Symmetry-Breaking Transition in Finite Frenkel-Kontorova Chains

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In this Letter we investigate a symmetry-breaking transition in the Frenkel-Kontorova model for finite chains with free-end boundary conditions. We present a detailed study of the behavior in the vicinity of the transition. It is shown that the gap in the phonon spectrum, the disorder parameter, and the reflection-symmetry parameter display scaling properties close to the transition. Their associated critical exponents are discussed and related to the displacements of the particles in the chains.

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The discrete sine-Gordon problem, first introduced by Frenkel and Kontorova,[1,2] has been widely studied as a model for crystal dislocations, adsorbed epitaxial monolayers, and incommensurate structures.[3-7] The problem deals with a linear chain of particles subject to an external periodic potential. One considers a chain of N particles with nearest-neighbor harmonic interactions, placed in a periodic potential, the substrate potential of periodicity a. The total potential energy of the system is[3]

$$V=\frac{1}{2}\alpha\sum_{i=1}^{N-1}(x_{i+1}-x_i-b)^2+\frac{1}{2}W\sum_{i=1}^{N}\left(1-\cos\frac{2\pi x_i}{a}\right), \tag{1}$$

where x_i is the position of the ith particle, b is the equilibrium spacing of the harmonic chain in the absence of the substrate potential, α is the harmonic force constant, and W is the depth of the substrate wells. The potential in Eq. (1) can be rewritten in units of $\alpha a^2/2$ as

$$V=\sum_{i=1}^{N-1}\left(\xi_{i+1}-\xi_i-\frac{1}{P_0}\right)^2+\frac{1}{2\eta^2}\sum_{i=1}^{N}\left(1-\cos\frac{2\pi x_i}{a}\right), \tag{2}$$

where $1/P_0$ is the misfit length, defined as $1/P_0=(b-a)/a$, and η is given by $\eta^2=\alpha a^2/2W$. The misfit length $1/P_0$ measures the amount by which the natural separation of the particles differs from the periodicity of the substrate potential. The parameter η measures the relative strength of the harmonic and substrate interactions, α and W, respectively, and ξ_i is the position of the ith particle given in units of a. Characteristic to the Frenkel-Kontorova problem is the existence of two competing periodicities, a and b, which may lead to a rich behavior of the state configurational properties of the particles.

It has been shown by Aubry and co-workers[6] that for an infinite chain of particles, which obeys Eq. (1), and under the conditions that the mean separation between the particles is kept constant and the chain is incommensurate with respect to the periodic potential, there is a critical value η_c below which the system undergoes a "transition of breaking of analyticity." This means that for $\eta>\eta_c$ the chain is unpinned and even an infinitesimal force can move it, but for $\eta<\eta_c$ a finite force is needed in order to move the chain.

Because of the fundamental role of the model in various related fields, there have been attempts to modify the basic assumptions by introducing anharmonicity in the chain, two-dimensional effects, finite temperatures, etc.[9-12] In the present work we concentrate on finite chains with an odd number of particles and with free-end boundary conditions[8] (an even number of particles will be discussed elsewhere). Such a case is of interest as it models symmetry properties of aggregates adsorbed on a finite substrate. We consider both the stable and the metastable configurations of the particles as a function of the strength of the substrate potential W. We observed that when the interaction between the chain particles and the periodic potential is weak ($\eta>\eta_c$), the chain is in the so-called analytical regime.[6] The important property of the chain in this regime is that it has a reflection symmetry with respect to the middle particle, which is at the top or at the bottom of the well in both ground and metastable states. We focus only on configurations in which the middle particle is at the top of the well. Below the transition point ($\eta<\eta_c$), this reflection symmetry is destroyed, and the middle particle leaves its position at the top of the well.

We will discuss some critical quantities which are relevant to the transition of breaking of symmetry in the Frenkel-Kontorova model. Applying the conventional procedure[6,7] of minimization of the energy with respect to $\{\xi_i\}$, but for a finite chain, we obtain the following equations:

$$\xi_2-\xi_1-1/P_0=(\pi/2\eta^2)\sin(2\pi\xi_1)\,, \tag{3a}$$

$$\xi_{i+1}-2\xi_i+\xi_{i-1}=(\pi/2\eta^2)\sin(2\pi\xi_i), \quad 2\le i\le N-1, \tag{3b}$$

$$\xi_{N-1}-\xi_N+1/P_0=(\pi/2\eta^2)\sin(2\pi\xi_N)\,. \tag{3c}$$

Unlike the Aubry case[6] where the mean particle separation in the chain is kept fixed, here Eqs. (3a) and (3c) account for the free-end boundary conditions. The two cases describe different realizations: a fixed-density chain and a chain with a constant pressure, correspondingly.

