Energy Transport in One- and Two-Dimensional Anharmonic Lattices with Isotopic Disorder

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We present results from computer simulations of anharmonic vibrations of one- and two-dimensional lattices. For disordered systems we have found that anharmonicity destabilizes the localized modes and that when energy is fed locally to the lattice, it spreads out beyond the localization length via some kind of anomalous diffusion. Moreover, the diffusion exponent ν seems dependent on the strength of anharmonicity but not on the amount of disorder. In perfect lattices we have observed the $(-\frac{1}{2},1,-\frac{1}{2})$ localized mode predicted recently [S. Takeno, K. Kisoda, and A. J. Sievers, Prog. Theor. Phys. Suppl. **94**, 242 (1988)].

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Vibrations in discrete lattices have been extensively studied in the context of phonons in condensed matter and in discrete versions of nonlinear soliton field theories. For pure harmonic restoring forces in disordered lattices, it is well known that the vibration modes are localized in one and two dimensions. At $T=0$ no energy can be transferred across lattices as described first by Anderson.[1] Conversely, perfect but weakly anharmonic lattices can support solitary wave pulses that progress ballistically[2] thus transporting energy through the lattice. However, it has been found that when the anharmonicity is large enough one recovers an ergodic behavior[3] indicating that the solitary waves must be unstable for strong anharmonicity. The problem of stability for weak anharmonicity and very long times is today an open question. Also, what happens when both disorder and anharmonicity are involved is of crucial interest since it is the most common situation in crystals and amorphous solids. This problem had been considered early[4] in numerical simulations where it was observed that anharmonicity produces an enhancement of the thermal conduction in isotopically disordered lattices. More recently, anharmonic resonant modes have been found in anharmonic lattices[5] and it was assumed that they move diffusively when disorder is present.[6] In order to test this assumption, we have studied numerically the energy transfer in anharmonic lattices with random masses in one and two dimensions. We have effectively observed that, after an initial local excitation where energy is given to the lattice, a regime of diffusion occurs at long times. However, our results indicate a process of *anomalous diffusion*. This regime is characterized by an exponent ν which depends strongly on anharmonicity but is insensitive to disorder.

We consider networks of N atoms connected by nonlinear springs between nearest neighbors. At each site the mass is m_i and vibrations are described by scalar field displacements $U_i(t)$ and their time derivatives $V_i(t)=\dot{U}_i(t)$. The nonlinearity comes from a "quartic" anharmonic interaction in the Hamiltonian which takes the following form:

$$\mathcal{H}=\tfrac{1}{2}\sum_i m_i V_i^2+\tfrac{1}{2}\sum_{i,j\,\mathrm{nn}}\{[U_i(t)-U_j(t)]^2+K_4[U_i(t)-U_j(t)]^4\}, \quad (1)$$

where the second sum runs over all pairs of nearest neighbors. K_4 is a positive constant describing the strength of the anharmonic potential.

We proceed by numerical integration of the equations of motion using a standard Euler-Cromer method (leap-frog algorithm) which has been specifically implemented and optimized for a parallel computer built at the laboratory. The viability of our computations has been checked against two types of numerical approximations, namely, the time discretization and the roundoff errors. We varied the time step from 1/50 to 1/4000 of the period of oscillation of the excitation force and the U_i and V_i have been represented as 32- and 64-bit numbers without affecting the qualitative aspect of the results. Also the conservation of total energy (to within 1% in the worst cases) has been used as an indicator of numerical stability.

We first study the combined effect of disorder and anharmonicity on the vibrations resulting from a local pulse. Some results on perfect lattices are also reported below. Disorder has been included in the model using a random mass distribution of the following type:

$$m_i=m_0 e^{\beta x_i}, \quad (2)$$

with m_0 the typical mass, β the strength of disorder ($\beta\simeq 1$), and x_i a random number uniformly distributed within $[-1,1]$. This disorder has the property that all the moments of the m_i/m_0 distribution are equal to the corresponding moments of the m_0/m_i distribution. The relative mass fluctuation σ has been used to characterize the isotopic disorder.

