Localized excitations of uniform anharmonic lattices

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The localized and resonant intrinsic vibrations in an anharmonic lattice which have been predicted theoretically [A. J. Sievers and S. Takeno, Phys. Rev. Lett. **61**, 970 (1988); S. Takeno and A. J. Sievers, Solid State Commun. **67**, 1023 (1988); S. Takeno *et al.*, Prog. Theor. Phys. **94**, 242 (1988)] and which have been observed in a numerical simulation [V. M. Burlakov *et al.*, Preprint 12, Institute of Spectroscopy, Academy of Sciences of the USSR, Troitsk] are shown to be genetically related to envelope solitons. An instability of a uniform excitation of the lattice with respect to decay into localized intrinsic vibrations has been observed.

Sievers and Takeno[1–3] noted in 1988 that localized or resonant (depending on the sign of the anharmonicity constant) intrinsic vibrations could exist in uniform lattices whose particle interaction potential contains a quartic anharmonicity. The studies in Refs. 1–3 and 5 were carried out in the strong-anharmonicity limit, in which the characteristic frequency of the localized intrinsic vibrations satisfies $\omega_l \gg \omega_m$, or that of the resonant intrinsic vibrations satisfies $\omega_r \ll \omega_m$ (ω_m is the upper limit of the phonon spectrum). The relationship between the localized excitations which were found and excitations which had already been studied thoroughly—solitons—therefore remained unclear. The discussion below is an effort to resolve this question.

1. To determine the genealogy of localized and resonant intrinsic vibrations, we consider the motion of particles of mass m of a monatomic anharmonic chain described by the equation

$$m\ddot{u}_n = K_2(u_{n+1} + u_{n-1} - 2u_n) + K_4((u_{n+1} - u_n)^3 + (u_{n-1} - u_n)^3), \tag{1}$$

where u_n is the displacement of atom n from its equilibrium position, and K_2 and K_4 are the harmonic and anharmonic constants of the potential.

Assuming the vibration spectrum of a particle in a localized intrinsic vibration to be harmonic, we seek a solution of Eqs. (1) in the form

$$u_n = \xi_n \cdot \exp(-i\omega t + ikx) + \xi_n^* \exp(i\omega t - ikx), \tag{2}$$

where ξ_n is a slow vibration amplitude. Substituting (2) into (1), and averaging the high-frequency harmonics over a period of $2\pi/\omega$, we find the equations

$$\left.\begin{aligned}&\frac{8i\omega}{\omega_m^2}\dot{\xi}_n + \xi_{n+1}\exp(ikh) + \xi_{n-1}\exp(-ikh) + \left(\frac{4\omega^2}{\omega_m^2} - 2\right)\xi_n \\ &+ 3\lambda\big((\xi_{n+1}\exp(ikh) - \xi_n)\,|\xi_{n+1}\exp(ikh) - \xi_n|^2 \\ &+ (\xi_{n-1}\exp(-ikh) - \xi_n)\,|\xi_{n-1}\exp(-ikh) - \xi_n|^2\big) = 0,\end{aligned}\right\} \tag{3}$$

where $\omega_m = (4K_2/m)^{1/2}$ is the frequency of the phonon band edge, $\lambda = K_4/K_2$ is the anharmonicity parameter, and h is the lattice constant. Assuming that ω is near the phonon band edge ($\omega = \omega_m + \Delta\omega$, where $|\Delta\omega| \ll \omega_m$), that λ is small, and that the variation of ξ_n along the chain is smooth, we can reduce system of nonlinear difference equations (3) to the differential equation

$$h^2 \cos(\Delta kh) \frac{\partial \xi^2}{\partial z^2} = 2(1 - \cos(\Delta kh) - \frac{4\Delta\omega}{\omega_m})\,\xi - 48\lambda\xi^3, \tag{4}$$

where $k = \pi/h + \Delta k$, $z = x - vt$, x is the coordinate along the chain, and v is the wave velocity, which is determined by

$$\frac{4v}{h\omega_m}(1 + \frac{\Delta\omega}{\omega_m}) + \sin(\Delta kh) = 0. \tag{5}$$

From Eq. (4) we can find the shape of the envelope of localized vibrations of the chain with an anharmonicity parameter λ. The resulting solutions are envelope solitons (Fig. 1).

