et al. [4]. It is well known that nonconvex interparticle interactions can exist in condensed matter systems. Example are, the RKKY oscillatory exchange interactions between localised spins in metals, and oscillating indirect interactions mediated by elastic strains [5]. Nonconvex interparticle interactions are also present in a Ginzburg Landau energy functional for the strains in materials undergoing elastic phase transitions (e.g. Barsch and Krumhansl [6]).

To study the effects of nonconvexity we use here an extention of the familiar (e.g. Aubry and LeDaeron [1]) Frenkel-Kontorova model into which we introduce degenerate double well interparticle springs. The Hamiltonian for the system is given by:

$$H = \sum_n \frac{1}{2}\dot{u}_n^2 + A(u_{n+1} - u_n - a)^4 - B(u_{n+1} - u_n - a)^2 - \cos(u_n) \quad (1)$$

This is in general a model with <u>three</u> competing lengths: $L_{1,2} = a \pm L_0$, the minima of the double well spring $L_0^2 = B/2A$) and $L_3 = 2\pi$, determining the minima of the substrate potential. However, we limit ourselves here to the study of the homogeneous and dimerized phases by setting a = 0, i.e. <u>two</u> competing lengths. For this case the configuration where the particles are at the minima of the substrate potential, $u_n = 0$, is such that the interparticle interaction energies are at their maxima. It is then easy to see that the system can lower its energy (for a large enough value of B) by dimerization, and the ground state configuration is $u_n = \frac{1}{2}(-1)^n u_0$ where u_0 is determined by the competition between the substrate and interparticle energies: Substituting in (1) and minimizing with respect to u_0 we obtain

$$4Au_0^3 - 2Bu_0 + 1/2\,\sin(u_0/2) = 0 \tag{2}$$

Eq. (2) has the solutions $u_0 = 0$ and $u_0 \pm[(B-1/8)/(2A-1/192)]^{1/2}$ where we have approximated $\sin(u/2)$ by $u/2 - 1/6u$). Thus, for $B < 1/8$ the ground state will be homogeneous, $u_n = 0$, while for $B > 1/8$ it will be dimerized.

To study excitations of the system in the dimerized phase, we consider first the staggered order parameter $v_n = (-1)^n u_n$. In the ground state $v_n = 0$ (homogeneous phase) and $v_n = +(-)u_0/2$ dimerized long-short (short-long) springs, respectively. Substituting a continuum approximation $v_{n\pm 1} = v_n \pm hv' + \frac{1}{2}h^2v''$, in the Hamiltonian and equations of motion we obtain:

$$H = \dot{v}^2/2 + v'^2/2\,(2B - 48Av^2) + 16Av^4 - 4Bv^2 - \cos(v) \tag{3}$$

$$\ddot{v} = 8Bv - 64Av^3 - \sin(v) + (2B - 48Av^2)v'' - 48Avv'^2 \tag{4}$$

We have obtained traveling wave solutions to equation (4) numerically (Fig. 1), a limit of which are the solitary wave solutions of Fig. 2. The physical meaning of the kink solutions in the context of our model is a change between two topologically inequivalent ground states from a "short-long" spring length configuration at one end of the chain, to a "long-short" one at the other end. The main properties of the kink solutions are: (i) their width d is a decreasing function of the velocity and of B; and (ii) pinning of the kink occurs for $B = 3/16$ where the static kink width vanishes and the continuum approximation breaks down. Since equations (3) and (4) were obtained in a continuum approximation, we have checked that the above properties of the kinks are valid for the discrete model (1) as well. To do this we numerically solved the equations of motion derived from (1), imposing, via boundary conditions, a single kink in the chain. To obtain the static defect configuration, we started from homogeneous initial positions and random velocities for the particles, and "cooled" the chain by adding a damping term $\epsilon \dot{u}_n$ to the equations of motion. After the velocities became sufficiently small, we turned off the damping and checked that the final configuration obtained is indeed a static solution of the equations of motion. For $B < 3/16$ (Fig. 3a) the change from $u_n = \frac{1}{2}(-1)^n u_0$ at the left of the chain to $u = \frac{1}{2}(-1)^{n+1} u_0$ at the right is indeed gradual and the continuum approximation is appropriate, while for $B > 3/16$ (Fig. 3b) the kink is pinned to one site having an abrupt "Ising wall" shape. All these properties can be analysed by mapping our Hamiltonian to an on-site ϕ^4 model, as we now show.

