Solitons in an anharmonic chain of the Frenkel'–Kontorova model

S. A. Beklemishev and V. L. Klochikhin
L. Ya. Karpov Scientific-Research Physicochemical Institute, 103064 Moscow, Russia

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Equations of motion incorporating an anharmonicity of the interatomic interaction are derived for the Frenkel'–Kontorova model. Corrections to existing solutions in the harmonic approximation are also derived. A limit is found on the velocity of an extension soliton, corresponding to an energy of the soliton which is still finite. New solutions due to the anharmonicity are found. One is a soliton with a topological charge of 2.

Frenkel' and Kontorova[1] have proposed an extremely simple 1D model of a chain in a periodic potential to describe the structure of dislocations. Later generalizations of this model to various periodic potentials, e.g., the ϕ^4 potential,[2] have been used to study structural phase transitions caused in ferroelectric materials by displacements of atoms from their equilibrium positions. These generalizations have also been used in discussions of the mobility of protons in chains of hydrogen bonds in certain macromolecules, biological membranes, and ice (as well as in other applications). Research on chains of hydrogen bonds is benefiting from the use of the ϕ^4 potential and the double periodic harmonic potential.[3] The problem reduces[4] to one of solving the double sine-Gordon equation with a minus sign.[5] The model becomes more similar to the original Frenkel'–Kontorova model which incorporates the features of the ϕ^4 model.

Pnevmatikos *et al.*[2] justified the standard assumption that the interatomic interaction is linear for a model of this type[6,7] on the basis that no analytic expressions are available for the solutions of the Frenkel'–Kontorova model with an anharmonic binding of nearest neighbors, other than some partial solutions[8] for a special type of quaternary anharmonicity and solutions with fixed parameters for the case of a cubic anharmonicity. A numerical study,[2] in which the parameters of a solution of the latter type were varied, demonstrated that this solution is not sufficient for studying an anharmonic chain in this model. Studies[9,10] of small anharmonic corrections to known solutions of the Frenkel'–Kontorova model have also failed to yield new types of solutions.

The assumption that the interatomic interaction is anharmonic is considerably more realistic. An inflection point in the anharmonic interatomic potential of the chain gives rise to new solutions in the model.[11,12] In the present letter we derive corrections and also new solutions in this model which are consequences of the anharmonicity of the chain.

The Frenkel'–Kontorova model deals with a 1D chain consisting of spring-coupled particles of mass m in a periodic potential g with a period h. We find travelling-wave solutions with a coordinate $(x-v\tau)$, where x is a Lagrange coordinate, v is the wave velocity, and τ is the time. The Hamiltonian H of such a system in the continuum

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approximation, normalized to the product of the stiffness coefficient f of the interatomic bond in the chain and the square of the chain period h, is

$$H=\int_{-\infty}^{\infty}[\nu(y'(n))^2/2+g(y(n))+u(r(n))]dn, \tag{1}$$

where $\nu=v^2/c^2$, $c^2=h^2f/m$ is the square of the sound velocity in the chain, $y(n)$ is the displacement of the nth atom of the chain from the nth minimum of the periodic potential well $g(y)$, divided by h, and $r(n)$ is the deformation of the nth bond. The external harmonic potential $g(y)$ can be chosen in the standard form[1,6] $g(y)=a[1-\cos(2\pi y)]/2\pi$, where a is the dimensionless amplitude of the potential. The prime means the derivative with respect to the variable n, which is continuous in the continuum limit. We choose the interatomic potential in the chain to be

$$u(r)=r^2/2-\gamma r^3/3, \tag{2}$$

where γ is a dimensionless anharmonicity constant.

From Hamiltonian (1) we find the equation of motion,

$$\beta y''=dg(y)/dy+2\gamma y'y'', \tag{3}$$

where $\beta=1-\nu$. This equation has three branches of solutions:

$$3ky'=\begin{cases}1-\sqrt{3}\,\sin(s)-\cos(s), & 3ky'<0, \quad (4a)\\ 1+\sqrt{3}\,\sin(s)-\cos(s), & 0<3ky'<2, \quad (4b)\\ 1+2\,\cos(s), & 3ky'>2, \quad (4c)\end{cases}$$

where $s=\arccos(1-q)/3$, $k=4\gamma/(3\beta)$, $q=81k^3[E+g(y)]/(4\gamma)$, and E is an integration constant. At values of the argument $|1-q|>1$, Eqs. (4a) and (4c) should be understood in the sense of an analytic continuation of the function $\arccos(1-q)$, where these formulas are applicable and have the form of the Cardan formula. The third branch of solutions, (4c), is due to the anharmonicity of the interatomic interaction. It corresponds to supercritical deformations, which have not previously been studied analytically. The new types of solutions derived below stem from the existence of this branch.

