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Mechanism of the generation of dislocations in the one-dimensional Frenkel-Kontorova crystal model

S. V. Dmitriev[a], L. V. Nauman[b], M. D. Starostenkov[b] and T. Shigenari[a]

[a]Department of Applied Physics and Chemistry, University of Electro-Communications, Chofu-shi, Tokyo 182, Japan

[b]General Physics Department, Altai State Technical University, Lenin St. 46, 656099, Barnaul, Russia

In the frame of one-dimensional Frenkel-Kontorova crystal model the collision between two breathers was studied. The range of parameters of quasiparticles where the interaction is accompanied by converting energy from kinetic form to potential form or conversely was found. The exchange of energy can, under certain circumstances, lead to the appearance of kink-antikink pairs which represent the dislocation loops in the frame of the present model. The condition for inelastic interaction of quasiparticles was found.

1. INTRODUCTION

The Frenkel-Kontorova model [1] has played an important role in the understanding of the essential properties of dislocations. The success of the model is attributable to the fact that in the longwave approximation it leads to the wellknown nonlinear sine-Gordon equation for which some analytical solutions were obtained. Due to this fact the discreteness of the model was leaved aside and it has been used only in special cases, such as for the determination of Peierls barrier [2]. However a series of important effects are lost when we assume continuous sine-Gordon equation instead of a set of difference-differential equations of the Frenkel-Kontorova model. The most important effect is a nontrivial interaction between quasiparticles which leads to changes of their properties or even to their transmutations. It is known that for the sine-Gordon equation the effects of inelastic interaction of solitons are absent and the number of solitons is conserved [3]. The set of equations of the Frenkel-Kontorova model may be considered as the sine-Gordon equation perturbed by the discretization process. Such a perturbation is an essential prerequisite to the inelastic interaction. The sine-Gordon equation perturbed by various Hamiltonian and/or dissipative terms was studied analytically as well as numerically and the effects of nontrivial collision of solitons were found. The extensive literature on this matter is reviewed in the review [4]. The purpose of this paper is to show that the discretization perturbation gives rise to inelastic interaction of solitons and study the features of the interaction.

2.FRENKEL-KONTOROVA MODEL OF CRYSTAL AND THE SINE-GORDON EQUATION

Let us consider an infinite, linear array of identical point-mass atoms situated along x axis with position coordinates defined by $x_i=ia$, where i is an integer. Neighboring atoms are bonded by linear springs of length a and stiffness c. Influence of other atoms on the array is represented by cosinusoidal potential function with the amplitude A and the period a:

$$U(u_i)=-A\cos(2\pi u_i/a). \quad (1)$$

The equation of motion of the i-th atom is:

$$m(d^2u_i)/(dt^2)=c(u_{i-1}-2u_i+u_{i+1})-(2\pi A/a)\sin(2\pi u_i/a), \quad (2)$$

where $u_i=u_i(x_i)$ is the displacement of the i-th atom; m is the mass of atom.

It is convenient to replace u_i and t by a new variables φ_i and τ related to u_i and t by the equations:

$$\varphi_i=2\pi u_i/a, \qquad \tau=t(2\pi/a)(A/m)^{1/2}. \quad (3)$$

With Eqs. (3), Eq. (2) may be written as:

$$(d^2\varphi_i)/(d\tau^2)-(\varphi_{i-1}-2\varphi_i+\varphi_{i+1})/h^2+\sin\varphi_i=0, \quad (4)$$

where

$$h=(2\pi/a)(A/c)^{1/2}. \quad (5)$$

If the magnitude of h is far less then 1, then the second term in Eq. (4) may be approximated by the second partial derivative of the continuous function $\varphi(\xi,\tau)$ with respect to the variable

$$\xi=x(2\pi/a^2)(A/c)^{1/2}. \quad (6)$$

In this case in parallel with Eq. (4) its long-wave approximation

$$(d^2 \varphi)/(d\tau^2)- (d^2 \varphi)/(d\xi^2)+\sin \varphi=0 \quad (7)$$

may be considered.

The long-wave approximation increases in accuracy with decreasing h. The step of approximation h may be considered here from two points of view. On the one hand, if the finite difference solution of Eq. (7) is wanted, h represents the density of finite difference mesh with respect to coordinate ξ. On the other hand, if the exact equation of a model is (4) then h represents the degree of nonlinearity of crystal. As may be seen from Eq. (5), h depends on the ratio A/a which characterizes the function $U(u_i)$ and on the stiffness of springs ac or one can say that h depends on ratio A/c.

A few solutions to the Eq.(7) have been obtained [5]. Here is one of them, which is called kink (antikink):

$$\varphi=4\arctan [\exp(\delta(\xi-\xi_0+d(\tau-\tau_0)))], \quad (8)$$

where $0<d<1$ is a parameter, which defines the velocity of kink; $\delta=(1-d^2)^{1/2}$; the magnitude of ξ_0 defines the position of the kink at a time $\tau=\tau_0$.

