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Phonon emission from a discrete sine-Gordon breather

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Abstract

Phonon emission from a large-amplitude discrete sine-Gordon breather was studied numerically for a small degree of discreteness. In contrast to the case of highly discrete system investigated by Boesch and Peyrard (Phys. Rev. B 43 (1991) 8491), it was found that the resonance between the breather's oscillation and the phonons of the lower phonon band edge ($\kappa = 0$) takes place for a small degree of discreteness. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Frenkel–Kontorova chain; Sine-Gordon equation; Breather; Phonon; Resonance effect

1. Introduction

The one-dimensional nonlinear systems which support soliton solutions, such as the sine-Gordon (SG) and φ^4 fields, play an important role in many branches of physics and chemistry [1–3]. In the last few decades it has been demonstrated that different kinds of perturbations give rise to many interesting phenomena (see e.g., Refs. [4,5] and references therein). For the nonintegrable systems various resonance effects may take place [5–11]. The discreteness of media is a kind of perturbation which naturally appears in many applications of solid state physics and significantly modifies the properties of unperturbed soliton solutions [9,11–22].

The resonance between the breather oscillation and the phonons has been investigated for a highly discrete SG system by Boesch and Peyrard [11]. They studied the emission of phonons from breather. In the course of the oscillation, the breather constantly loses energy and its frequency ω_b gradually increases. When $3\omega_b$ becomes greater than the frequency of the upper phonon band edge, the energy emission drops down and the lifetime of the breather drastically increases [11].

In the present paper, we study numerically the breather-phonon resonance in the case of weak discreteness. In this case, the phonon band is very wide and the effect observed by Boesch and Peyrard [11] cannot take place because $3\omega_b$ cannot reach the upper phonon band edge. However, an interesting resonance effect takes place for a large-amplitude breather when $(2m+1)\omega_b$ with a positive integer m becomes greater than the frequency of the lower

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phonon band edge. Under this condition, the breather emits large bursts of phonon radiation. The remarkable fact is that this resonance effect is noticeable even for a weak discreteness.

2. Frenkel–Kontorova model and sine-Gordon equation

We consider the Hamiltonian of the Frenkel–Kontorova model [23] in a dimensionless form

$$H = \sum_n \left[\frac{p_n^2}{2} + \frac{1}{2h^2}(u_{n+1} - u_n)^2 + (1 - \cos u_n) \right], \tag{1}$$

where u_n is the displacement of the nth particle from an initial point with coordinate $x = nh$, p_n the momentum of the particle with a unit mass, H/h the density of energy and h is the only parameter of the system, which gives a measure of discreteness. The dynamics of the system are given by a set of equations of motion

$$\frac{d^2 u_n}{dt^2} - \frac{1}{h^2}(u_{n-1} - 2u_n + u_{n+1}) + \sin u_n = 0. \tag{2}$$

In the continuum limit ($h \to 0$), Eq. (2) takes the form of SG equation

$$u_{tt} - u_{xx} + \sin u = 0. \tag{3}$$

The breather solution to Eq. (3) in its center-of-mass frame can be written as

$$u(x,t) = 4 \arctan \frac{\eta \sin[\omega_b (t - t_0)]}{\omega_b \cosh[\eta (x - x_0)]}, \tag{4}$$

where $0 < \omega_b < 1$ is the frequency of the breather, $\eta = \sqrt{1 - \omega_b^2}$, and x_0 is the position of the breather.

In the continuum limit the period T_b, the amplitude A_b, and the energy E_b of the breather are given by the frequency of the breather ω_b as follows:

$$T_b = \frac{2\pi}{\omega_b}, \quad A_b = 4 \arctan\left(\frac{\eta}{\omega_b}\right), \quad E_b = 16\eta. \tag{5}$$

From the linearized SG equation, the following dispersion relation for small-amplitude oscillation modes (phonons) with a wave vector κ can be obtained:

$$\omega_\kappa^2 = 1 + \frac{4}{h^2} \sin^2(\pi\kappa), \tag{6}$$

with $0 \leqslant \kappa \leqslant 1/2$.