The lattice, initially immobile ($U_i=V_i=0$), is excited on a single site by a pulse of an external oscillatory force

acting at frequency Ω with a Gaussian envelope at half-width equal to 3 (expressed in our time unit $2\pi/\Omega$). Hence the wave packet excited in the harmonic regime has a relative width $\sigma_\Omega/\Omega \approx 1/10$. For a given lattice excited at frequency Ω, the anharmonic situation is completely characterized by three parameters, namely, the amplitude of the acting force F_0, the typical mass m_0, and the anharmonic constant K_4. To express the strength of the anharmonicity by a single parameter is a complex problem since the anharmonic potential itself is not a constant of motion. One can define the ratio η of anharmonic energy to the total energy but it varies in time and, for a given total energy, it is dependent on the *global* mode pattern. Takeno, Kisoda, and Sievers[7] have described an anharmonic stationary mode using a parameter Λ that characterizes the anharmonic situation *locally* but this is not extensible to the present regime. All our simulations have been done at constant $F_0 = 0.062$ and $m_0 = 260$ while the anharmonicity has been varied through the parameter f_{anh} related to K_4 via the relation $K_4 = 2^{3f_{\text{anh}}-1}$. One should note that even with the largest value of K_4, the ratio η of anharmonic energy over total energy has never exceeded 6% in one dimension (1D) and 12% in two dimensions (2D). Conversely, when $f_{\text{anh}} = 0$, the ratio η becomes so small that the situation is effectively harmonic.

During the short initial pulse, energy is fed on a single site and starts to spread on the lattice. When $K_4 = 0$ the harmonic system is governed by Anderson localization and the energy cannot spread beyond the localization length ξ. Figures 1(a) and 1(b) show "maps" of the energy distribution, respectively, on the 1D and 2D lattices.