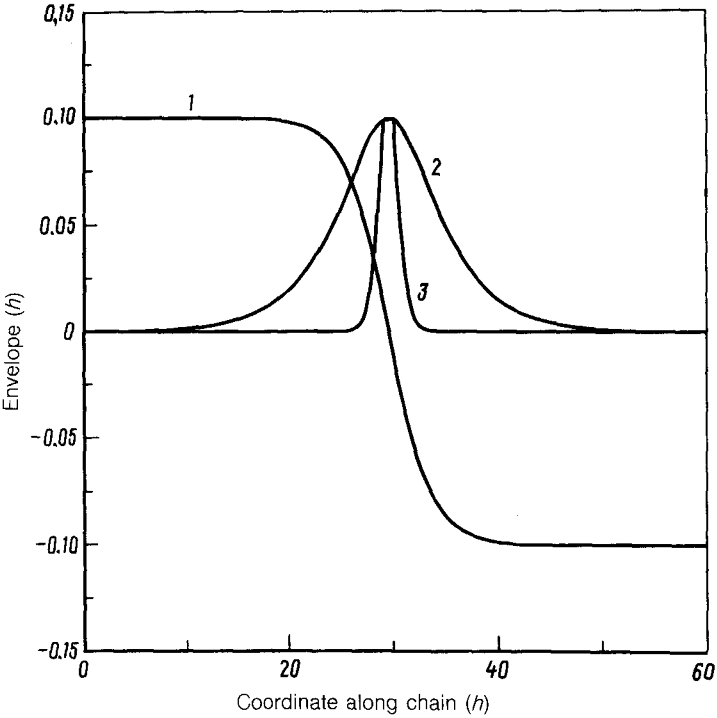

FIG. 1. Shape of the envelope of steady-state local vibrations of a chain. 1—Kink, $u_n = A\tanh(A(n-29.5)\sqrt{-6\lambda})$, $\lambda A^2 = -0.01$, where A is the amplitude; 2—envelope soliton, $u_n = A\,\mathrm{sech}[A(n-29.5)\sqrt{6\lambda}]$, $\lambda A^2 = 0.01$; 3—envelope found from the solution of Eqs. (3) with $\lambda A^2 = 1.0$.

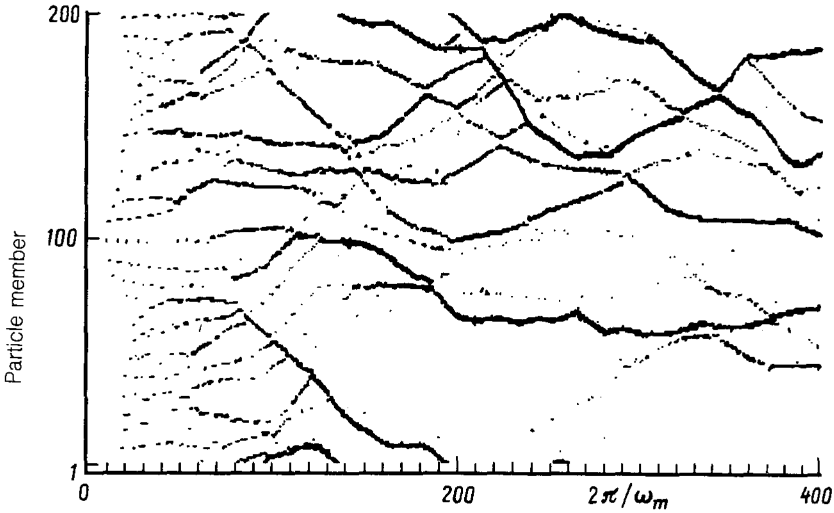

FIG. 2. Temporal Fourier spectrum of the motion of a particle at the center of a steady-state localized vibration found by the molecular dynamics method for the excitation of a localized intrinsic vibration with $\lambda A^2 = 1.0$ in a chain of 100 particles of mass $m = 1$. The motion of the particles was observed for a time of $1024\pi/\omega_m$. The peak is at the frequency $\omega_l = 1.644\,\omega_m$; a numerical calculation based on (3) yields $\omega_l = 1.656\,\omega_m$.

If instead the anharmonicity is not weak (a short localization radius), we must abandon the approximation of a continuous medium, and solve Eq. (3) numerically. The displacements u_n of the particles of a localized vibration, which have been found as a result of the numerical solution [Fig. 1(c)], were used as initial values for a study of the motion of the chain by the method of molecular dynamics.[6] A vibration retained its shape (within better than 1% in terms of the amplitude) over a time of $2048\pi/\omega_m$; a Fourier spectrum of the particle vibrations is shown in Fig. 2. The frequencies found for the steady-state envelope soliton by the molecular dynamics method and solutions of the envelope kink type are essentially the same as those found from the solution of Eqs. (3).