The phonon spectrum varies through the range $\omega_0 \leqslant \omega_\kappa \leqslant \omega_{1/2}$, where the frequency of the $\kappa = 0$ phonon and that of the $\kappa = 1/2$ phonon are

$$\omega_0 = 1, \quad \omega_{1/2} = \sqrt{1 + 4/h^2}. \tag{7}$$

Boesch and Peyrard have shown that the effect of the increase of breather lifetime [11] takes place at $3\omega_b > \omega_{1/2}$. However, since ω_b does not exceed 1, the effect can be observed only for $h > 1/\sqrt{2} \approx 0.71$.

3. Molecular dynamics simulation

The equations of motion Eq. (2) were integrated numerically with the use of the Störmer method of order six [24]. For the time step we set $\Delta t = (10^{-4} \sim 10^{-5})(2\pi/\omega_{1/2})$. For each set of parameters, we carried out several runs with different magnitudes of Δt in order to control the accuracy of simulation. Eq. (4), after the substitution $x \to nh$, was used for the initial conditions. A large-amplitude breather (with ω_b approaching zero) was placed in the middle of a chain containing from 801 ($h = 0.5$) to 5001 ($h = 0.1$) particles. Particles are numbered in a way that $-N \leqslant n \leqslant N$. A kind of absorbing boundary condition was used in order to prevent the breather from suffering the effect of the radiation reflected from the boundaries.

The discreteness parameter was varied in the range $0.1 \leqslant h \leqslant 0.5$. Eq. (4), besides ω_b, contains two more parameters, t_0 and x_0. The parameter t_0 defines the initial phase of breather oscillation and we put $t_0 = T_b/4$. The parameter x_0 defines the location of the breather center with respect to the lattice of particles and hence, it is sufficient to consider $0 \leqslant x_0 \leqslant h/2$. Our calculations showed that even for the largest studied magnitude of $h = 0.5$, the results do not depend on x_0 and one can put $x_0 = 0$.

In the course of the numerical experiment we calculated the breather energy after each half-period of its oscillation, when the breather has the minimum kinetic energy. The breather energy $E_b(l)$ was calculated with the use of Eq. (1) by summing over $-10/h \leqslant n \leqslant 10/h$ (center of breather is at $n = 0$). Thus, we numerically obtained the function $E_b(l)$, where l is the number of half-oscillation of the breather. The energy lost by breather in the lth half-oscillation can be defined as

$$\Delta E_b(l) = E_b(l+1) - E_b(l). \tag{8}$$

Eq. (5) for $h \leqslant 0.5$ gives the breather parameters with a good accuracy. It means that knowing the breather energy E_b, one can calculate the other parameters of the breather. In the present study, however, we calculated the frequency of breather $\omega_b(l)$ (where l is the number of half-oscillation) numerically, taking into account a small influence of discreteness on the frequency. The half-period of the breather can be obtained as the time between two sequential maximums of kinetic energy of the breather.

4. Numerical results and discussion

Eq. (4) predicts the oscillatory motion of the breather without the loss of energy. However, in the discrete system a breather constantly loses energy in the form of small-amplitude radiation. The reduction of breather energy E_b implies the increase in breather frequency ω_b (simulation starts from $\omega_b \approx 0.05$).

Having the two functions, $\Delta E_b(l)$ and $\omega_b(l)$, one can consider l as a parameter and study how ΔE_b varies with ω_b. In Fig. 1, the variation of ΔE_b as a function of ω_0/ω_b is presented for $h = 0.2$. One dot corresponds to one half-oscillation of the breather or, in other words, to a certain l. As one can see from Eq. (7), $\omega_0 = 1$, but we keep the symbolic notation to stress the physical meaning of the parameter. As Fig. 1 suggests, the energy emitted in a half-oscillation ΔE_b, on the average, sharply increases at $(2m+1)\omega_b = \omega_0$, where m is a positive integer. The smaller the m, the sharper the increase, so the most prominent resonance takes place when $3\omega_b$ becomes equal to ω_0.

