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Frenkel-Kontorova model with anharmonic interactions

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It is shown that allowing for anharmonicity of the interatomic forces within the framework of the Frenkel-Kontorova model may have a dramatic effect on the soliton picture arising in systems with competing periodicities. An approximate analytical treatment, as well as numerical iterations of the corresponding two-dimensional area-preserving mapping, reveal discontinuities which indicate a disintegration (rupture) of the entire system beyond some critical values of the characteristic parameters.

The study of commensurate-incommensurate phase transitions, such as observed in some spin- and charge-density wave systems, nonregistered to registered adsorbed (or interstitial) atomic monolayers, intercalation compounds, and magnetically ordered structures[1] has recently been of considerable interest both for experimentalists as well as for theoreticians. Among the variety of phenomenological models proposed to describe such systems, the simple model of a chain of atoms interacting via next-neighbor *harmonic* forces and placed in a periodic external (substrate) potential, due originally to Frenkel and Kontorova (FK)[2] and developed further by Frank and van der Merwe,[3] has proved the most suitable for the theoretical description of various phenomena arising from competing periodicities. It has been extended in a number of works to more than one dimension and to nonzero temperatures,[1] including soft substrates or substrates with more complicated periodicity, etc. A new insight into the problem has been brought by Aubry,[4] who introduced the concept of transitions by the breaking of analyticity, considering the effects of discreteness of the lattice for a general class of models which include the FK model as a particular case.

Meanwhile, in all these studies the implications of a major limitation of the FK model, namely, the assumed purely harmonic nature of the interatomic forces acting between the atoms of the chain, have been largely ignored. In the present work we show that accounting for the anharmonicity of atomic interactions leads to qualitatively new effects, such as a possible breakdown of the collective soliton picture in the adphase even at moderate degrees of anharmonicity. Besides the amplitude of the periodic potential of the substrate (measured in units of the elastic energy of a single atom), it is the magnitude of the natural lattice misfit, and its sign, which, in contrast to the harmonic case, appear essential for the disintegration of the entire system into smaller fractions and thus set clear limits on the applicability of the FK picture.

Consider a one-dimensional (1D) string of atoms, assumed to interact via Toda forces,[5] the corresponding potential being

$$V(r)=\mu/\beta\{(1/\beta)\exp[-\beta(r-b)]-1/\beta+r-b\}\ , \qquad (1)$$

where μ denotes the elastic constant, β reflects the degree of anharmonicity, and b is the equilibrium interatomic distance in the unperturbed chain. By varying β, one may go smoothly from the purely harmonic limit of the FK model, $\beta\to 0$, $V(r)\to\mu/2(r-b)$,[2] with growing asymmetry to the hard-sphere limit: $\beta\to\infty$, $V(r\leq b)=\infty$, and $V(r>b)=0$. The Hamiltonian of the system (after appropriate scaling) is

$$H=\sum_{i=1}^{N}((1/\beta)^2\{\exp[-\beta(\phi_{n+1}-\phi_n-P)]-1\}+(1/\beta)(\phi_{n+1}-\phi_n-P)+(\lambda/2)(1-\cos\phi_n))\ , \qquad (2)$$

where ϕ_n denotes the relative displacement of the nth atom from the bottom of the nth potential well of the substrate (in periods of the substrate, a), λ represents the scaled barrier for surface diffusion, and P stands for the natural lattice incompatibility between substrate and overlayer, $P=(b-a)/a$.

The stationary configurations of (2), following from $\delta H/\delta\phi_n=0$, must satisfy

$$\exp[-\beta(\phi_{n+1}-\phi_n-P)]=\exp[-\beta(\phi_n-\phi_{n-1}-P)]-\lambda\beta\sin\phi_n\ . \qquad (3)$$

From the form of Eq. (3) it is immediately clear that for large enough λ and $\beta\neq 0$, depending on P, the right-hand side may become negative, so that no value of ϕ_n could satisfy the equation.

In order to study Eq. (3) more closely, one may apply the operation rule $\exp[\pm\nabla f(n)]=f(n\pm 1)$ to ϕ_{n+1} and ϕ_{n-1} and convert (3) into[6]

$$\exp[-\beta(\sinh\nabla)\phi]\sin[\beta(\cosh\nabla-1)\phi]=\gamma\sin\phi \qquad (4)$$

with $\gamma=(1/4)\lambda\beta\exp(-\beta P)$ which in the limit $\beta\to 0$ yields the well-known sine-Gordon equation,[3] $\nabla^2\phi=2\gamma\sin\phi$.