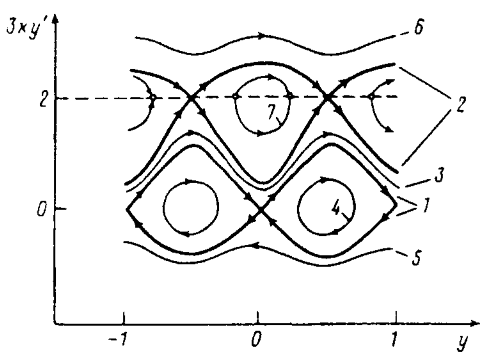

FIG. 1. Phase trajectories for the case $\epsilon>0$. 1—$E=0$; 2—$E=a\epsilon/\pi$, 3—$0<E<a\epsilon/\pi$, extension; 4—$a/\pi<E<0.5$; 5—$0<E<\infty$, contraction; 6—$-\infty<E<a\epsilon/\pi$, supercritical extension; 7—$a\epsilon/\pi<E<\beta^3/24\gamma^2$.

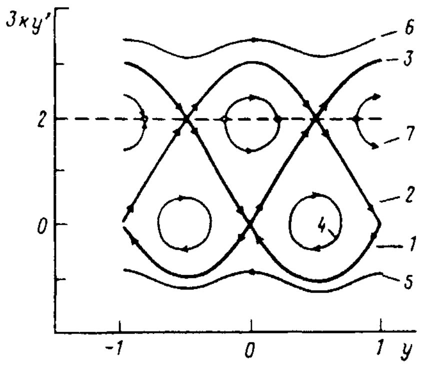

FIG. 2. Phase trajectories for the case $\epsilon=0$. 1,2,3—$E=a\epsilon/\pi=0$, separatices; 4— $-a/\pi<E<0.5$; 5—$0<E<\infty$, contraction; 6— $-\infty<E<0$, supercritical extension; 7—$0<E<\beta^3/24\gamma^2$.

Let us consider the waves with $\nu<1$. The phase portrait of the model described by Eqs. (1) takes different forms, depending on the sign of the parameter

$$\epsilon=\pi\beta^3/24\gamma^2a-1 \tag{5}$$

(see Figs. 1–3 for $\epsilon>0$, $\epsilon=0$, and $\epsilon<0$, respectively). The different types of phase trajectories are separated by separatrices (the heavy curves in Figs. 1–3) which correspond to two values of the integration constant, $E=0$ (curve 1 in Figs. 1 and 3) and $E=a\epsilon/\pi$ (curve 2 in Figs. 1 and 3). In the case $\epsilon=0$, all the separatrices correspond to a common value of the integration constant, $E=a\epsilon/\pi=0$, and they merge (curves 1–3 in Fig. 2).

The anharmonicity influences the solutions which have been found previously (1 and 3 in Fig. 1; 4 and 5 in Figs. 1–3) in the Frenkel'–Kontorova model.[1,6,7] Under the condition $3ky'\ll 1$ we find from (4)

$$y'=\pm[2(E+g)/\beta]^{1/2}+3k^2(E+g)/4\gamma, \tag{6}$$

where the plus sign corresponds to an extension, and the minus sign to a contraction. Incorporating the first term gives us the wave profile in the Frenkel'–Kontorova model. The second term, which is the anharmonic correction, is proportional to the constant γ. The sign of this correction depends on whether we are dealing with subsonic waves ($\nu<1$) or supersonic ones ($\nu>1$). It follows from (6) that for subsonic waves (including

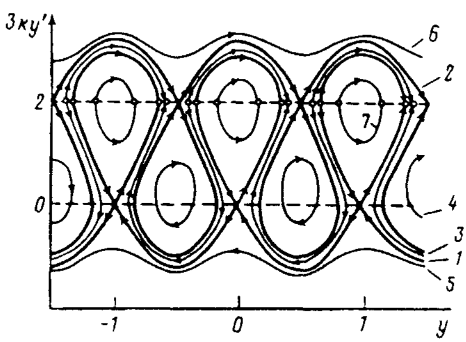

FIG. 3. Phase trajectories for the case $\epsilon<0$. 1—$E=0$; 2—$E=a\epsilon/\pi$; 3—$a\epsilon/\pi<E<0$; 4—$-a/\pi<E<a\epsilon/\pi$; 5—$0<E<\infty$, contraction; 6—$-\infty<E<a\epsilon/\pi$, supercritical extension; 7—$0<E<\beta^3/24\gamma^2$.

standing waves) the regions of extension of the chain (with $y'>0$) are shortened by the anharmonicity. The regions of contraction ($y'<0$) become longer. The anharmonicity has the opposite effects for supersonic waves.