The rest-energy of a kink i.e. its energy when d=0 is

$$E_k=8. \quad (9)$$

One more solution to the Eq.(7), which is called breather is:

$$\varphi=4\arctan(B/C), \quad (10)$$

where $B = \eta \sin [\delta\omega\sigma ((\tau-\tau_0) - (\xi-\xi_0+d\tau_0))]$, $C= \omega \cosh [\delta\eta\sigma ((\xi-\xi_0+d\tau_0) - (\tau-\tau_0))]$. $0<d<1$, $0<\omega<1$ are the parameters which define the velocity and amplitude of breather respectively; ξ_0, τ_0 are the position and the phase of the breather at the initial time $\tau=0$; $\delta=(1-d^2)^{1/2}$, $\eta=(1-\omega^2)^{1/2}$.

The velocity of the breather d, its wavelength λ and period T are related to each other by the expressions

$$d=\lambda/T, \quad \lambda=2\pi\delta d/\omega, \quad T=2\pi\delta/\omega. \quad (11)$$

The breather amplitude D depends on ω only:

$$D=4\arctan (\eta/\omega). \quad (12)$$

The amplitude D increases as the magnitude of ω decreases and as ω tends to zero, D approaches 2π.

If the breather does not move along the crystal (d=0), it has the energy

$$E_b=16\eta=16(1-\omega^2)^{1/2}, \quad (13)$$

which is its rest-energy. So, E_b may vary from 0 to $2E_k$ (see Eq. (9)). The kinetic energy is added to the rest energy of a quasiparticle if it is in motion along the crystal.

In the following section the results of numerical solution of Eq.(4) are reported.

3. RESULTS AND DISCUSSION

Let us consider the collision between two breathers moving towards each other with equal in magnitude but opposite in sign velocities and with the same phases, i.e. collision between breathers which are mirror images of each other. In such a situation, only one breather may be considered using the mirror boundary conditions. The initial conditions were defined by the Eq.(10), where we put $\tau=0$ and $\xi_i=i(2\pi/a)(A/c)^{1/2}$. The distance $2\xi_0$ between breathers at a time $\tau=\tau_0$ was varied. In view of the fact that the motion of breather is periodic, it is sufficient to examine $0<2\xi_0<\lambda$.

First we consider the influence of nonlinearity factor h on the collision between the breathers. Magnitude of h should be chosen small enough so that the Eq. (7) is in rather good agreement with Eq.

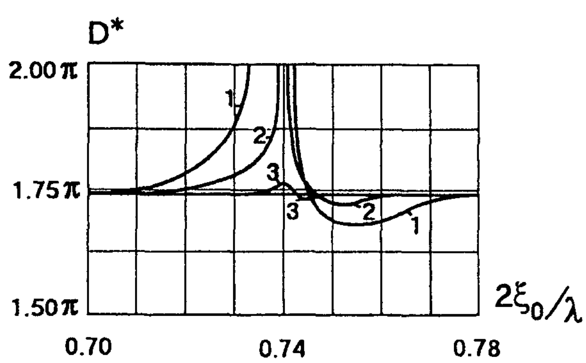

Figure 1. The dependence of the amplitude of breathers after encounter D* on dimensionless distance $2\xi_0/\lambda$ between breathers at a time $\tau=0$. Curves 1,2,3 correspond to $h=0,5\pi 10^{-3/2}$, $h=\pi 10^{-3/2}$, $h=2\pi 10^{-3/2}$.

(4), at the same time h should not be too small, so that the effect of discreteness of the Frenkel-Kontorova model could manifest itself.

Fig. 1 shows the dependence of the amplitude of the breathers D* after the encounter on the dimensionless distance $2\xi_0/\lambda$ between breathers at a time $\tau=0$. Curves 1,2,3 correspond to $h=0,5\pi 10^{-3/2}$, $h=\pi 10^{-3/2}$, $h=2\pi 10^{-3/2}$. The magnitudes of other parameters were $d=0,2$, $\omega=0,2$, $\tau_0=0$. The amplitude of breathers before the encounter is $D=1,744\pi$.

As may be seen from Fig. 1, there is a narrow range of parameter $2\xi_0/\lambda$, where the amplitude of breathers changes as a result of the encounter. The decrease of the amplitude of the breathers means that a part of their kinetic energy connected with the motion along crystal transforms into the potential energy. After such an interaction the breathers with larger amplitude (rest-energy) and smaller velocity are formed. In the case of increasing of amplitude the opposite situation occurs. Outside of the narrow range mentioned above when two breathers collide they go through one another recovering their initial properties. It is interesting that the greater is the velocity of breathers, the narrower is the range with the nontrivial interaction.