We consider the effect of nonvanishing anharmonicity ($\beta\neq 0$) by keeping the lowest-order derivatives in Eq. (4) which then reduces to

$$\exp(-\beta\nabla\phi)\beta\nabla^2\phi=2\gamma\sin\phi\ . \qquad (5)$$

A first integral of Eq. (5) is now readily obtained in the form

$$1-(1+\beta\omega)\exp(-\beta\omega)=2\beta\gamma(C-\cos\phi)\ , \qquad (6)$$

where $\omega=\nabla\phi$ and C is an integration constant. For $\beta\to 0$ Eq. (6) yields the first integral of the sine-Gordon equation[3]

$$\omega^2=\lambda(C-\cos\phi) \qquad (7)$$

with a single soliton solution $\phi = 4\arctan[\exp(\pm n\sqrt{\gamma}/2)]$ for $C=1$.

Following the approximate analytical treatment, suggested by Pokrovsky,[7] Eq. (6) may be viewed as giving the curves $\omega(\phi)$ which remain invariant in the phase space (ω, ϕ) under the area-preserving mapping transformation

$$\exp(-\beta\omega_{n+1}) = \exp(-\beta\omega_n) - 2\gamma \sin\phi_n \ ,$$
$$\phi_{n+1} = \omega_n + \phi_n \ , \tag{8}$$

defined by Eq. (3).

In Fig. 1 we plot the invariant curves, following from (6), within the cylinder $(\omega, \mathrm{mod}[\phi, 2\pi])$ as obtained for $\beta=1$ and $\gamma=1$ (thick lines), and compare them with those, following from the harmonic treatment (7) (the thin lines in Fig. 1).

Evidently, the whole picture consisting of closed curves (for $-1 < C < 1$), bounded by separatrices ($C=1$) and periodic open curves ($C > 1$) is now dramatically changed due to the presence of anharmonicity. For $\omega < 0$ (compressed overlayer) the curves are now much less modulated, due to the "hard" repulsive branch of the Toda potential (1). For $\omega > 0$ (expanded chain) most curves reveal discontinuities, the gap increasing with C, which are symmetric with respect to the top of the substrate potential at $\phi = \pi$. In particular, the separatrix, corresponding physically to a single soliton (an extra hole) which makes a smooth transition between neighboring configurations with $\phi = 0$, or $\phi = 2\pi$ at $n \to +\infty, -\infty$, is now discontinuous. The formation of a gap indicates that the integrity of the whole system is broken, i.e., the weaker attractive branch of (1) cannot withstand the expansion, due to the substrate or to negative pressure, and the system breaks into disconnected fractions. It is also clear from Eq. (4) that the critical amplitude γ, responsible for the rupture of the chain, depends both on λ as well as on the degree of anharmonicity β, whereby a negative misfit, $P < 0$, appears more dangerous [as effectively enhancing γ, cf. Eq. (4)] than a positive misfit of the same absolute value. Indeed, for small misfits, in the former case ($P < 0$) the substrate tends to expand the chain which resists with the weaker attractive branch of (1), while in the second case ($P > 0$) the

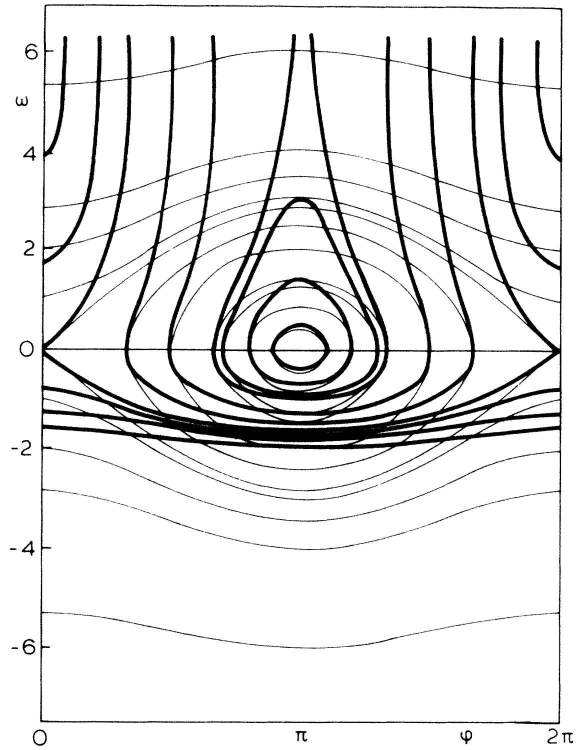

FIG. 1. Invariant curves of the conventional Frenkel-Kontorova model (thin lines), and after anharmonicity is accounted for (thick lines) according to Eq. (6) with $\beta=1$ and $\gamma=1$.