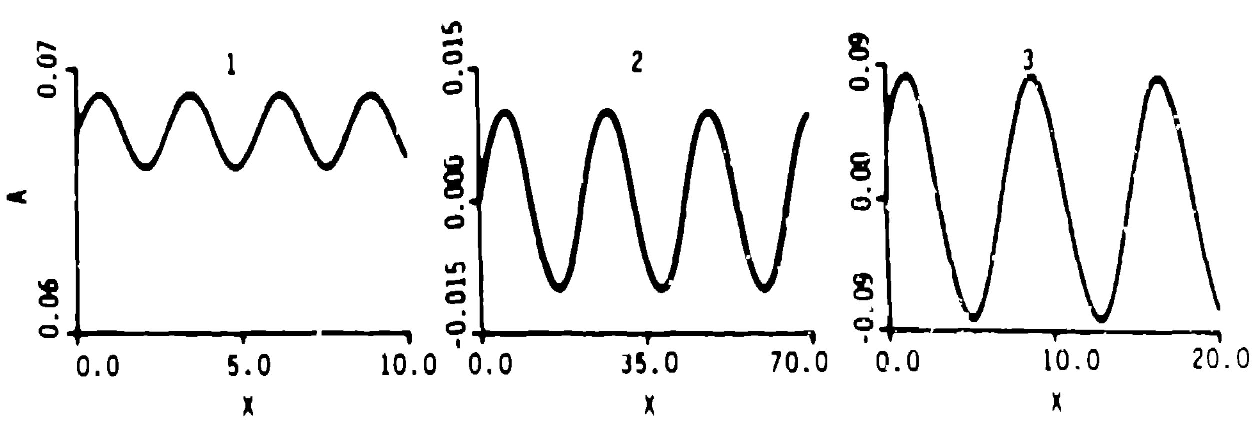

Fig. 1. Traveling wave solutions of eqn. (4). The numbers are from the ϕ^4 terminology [7].

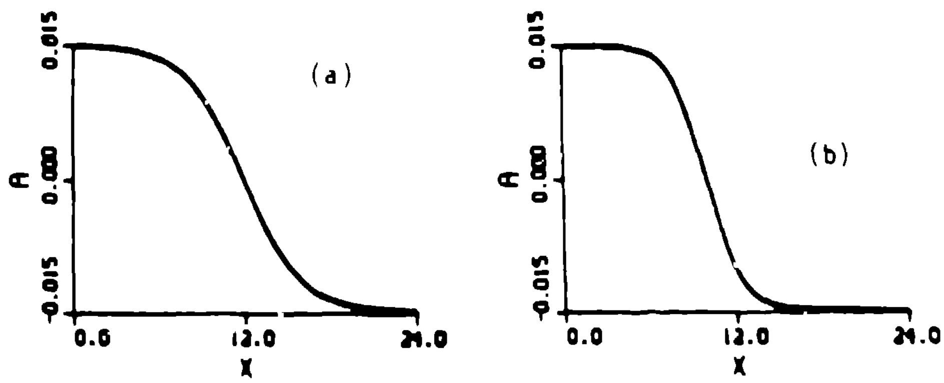

Fig. 2. The solitary kink solution obtained as an infinite period limit of solution No. 2 in Fig. 1.