A relevant parameter which characterizes the transition, as defined by Aubry,[6(c)] is the gap in the phonon spectrum. This phonon gap enters when the stabilization of the chain is considered. The time Fourier transform of the linearized equations which describe the small-amplitude motion of the atoms around their equilibrium positions (phonons) yields[6-8]

$$\begin{aligned} &\omega^2\epsilon_1(\omega)=(\pi^2/\eta^2)\epsilon_1(\omega)\cos(2\pi\xi_1)-[\epsilon_2(\omega)-\epsilon_1(\omega)]\,,\\ &\omega^2\epsilon_i(\omega)=(\pi^2/\eta^2)\epsilon_i(\omega)\cos(2\pi\xi_i)-[\epsilon_{i+1}(\omega)-2\epsilon_i(\omega)+\epsilon_{i-1}(\omega)],\quad 2\le i\le N-1\,,\\ &\omega^2\epsilon_N(\omega)=(\pi^2/\eta^2)\epsilon_N(\omega)\cos(2\pi\xi_N)-[\epsilon_{N-1}(\omega)-\epsilon_N(\omega)]\,. \end{aligned} \tag{4}$$

Equations (4) determine the phonon eigenfrequencies and the corresponding eigenmodes. In a stable configuration, all the eigenvalues, derived from Eqs. (4), are positive or zero. The gap in the phonon spectrum, ω_G, is defined as the positive square root of the smallest eigenvalue.[6(c)] At the transition point $\omega_G=0$, and Eqs. (4) become

$$\begin{aligned} &\epsilon_2-\epsilon_1=(\pi^2/\eta^2)\epsilon_1\cos(2\pi\xi_1)\,,\\ &\epsilon_{i+1}-2\epsilon_i+\epsilon_{i-1}=(\pi^2/\eta^2)\epsilon_i\cos(2\pi\xi_i),\\ &\qquad 2\le i\le N-1,\\ &\epsilon_{N-1}-\epsilon_N=(\pi^2/\eta^2)\epsilon_N\cos(2\pi\xi_N)\,. \end{aligned} \tag{5}$$

The transition point is found by solving a terminated continued-fraction equation.[6] For an infinite chain of the Aubry type, ω_G is zero above the transition ($\eta>\eta_c$); i.e., the chain can slide freely on the substrate. On the contrary, below the transition ($\eta<\eta_c$) the chain is pinned and unable to slide on the substrate, unless a finite force is applied. A critical exponent of ω_G has been introduced,[6(c)] $\omega_G\propto(\eta_c-\eta)^\chi$, with $\chi\simeq1.03$. For finite chains the situation turns out to be different; ω_G is zero only at a transition *point* η_c and is larger than zero both below and above it. The chain is then pinned *both* for $\eta>\eta_c$ and $\eta<\eta_c$ and is unpinned only at $\eta=\eta_c$. The meaning of the transition is therefore not a pinning-unpinning transition as in the Aubry case, but a symmetry-breaking transition. One has to distinguish between χ^- and χ^+ which determine the behavior of the chain below and above the transition, respectively:

$$\begin{aligned} &\omega_G^+\propto(\eta_c-\eta)^{\chi^+}\quad(\eta<\eta_c)\,,\\ &\omega_G^-\propto(\eta-\eta_c)^{\chi^-}\quad(\eta>\eta_c)\,. \end{aligned} \tag{6}$$

Another relevant parameter, introduced by Coppersmith and Fisher,[7] is the disorder parameter

$$\psi=\min_{j,m}|x_j-2\pi(m+\tfrac{1}{2})|\,. \tag{7}$$

ψ gives the minimum distance of any particle from the top of the well. In the symmetric regime, $\eta>\eta_c$, the middle particle is at the top of the potential well, i.e., $\psi=0$. Below the transition, $\eta<\eta_c$, it is found that

$$\psi\propto(\eta_c-\eta)^\sigma\,. \tag{8}$$

This defines the second critical exponent σ, which in the Aubry case obtains the value $\sigma=0.721$.[11] In our case ψ measures the distance of the middle particle from the top of the potential well. We introduce a new parameter ϕ which characterizes the reflection symmetry of finite chains:

$$\begin{aligned}\phi&=\frac{1}{N-1}\left|\sum_{i=1}^{N-1}(-1)^i(\xi_{i+1}-\xi_i)\right|\\ &\equiv\frac{1}{N-1}\frac{\pi}{2\eta^2}\left|\sum_{i,1,3,5,\ldots}\sin(2\pi\xi_i)\right|.\end{aligned} \tag{9}$$

The parameter ϕ follows the breaking of symmetry of a chain as η decreases. We expect that above the transition point $\phi=0$, and below it, scales as

$$\phi\propto(\eta_c-\eta)^\kappa\,. \tag{10}$$

We now turn to a detailed study of the quantities ω_G, ψ, and ϕ in the vicinity of the transition point η_c.