2. As was found by the molecular dynamics method, the excitation of local intrinsic vibrations through the specification of a one-, two-, or three-particle configuration of initial displacements is a process in which a threshold is involved.[4] The present study has shown that this fact is a consequence of the great disparity between the localization radii of the initial and stable excitations, as can be seen in the threshold nature of the energy loss of the fast particles which interact locally with the solid.

3. It is also interesting to study the stability of the highest-frequency mode of an anharmonic chain in the regime of slightly anharmonic vibrations. It turns out that the introduction of a weak random perturbation (with an amplitude of less than 1%) leads to a rapid decay of the mode, accompanied by the formation of several local intrinsic vibrations. In the latter vibrations, the particle vibration energy is an order of magnitude greater than the average value[7] (Fig. 3). This result may reflect the specific

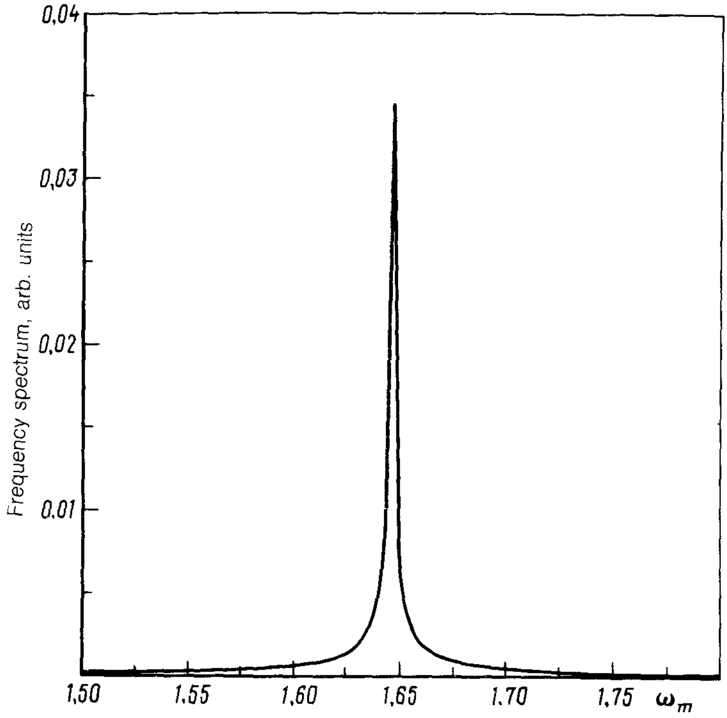

FIG. 3. Tracks of a localized intrinsic vibration in a chain of 200 particles ($m = 1$, $h = 1$) formed during the decay of the mode with $k = \pi/h$ ($u^0 = 0.1h$). The points correspond to a particle energy three times the average energy per particle. The parameters of the potential are $K_2 = 9.87$ and $K_4 = 9.87$ ($\lambda A^2 = 0.1$).

mechanism for the generation of defects (when the energy of a local intrinsic vibration exceeds the threshold for defect formation) in a uniform medium during intense coherent excitation. The long lifetime of local intrinsic vibrations, we should point out, leads to a substantial increase in the probability for a generation of defects by a tunneling (below-threshold) mechanism.

[1]A. J. Sievers and S. Takeno, Phys. Rev. Lett. **61**, 970 (1988).
[2]S. Takeno and A. J. Sievers, Solid State Commun. **67**, 1023 (1988).
[3]S. Takeno *et al.*, Prog. Theor. Phys. **94**, 242 (1988).
[4]V. M. Burlakov *et al.*, "Local normal vibrations in anharmonic chain," Preprint 12, Institute of Spectroscopy, Academy of Sciences of the USSR, Troitsk, 1989.
[5]J. B. Page, accepted for publication in Phys. Rev. B.
[6]R. W. Hockney and J. W. Eastwood, *Computer Simulation Using Particles*, McGraw-Hill, New York, 1981.
[7]Solitons are known to contain a large fraction of the energy of the initial "quasiclassical" excitation of the system. V. E. Zakharov, S. V. Manakov, S. P. Novikov, and L. P. Pitaevskiĭ, *Theory of Solitons*: *Method of the Inverse Problem*, Nauka, Moscow, 1980.

Translated by Dave Parsons