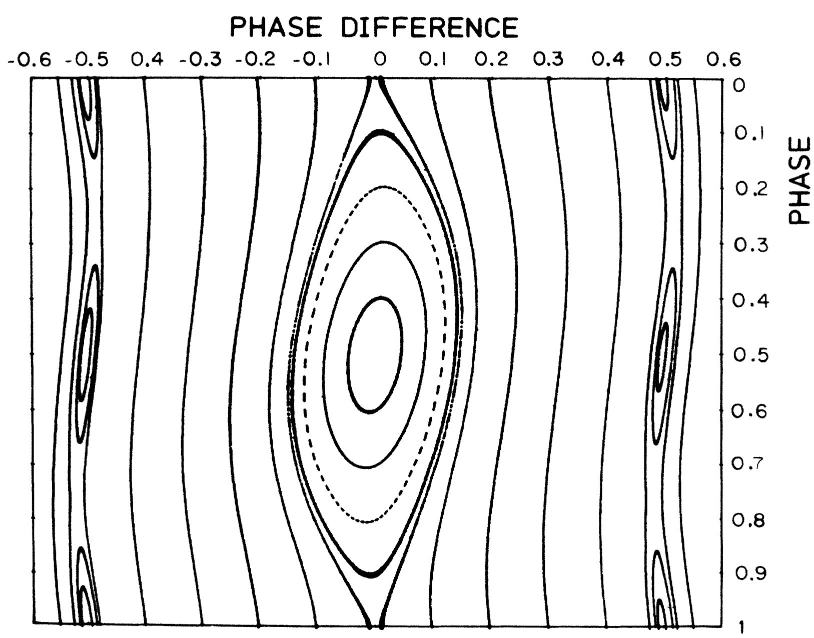

FIG. 2. Invariant trajectories of the mapping (8) with $\lambda = 0.43864$ and $\beta = 0.002$ (harmonic interactions). The number of steps used is 2000, the misfit is 0.05, $\alpha = 6000$, and $\omega = 1.2$. Both axes are in units of 2π.

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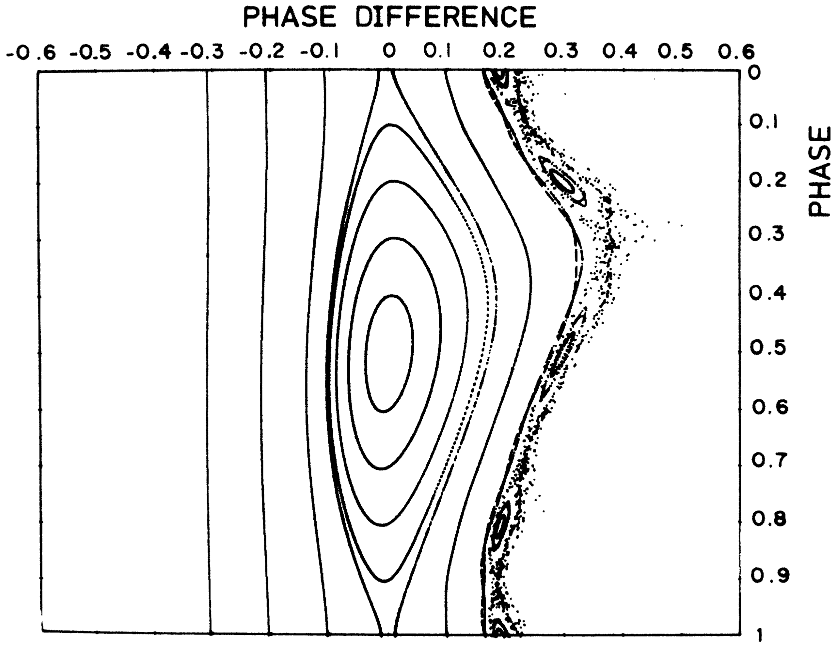

FIG. 3. Invariant trajectories of (8) with $\lambda = 0.438\,64$, positive misfit $P = 0.05$, and degree of anharmonicity $\beta = 2$. The number of steps used is 2000, $\alpha = 6$, and $\omega = 1.2$. Both axes are in units of 2π.

overlayer at first relaxes upon expansion from the substrate-enforced repulsion between the adatoms.