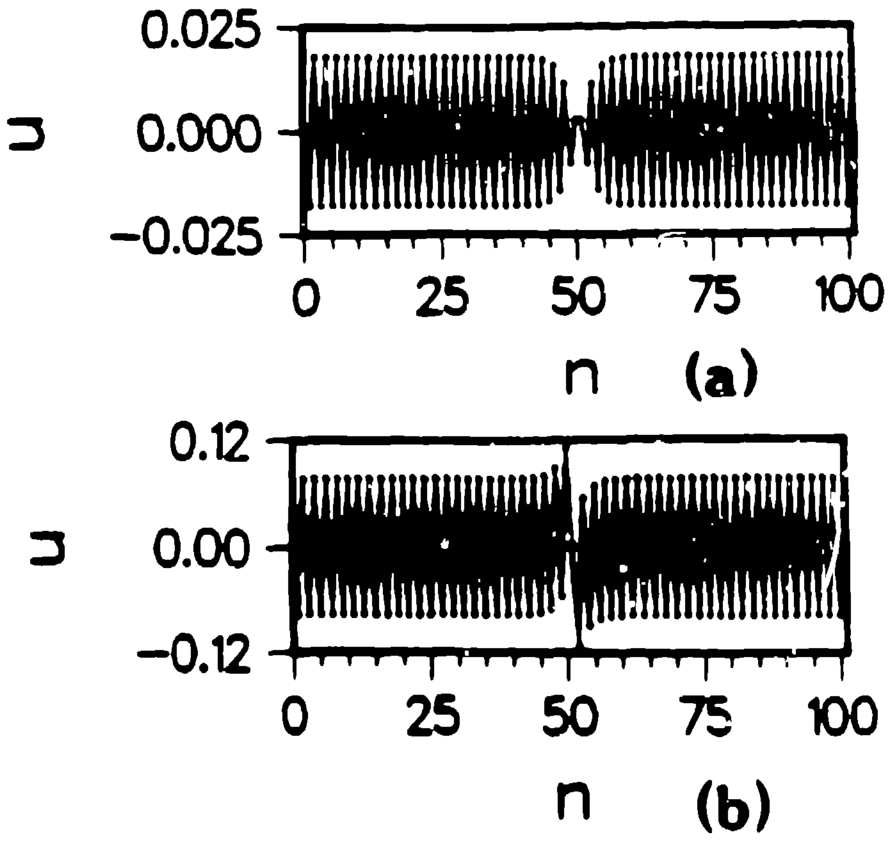

Fig. 3 The discrete solutions with one kink: (a) $1/8 < B < 3/16$; (b) $B > 3/16$.

We assume v to be small and expand sin(v) and cos(v) in equations (3) and (4) to $O(v^4)$. Defining a dimensionless displacement $W = v/(u_0/2)$ we obtain:

$$H = (u_0/2)^2(\dot{W}^2/2 + B(1 - 3(u_0/L_0)^2 W'^2)W'^2 + 2(B - 1/8)(W^2 - 1)^2 \tag{5}$$

This is the Hamiltonian for the on-site ϕ^4 problem [7] with an effective spring constant $C = 2B(1 - 3(u_0/L_0)^2 W'^2)$, and a depth $E = (u_0/2)^2(B - 1/8)$. We can therefore apply known results to the present problem. The main effect of the nonlinear interparticle interaction is to introduce a dependence on W in the effective spring constant C. This plays an important role, determining the stability limits of the different traveling wave solutions to (5), as will be discussed elsewhere. In this report we focus on the effects of the nonlinearity on the traveling kinks (fig. 2). The asymptotic values of W in these solutions are $W = +\frac{1}{2}u_0$ as $z \to +\infty$, where $z = x - ct$ and c is the kink velocity. the kink width d and its energy E will thus be given from the ϕ^4 theory as:

$$d = \frac{u_0}{2}\left\{2B[1-3(u_0/L_0)^2]/[B-1/8]\right\}^{1/2} \tag{6}$$

$$E = \frac{1}{4}u_0^2\left\{2B[1-3(u_0/L_0)^2][B-1/8]\right\}^{1/2} \tag{7}$$

The kink's width is infinite at the phase transition ($B = 1/8$) and decreases to $d = 0$ when u reaches the value $L_0/\sqrt{3}$ (at $B = 3/16$). It has zero creation energy both at the phase transition, where its amplitude vanishes, and when $u_0 = L_0/\sqrt{3}$, where the whole chain except one atom is in its ground state. It is now easy to see that at the point $u_0 = L_0/\sqrt{3}$ the interparticle interaction changes from concave (for $u < L_0/\sqrt{3}$) to convex (for $u_0 > L_0/\sqrt{3}$). A similar effect was noted by Barsch and Krumhansl (1984) in their study of solitons in ferroelastic materials. This point is seen more clearly when we consider the linearized phonons in the dimerized ground state. The dispersion relation is then:

$$\omega^2 = \cos(u_0/2) + 4B[3(u_0/L_0)^2 - 1]\sin^2(k/2) \tag{8}$$

For $k = \pi$, this has a homogeneous component plus upward (downward) curvature when the ground state is in the concave (convex) region of interparticle interactions. Note that although the ground state is dimerized the linearised phonon spectrum consists of one branch only. Splitting into acoustic and optic branches and in particular opening a gap at $k = \pi$ occurs only if nonlinear effects are included. As will be shown elsewhere, these will become important only at large enough amplitudes A: viz.