In order to confirm the scaling relationships and evaluate χ^-, χ^+, σ, and κ for finite chains, we used an algorithm due to Snyman and Van Der Merwe[13] to calculate all the strain-free stable configurations of small odd finite chains ($N=5$, 7, 11, 13, 25, 29, and 41). To identify the stable configurations, a normal-mode analysis was performed. We concentrated on the configurations with the middle atom at the top of the potential well (above the transition). Both ground and metastable states were considered. The misfit parameters $1/P_0$ were chosen as 0.3001... and $\frac{1}{3}$. The properties of the chains close to the transition point were studied by using the above algorithm.[13] Our results show that all the critical exponents describing the symmetry-breaking transition for finite chains with free-end boundary conditions are equal to 0.5, and do not depend on the number of particles in the chain.[14] These results emphasize that finite chains with free ends differ from the case studied by Aubry and co-workers,[6] where the mean interparticle distance was kept constant and incommensurate with the substrate potential.

In Figs. 1 and 2 we show the behavior of the critical quantities ω_G^- and ω_G^+, respectively, for various chain lengths as a function of $\Delta\eta=|\eta-\eta_c|$. Around η_c ($\eta<\eta_c$) a decrease in the phonon gap is observed as η increases until a minimum is reached at $\eta=\eta_c$, where $\omega_G=0$. As η increases beyond η_c, a phonon gap opens

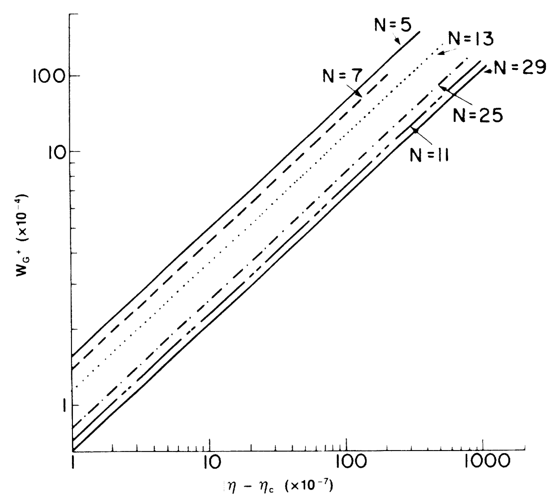

FIG. 1. ω_G^+ as a function of $|\eta-\eta_c|$ for $N=5$, 7, 11, 13, 25, and 29 particles. The corresponding values of η_c are 3.04346, 3.1544, 3.4060, 3.152, 3.232, and 3.307. The corresponding value of the misfit parameter is $1/P_0=0.300111111$.

again. The behavior of ψ near the transition point as a function of $\Delta\eta$ is shown in Fig. 3 for the same chain lengths. In Fig. 4 we present the behavior of the reflection parameter ϕ in the vicinity of the transition. All these curves have the same slope of 0.5 and the scaling relationships in Eqs. (6), (8), and (10) are confirmed. The $\Delta\eta$ interval in Figs. 1-4 is taken to be $10^{-7}<\Delta\eta<10^{-3}$, which is extremely close to criticality.

The same problem has been recently studied by Sharma, Bergersen, and Joos.[8] They have investigated finite chains of length $N=13$, 25, 41, and 99 with free-end boundary conditions and with different misfit parameters $1/P_0$. For $N=13$ and 25 we have obtained almost the same critical value of η_c, but our critical exponents differ

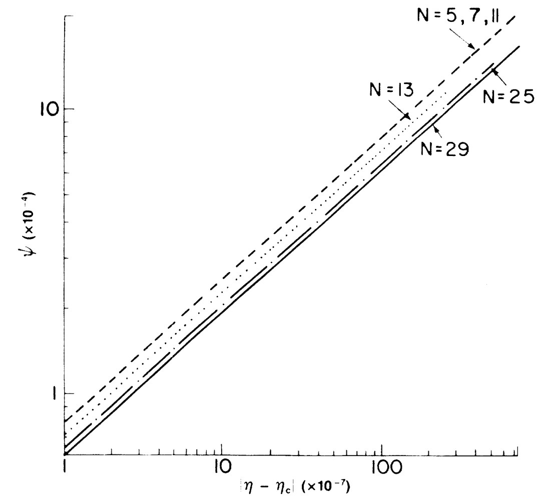

FIG. 3. ψ, the disorder parameter, as a function of $|\eta-\eta_c|$ for the same chains as in Fig. 1.

from those reported by Sharma, Bergersen, and Joos,[8] as evident from our figures and their Table III.