These results of the approximate treatment are substantiated further by a numerical investigation of the recursion relation (8). Since the character of the invariant curves of area-preserving maps, as Eqs. (8), has been extensively studied in a number of works,[8] it is now well established[4] that these curves may either consist of a finite number of discrete points (fixed points of order q corresponding to commensurate configurations) or be continuous smooth curves, known as Kolmogorov-Arnold-Moser (KAM) curves (corresponding to incommensurate phases), or be a chaotic trajectory whose points form a Cantor set. Without going into details, we present in Fig. 2 results of the purely harmonic FK model with $\beta = 0$ and $\lambda = 0.438\,64$ (P is thereby irrelevant) to be compared to Figs. 3 and 4 where the *same* λ is used, but with $\beta = 2$ and $P = 0.05$ (Fig. 3), and $P = -0.05$ (Fig. 4). Everywhere the phase difference ω_n is plotted as function of the phase ϕ_n (mod 1) in units of 2π, whereby points on the ω and ϕ axes were generally chosen

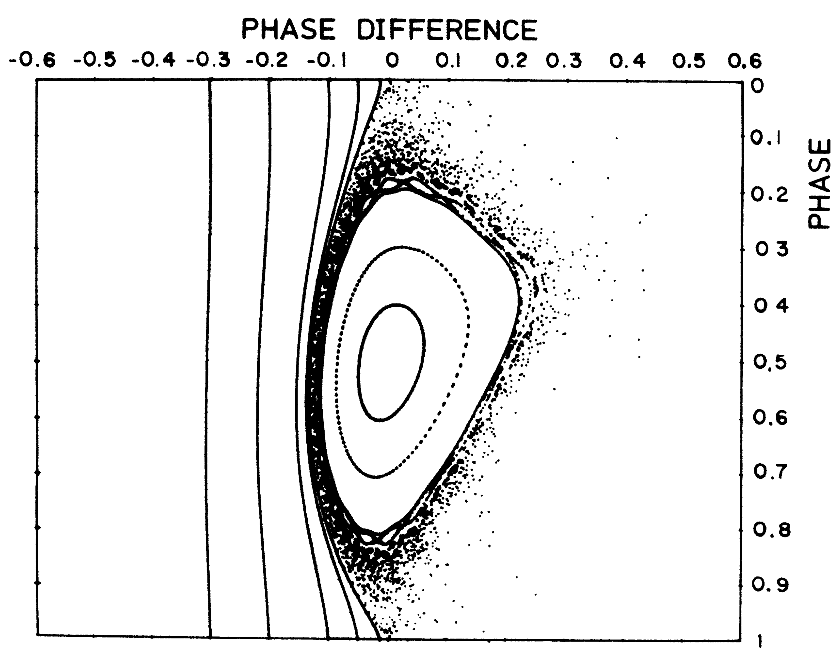

FIG. 4. The same as in Fig. 3 at negative misfit, $P = -0.05$.

as starting points and typically 2000 iterations were performed.

The general agreement between predictions of the analytical treatment, Eq. (6), and the numerical calculations is evident. Despite the fact that the amplitude λ is always kept equal to that of the harmonic case, the presence of anharmonicity leads to the expected drastic changes in the maps.

Compressed systems ($\omega < 0$) manifest vanishing fluctuations in ω due to the (nearly) hard-core repulsion; moreover, at high pressure ($\omega < -0.4$) the iteration produces only a finite number of points. For the expanded state of the system ($\omega > 0$) both maps end with a chaotic set of points indicating an instability in the system which leads to rupture. For $P > 0$ the (less vulnerable) system still bears some resemblance to the harmonic original (cf. Figs. 3 and 2), exhibiting several open KAM curves (incommensurate phases) at moderate expansion ($\omega < 0.15$). For negative P no open curves are found to exist, although several closed ones (higher-order commensurate phases) are still there and the whole picture is, in fact, very similar to that of the analytical treatment (cf. Fig. 1).

Although the results presented here have been derived for a specific model, it can be shown[9] that they are not an artifact of the Toda potential. Since forces in nature are largely anharmonic, the picture which emerges may well apply to many different systems in statistical mechanics, magnetism, and other areas of solid-state physics where modulated structures occur. For example, anharmonicity seems to be directly responsible for the formation of cracks out of misfit dislocations. Also its influence on dynamic properties, such as mass and charge transfer, could impose important limitations on some current theoretical approaches and should be thoroughly examined.

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