The physical meaning of the anharmonic corrections can be outlined as follows. If a defect involving the disappearance of one atom arises in a commensurate system, the anharmonic chain, becoming softer in the extended state, reaches a match with the substrate over a shorter length of the chain than in the case of a harmonic chain. If an atom is instead added to an anharmonic chain, which becomes stiffer in the course of contraction, the contraction spans a section of the chain wider than in the harmonic case. The size of the region of contraction or extension is characterized by the width of the corresponding kink or topological soliton of the given model.

In the case $E=a\epsilon/\pi>0$, the phase trajectories of sub- and supercritical extension at the points $y=\pm 1/2, \pm 3/2...$, $3ky'=2$ connect, forming separatrices 2, which consist of solutions (4b) and (4c). These trajectories are distinguished by the circumstance that their period is twice that of the period of an unclosed phase trajectory for the Frenkel'–Kontorova model (curve 3 in Fig. 1). In the case $\epsilon\rightarrow 0$, separatrices 2 and 1 in Fig. 1 merge and form separatrices 1–3 in Fig. 2. In the case $3ky'>0$ these separatrices describe a kink with a topological charge (i.e., the total displacement y along the length of the chain) of 2 (separatrices 2 from $y=-1$ to $y=1$ in Fig. 2). In the case $E=a\epsilon/\pi=0$, the velocity of the extension soliton described by the separatrix in Fig. 2 is at its maximum value,

$$v_c=c[1-(24a\gamma^2/\pi)^{1/3}]^{1/2}. \tag{7}$$

In the case $E=a\epsilon/\pi>0$ (Fig. 1) each separatrix 2 describes a lattice of solitons with a velocity $v<v_c$. For example, if we are dealing with a soliton mechanism for the transport of protons in a chain of hydrogen bonds,[4] we must bear in mind that the transport velocity is limited to the value v_c, at which the soliton energy is still finite, as was known previously. In the model of Ref. 4, idealized to the case of defects of only a single type, the magnitude of the electric charge that can be transported can double in accordance with the topological charge of 2.

In a description of a soliton in a system with critical parameter values ($\epsilon=0$; Fig. 2), Eqs. (4) for the separatrices simplify:

$$3ky'=1+2\cos[2\pi(y+j)/3], \quad j=+1,0,-1. \tag{8}$$

Equations (8) describe separatrices 1–3, respectively, in Fig. 2. From them we find an expression for the profile of the corresponding critical extension kink with a topological charge of 2:

$$y=(3/\pi)\arctan[\sqrt{3}\tanh(n\pi/2L)]. \tag{9}$$

In the case $3ky'<0$, separatrices 1–3 in Fig. 2 describe a contraction antikink, for which the given velocity is not critical:

$$y=(3/\pi)\arctan[(2\exp(n\pi/L)+1)/\sqrt{3}], \tag{10}$$

where the quantity $L(\beta_c \pi/2a)^{1/2} = (\sqrt{3}\gamma\pi/a)^{1/3}$ is formally equal to the width of the soliton in the Frenkel'–Kontorova model[1] with the critical parameter $\beta_c \equiv \beta(v_c) = (24a\gamma^2/\pi)^{1/3}$.

In the case $\epsilon < 0$, separatrix 2 separates closed continuous trajectory $4(-a/\pi < E < a\epsilon/\pi)$ and unclosed continuous trajectory 6 $(-\infty < E < a\epsilon/\pi)$ from trajectories 1, 3, and 7, with a discontinuity at the critical point $(3ky' = 2)$. Separatrix 2 corresponds to a travelling wave in which the displacement of the extension grows in the course of an alternation of contraction and extension.

There can be no cyclic motion along trajectories 7 (Figs. 1 and 2) or 1, 3, and 7 (Fig. 3) (the permissible direction of the motion is specified by the arrows on the phase trajectories), and in the continuum approximation there is no configuration of the chain which corresponds to such a motion.

The results of this study can be summarized as follows. First, a limit is imposed on the velocity of an extension soliton by the velocity at which the energy of the soliton is still finite (as was assumed previously). This point is of importance for (among other things) explaining the mobility of ions in the case of a proton conductivity. Second, among new solutions stemming from an anharmonicity we have found a soliton with a topological charge of 2. This solution, not previously known, is a 4π pulse not for the double sine-Gordon equation[5] but for the ordinary Frenkel'–Kontorova model with an anharmonic chain. Consequently, both the choice of substrate potential in the given model[3,4] and the interatomic anharmonicity may give rise to new types of solutions.

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