$$A > \{2B[1 - 3(u_0/L_0)^2] + \cos(u_0/2)\}/\{3(u_0/L_0)\} \tag{9}$$

The analogy with the ϕ^4 theory can be applied to moving kinks and to finite temperature effects as well. For traveling kinks the limiting sound velocity is $c = 2B[1 - 3(u_0/L_0)^2]$, which vanishes when $u_0 = L_0/\sqrt{3}$. This explains both the decrease of the kink's width with velocity (fig. 2) and the pinning of the kink when $u_0 = L_0/\sqrt{3}$.

When finite temperatures are considered, we can distinguish two regions (Aubry 1975): (1) the displacive region near $B = 1/8$ with a characteristic "transition" temperature $k_BT \approx (0.4)\, 2B[1-3(u_0/L_0)^2][B-1/8](u_0/2)$, which is the creation energy of the kink (eq. 7); and (2) the order-disorder region near $B = 3/16$ with a transition temperature $k_BT \approx 0.2(B-1/8)(u_0/2)$, which is the barrier height of the effective double well. These have the following interpretation for the present model: At $B = 1/8$ the "melting" of the dimerized springs is characterised by large domains (of the order of the kink's width) of nearly undimerised portions of the chain separating dimerised phases. At $B = 3/16$, on the other hand, there exist many dimerised regions separated by Ising walls (i.e. a width of the order of a lattice constant) in which the chain's dimerization changes from a "long-short" to a "short-long" spring configuration.

Finally we return to the shape of the kink when $u_0 = L_0/\sqrt{3}$. The sharp jump in the value of W from $+u_0/2$ to $-u_0/2$ is smoothed out if we include higher derivatives in the continuum Hamiltonian or equivalently longer range interparticle interactions in the discrete version. Such terms are present if we consider, for instance, an expansion of the energy in the elastic string. To see the effect of such a term we add $1/2\, G\, (W'')^2$ to the Hamiltonian (eq. 5). Substituting a solution $v = \tanh(x/d)$ in the equation of motion we obtain to leading order in 1/d:

$$d = \left\{\sqrt{\frac{1-3(u_0/L_0)^2}{8G} + \frac{B-1/8}{8G}} - \frac{1-3(u_0/L_0)^2}{8G}\right\}^{-1/2} \tag{10}$$

Eqn. (10) shows a crossover from an infinite width at $B = 1/8$ to a finite nonzero one, $d = \sqrt{[8G/(B-1/8)]}$, at $u_0 = L_0/\sqrt{3}$. Note that for $G > 0$ we obtain well defined kink solutions for all values of B ($u_0 \to L_0$ as $B \to \infty$).

To summarize we have presented a study of the ground state and excitations of the Frenkel-Kontorova model with nonconvex interparticle interactions, emphasizing the special effects of the nonconvexity on the ground state and on the excitations. Our study here has been limited to nonconvexity with two competing length scales. As indicated earlier, a third length scale can be introduced by choosing a nonzero value for a in eqn. (1). This was done by Marchand, Hood and Caille [4] in their study of the ground states of (1), assuming small displacements u_n and thus replacing $\cos(u_n)$ by $1 - u^2_n/2$. The phase diagram obtained in this study consists of various modulated configurations with first and second order phase transitions between them. On the other hand Barsch et al. [6,8] have shown that the present model with a strain gradient term may be useful in the description of twin boundary dynamics in martensite materials. In this case the substrate potential models the parent phase and the other terms are the expansion of the free energy as a function of the strain and strain gradients. We are currently studying this model. We have obtained additional ground state configurations (as the strain gradient term is increased). These consist of configurations where $u_n = n \cdot a$ for $n = 1 \ldots N$ and $u_n = n \cdot b$ for $n = N+1 \ldots M$ (the dimerized phase is one with $M = N = 1$, but different M, N can be obtained as the parameters are varied). The case (N,N) with $N \gg 1$ corresponds to the twin boundary lattice described by Barsch et al. [8]. A complete phase diagram is in preparation and will be published elsewhere.

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