The functions $\Delta E_b(l)$ and $\omega_0/\omega_b(l)$ in the vicinity of the strongest resonance ($m = 1$) are presented for $h = 0.2$ in Fig. 2 and for $h = 0.4$ in Fig. 3. Before the resonance ($\omega_0/\omega_b(l) > 3$) breather loses in a half-oscillation the energy about 10^{-4} for $h = 0.2$ and about 2×10^{-3} for $h = 0.4$. In both cases, the energy emitted in a half-oscillation is a small fraction of breather energy, because, for $\omega_0/\omega_b = 3$, one has $\omega_b = 1/3$ and, according to Eq. (5), $E_b \approx 15.1$. When $\omega_0/\omega_b(l)$ becomes smaller than 3, the breather starts to emit comparatively large bursts of energy. This process is shown for $h = 0.4$ in Fig. 4, which is a three-dimensional plot of $u_n(t)$ (for the sake of convenience, instead of time t we

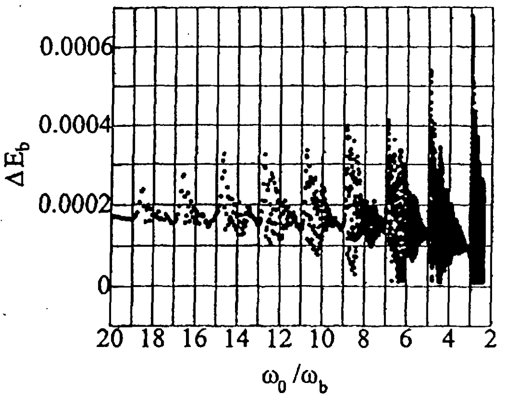

Fig. 1. Variation of ΔE_b as a function of ω_0/ω_b for $h = 0.2$.

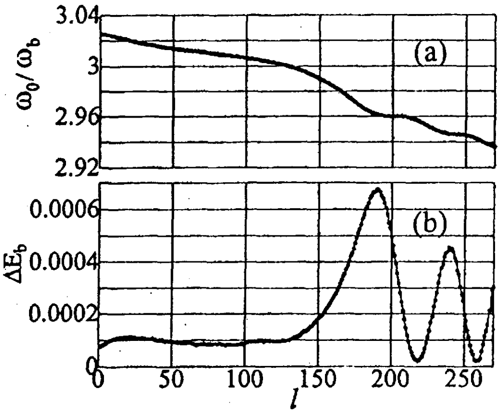

Fig. 2. (a) $\omega_0/\omega_b(l)$ and (b) $\Delta E_b(l)$ in the vicinity of the strongest resonance ($m = 1$) for $h = 0.2$ (l is the number of breather's half-oscillation).

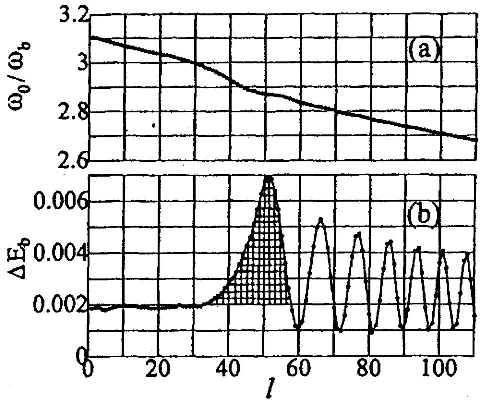

Fig. 3. The same as in Fig. 2 but for $h = 0.4$. The energy of the first, the largest, burst E_B is estimated from the shaded area.