To support our numerical results we have solved Eq. (3) near the transition point. Given a physically stable solution $\{\xi_i\}$ to the force equation we wish to know what a nearby stable solution $\{\xi_i'\}$ will be when η is changed by a small amount $\Delta\eta$. By nearby we mean that $\delta\xi_i=\xi_i'-\xi_i$ approaches zero as $\Delta\eta$ does. The force equation $\{\delta\xi_i\}$ is

$$\delta\xi_{i+1}-2\delta\xi_i+\delta\xi_{i-1}$$
$$=\frac{\pi}{2(\eta_c-\eta)^2}\sin[2\pi(\xi_i+\delta\xi_i)]-\frac{\pi}{\eta_c^2}\sin(2\pi\xi_i). \quad (11)$$

Expanding in $\delta\xi_i$ and assuming that the middle particle is at the top at the transition point, i.e., $\sin(2\pi\xi_{n+1}=0)$

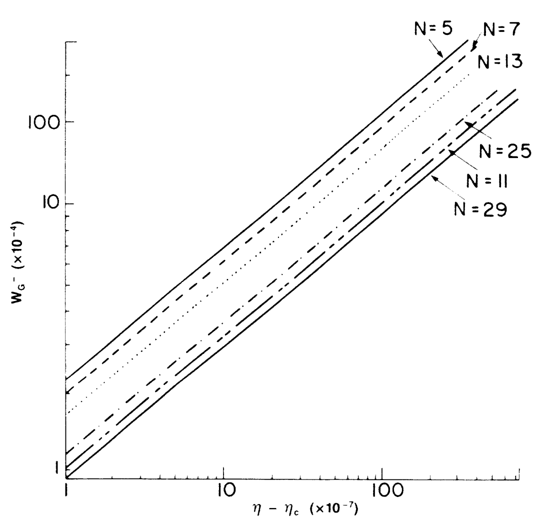

FIG. 2. As in Fig. 1, but for ω_G^-.

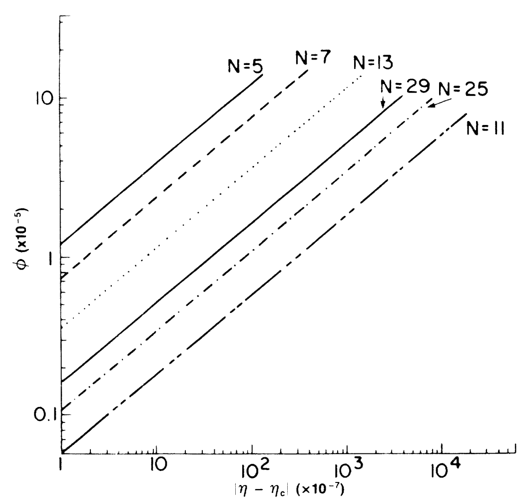

FIG. 4. ϕ, the reflection symmetry parameter, as a function of $|\eta-\eta_c|$ for the same chains as in Fig. 1.

and $\cos(2\pi\xi_{n+1}) = -1$ (the middle atom has the index $n+1$), we obtain

$$\delta\xi_{n+2} - 2\delta\xi_{n+1} + 2\delta\xi_n = -\frac{\pi^2}{\eta_c^2}\delta\xi_{n+1} + \left(\frac{2\pi^4\delta\xi_{n+1}^3}{\eta_c^2} - \frac{2\pi^2\Delta\eta\delta\xi_{n+1}}{\eta_c^3}\right). \quad (12)$$

We have shown[14] that $\delta\xi_i \propto (\Delta\eta)^\beta$, with $\beta = 0.5$, for any i independent of the length of the chain. This reduces Eq. (12), and to first order in $\delta\xi_{n+1}$ the following condition is satisfied:

$$\delta\xi_{n+2} - 2\delta\xi_{n+1} + \delta\xi_n = -(\pi^2/\eta_c^2)\delta\xi_{n+1}. \quad (13)$$

Equation (13) is analogous to Eq. (5) when $\omega_G = 0$, which defines the transition point η_c.

We conclude then that below the transition all the atoms have the same dependence on $\Delta\eta$. This defines the critical exponents χ^+, χ^-, σ, and κ to be equal to 0.5 as we indeed observed in our numerical calculations, $\chi^- = \chi^+ = \sigma = \kappa = 0.5$.

We have demonstrated that finite Frenkel-Kontorova chains with free-end boundary conditions may go through a symmetry-breaking transition. Various critical properties in the vicinity of the breaking of symmetry exhibits universal laws, which do not depend on the chain length.

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