It should be pointed out that the nonlinearity factor h strongly influences the width of range of values of $2\xi_0/\lambda$ where the nontrivial interaction occurs.

As Fig. 1 suggests, for curves 1,2 there is a range of parameter $2\xi_0/\lambda$ where the amplitude of breathers after collision is indeterminate (recall that according to Eq. (12) the amplitude of breather can not be more than 2π). In this area the transmutation of quasiparticles takes place. Two types of reactions were revealed. Two kink-antikink pairs or one kink-antikink pair and a breather with velocity $d=0$ were formed (see Fig. 2 and Fig. 3 respectively). The Eq. (4) is reversible in time, therefore the reactions described above can be

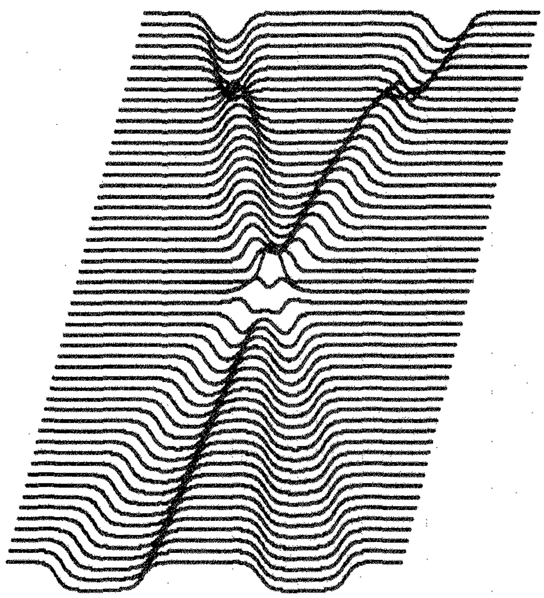

Figure 2. Collision of two breathers with two kink-antikink pairs formation.

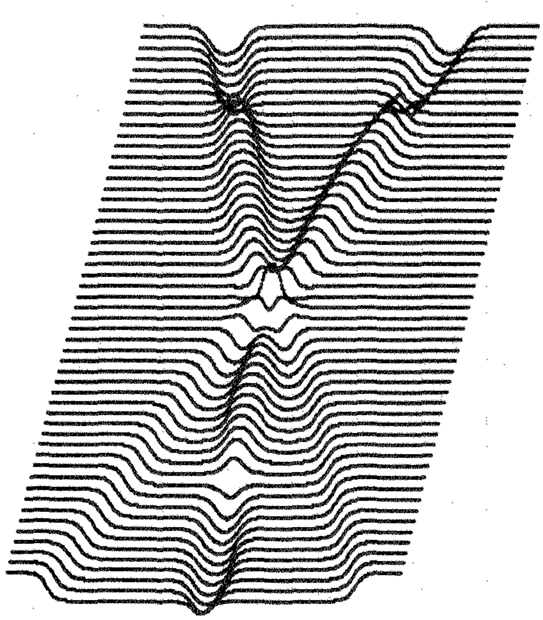

Figure 3. Collision of two breathers with one kink-antikink pair and a breather formation.

reversed.

The channel of nontrivial interaction was found. The dependence of maximum displacement of the atom which is in the encounter point of the two breathers as a function of $2\xi_0/\lambda$ has a sharp inflection which position completely corresponds to the region where the energy transformation occurs. This inflection indicates the location of a separatrix in the phase space of the considered system. Near the separatrix the discreteness of the model manifests itself.

4. CONCLUSIONS

The equations of the Frenkel-Kontorova model as the sine-Gordon equation perturbed by the discretization process were considered. The collision between the two mirror-like breathers was studied and the narrow range of parameters of quasiparticles where the nontrivial result of collision is observed was found. The way of finding of the range was described. Out of this range the perturbation and its influence on the change of properties of the quasiparticles after their collision are of the same order. By contrast, inside the specific range the small perturbation dramatically affect the result of the collision.

REFERENCES

1. Ya. T. Frenkel and T. Kontorova: Zh. Eksp. Teor. Fiz. 8 (1938) 1340.
2. R. Hobart: J. Appl. Phys. 36, 6 (1965) 1944.
3. R. K. Dodd, J. C. Eilbeck, J. D. Gibbon and H. C. Morries: Solitons and Nonlinear Wave Equations, Academic, London, 1982.
4. Yu. S. Kivshar and B. A. Malomed: Rev. Mod. Phys. 61, 4 (1989) 763.
5. V. E. Zakharov, L. A. Takhtadjan and L.D.Faddeev: Dok. Akad. Nauk SSSR 219 (1974) 1334.