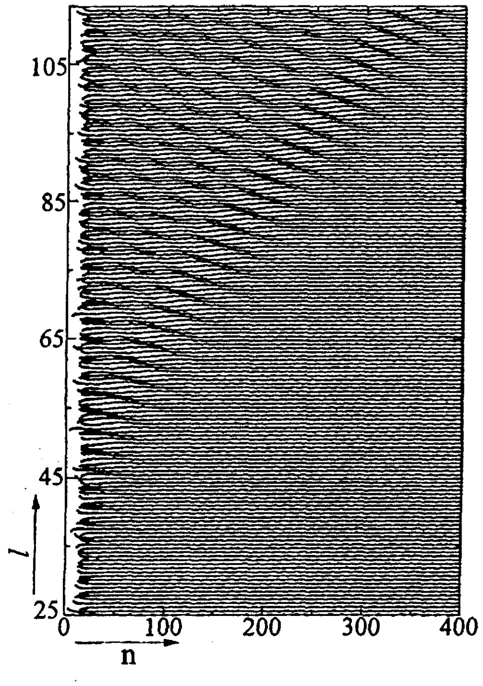

Fig. 4. The three-dimensional plot of $u_n(l)$, where l is the number of breather half-oscillation. $h = 0.4$. The breather locates at $n = 0$ and cannot be seen because only the particles with displacements $|u_n| \leqslant 0.1$ are plotted. Due to the symmetry, one-half of the picture is presented.

use the number of breather half-oscillation l). Due to the symmetry, one-half of the picture is presented. The breather is located at $n = 0$ and cannot be seen in Fig. 4, because we plot only the particles with displacements $|u_n| \leqslant 0.1$. Comparing Figs. 3 and 4, one can see that each maximum of the curve $\Delta E_b(l)$ corresponds to the emission of a burst.

Let us denote the energy of the first, the largest, burst as E_B. Energy E_B is emitted in the course of many half-oscillations of the breather. We estimated this energy by the shaded area shown in Fig. 3.

In Fig. 5, the influence of degree of discreteness h on the energy E_B is presented. On decrease of h from $h = 0.5$ $(1/h^2 = 4)$ to $h = 0.1$ $(1/h^2 = 100)$ the energy E_B decreases only by one order of magnitude, from 0.08 to 0.007. It is well known that many other manifestations of discreteness drop much faster with decreasing h. For example, the energy emitted by the breather in a half-oscillation in the pre-resonance regime drops by three orders of magnitude, from 5.5×10^{-3} to 7×10^{-6} on decrease of h from $h = 0.5$ to $h = 0.1$.

The reason of such slow decaying of E_B with decrease in h is quite clear. Indeed, on one hand, the smaller the h, the smaller the energy emitted by a breather in a half-oscillation, but on the other hand, the change of ω_b in a half-oscillation is also small and the resonance condition is fulfilled for a longer time.

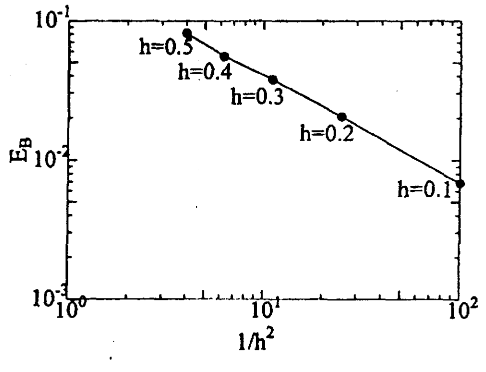

Fig. 5. The energy of the first resonance burst E_B vs $1/h^2$. Notice the logarithmic scale for both axes.

5. Conclusion

It was established numerically that in a weakly discrete SG system ($0.1 \leqslant h \leqslant 0.5$), the resonance between large-amplitude breather and phonons of the lower phonon band edge takes place when $(2m+1)\omega_b = \omega_0$, with a positive integer m. Under this condition the breather starts to emit comparatively large bursts of radiation in the form of small-amplitude wave packets. The most prominent resonance takes place for $m = 1$.

For a highly discrete system, the resonance effect does not manifest itself, because the breather passes through the resonance very quickly. This resonance effect is prominent for a moderate discreteness and it is noticeable for a weak discreteness.

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