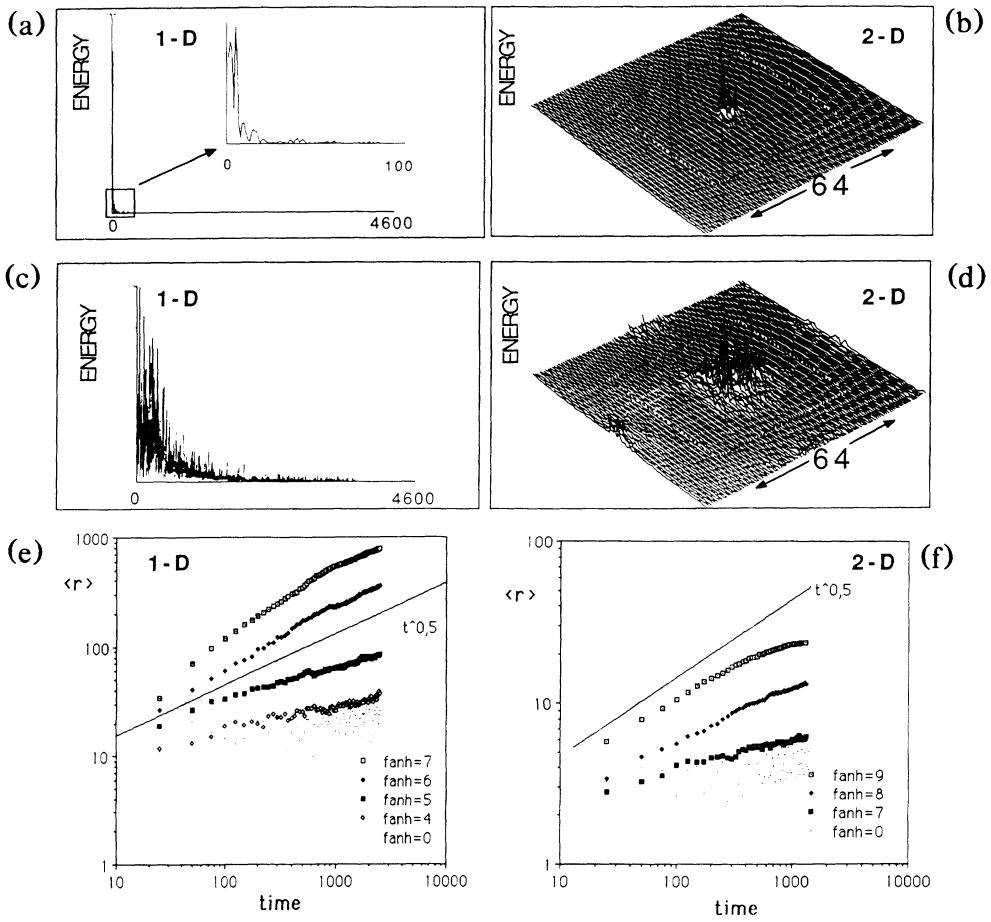

FIG. 1. Spreading of energy in 1D and 2D lattices. For the 1D case the number of sites is 4600 and free boundary conditions are used. The 2D lattice size is 64×64 and periodic boundary conditions are in effect. (b) and (d) are presented using a repeated zone scheme. (a),(b) Energy distribution function resulting from a local pulse in disordered harmonic lattices; (a) $\Omega/\omega_{\max} = 0.935$, $\sigma = 11.5\%$, and $t = 1000$; (b) $\Omega/\omega_{\max} = 0.8$, $\sigma = 81\%$, and $t = 100$. For this harmonic case the modes are localized. (c),(d) Energy distribution in disordered *anharmonic* lattices [(c) $f_{\text{anh}} = 7$ and (d) $f_{\text{anh}} = 8$] in otherwise the same conditions as (a) and (b). The energy spreads out markedly beyond the localization length. (e),(f) Evolution of the mean radius of the energy distribution function for different anharmonic cases. The $\langle r(t) \rangle$ follow power laws of time t^ν with $\nu \neq 0.5$ indicating anomalous diffusion. Moreover, ν depends on the anharmonic coefficient f_{anh}. In (f) the negative curvature for $f_{\text{anh}} = 9$ is a finite-size effect.

For the 1D case $\Omega/\omega_{max}=0.935$, $\sigma=11.5\%$, and the time $t=1000$; for the 2D case $\Omega/\omega_{max}=0.8$, $\sigma=81\%$, and $t=100$ (ω_{max} is the cutoff frequency of the acoustic band of each perfect lattice). In both cases the time is such that the mode patterns do not evolve any further. One can see from the figures that the size of the samples is much larger than the localization length; this validates these studies even though the sizes are only moderately large.

When anharmonicity is introduced, we observe the most striking feature of these simulations [Fig. 1(c), $f_{anh}=7$ and Fig. 1(d), $f_{anh}=8$; the conditions are otherwise the same as for Figs. 1(a) and 1(b), respectively]: *the energy spreads out markedly beyond the localization length* ξ. The energy is not confined around the excitation site but is distributed according to some law reminiscent of a diffusion profile. In order to describe quantitatively this process, the time evolution of the "center of mass" of the energy distribution has been measured. If $\epsilon_i(t)$ is the local energy on site i at time t then the mean radius $\langle r(t)\rangle$ of this distribution is defined by $\langle r(t)\rangle = \sum[\epsilon_i(t)r_i]/\sum\epsilon_i(t)$, where r_i is the distance to origin of the ith site (absolute value) and the sums run over all sites. We have represented in log-log plots the laws $\langle r(t)\rangle$ for different values of the anharmonic constant f_{anh} [Figs. 1(e) and 1(f) in one and two dimensions].

For each value of f_{anh} our data have been analyzed in terms of a power law of the type $\langle r(t)\rangle \propto t^{\nu}$, where ν is a conventional exponent of diffusion. The values of ν obtained from least-squares fits over about two decades of time are collected in Fig. 2. Note that ν is different from 0.5 for most cases, which can be considered as an indication of an anomalous diffusion process. Moreover, ν is a function of the strength of anharmonicity but does not seem to depend on disorder. This last result has been obtained by an ensemble of simulations where the disordered has been changed at fixed f_{anh}.

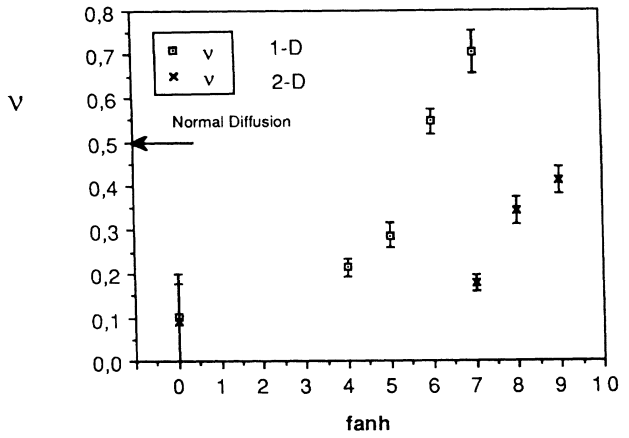

FIG. 2. Values of the anomalous diffusion exponent ν obtained from Figs. 1(e) and 1(f) as a function of the anharmonic coefficient f_{anh}. The error bars reflect the indetermination of the best line passing through the data points in Figs. 1(e) and 1(f).

The diffusion is remarkable in the sense that it does not seem to result from a random walk of some elementary excitation such as a solitary wave. Those waves do exist in the *perfect* lattice and we have observed them numerically but they tend to break down in *disordered* systems. This breakdown could be interpreted as an indication that the mean free path of those waves become comparable to their thickness or equivalently that hopping times become comparable to the periods of vibration. The diffusion seen here comes from a spreading of the energy distribution function in its entirety. There is no energy "grain" obeying a random-walk motion.

We will report elsewhere in more detail the results we obtained in perfect lattices (with no mass disorder). We enumerate here some interesting properties of those systems. First, we have observed that our pulsed excitation creates "peaks" that propagate ballistically on the lattices. Those peaks behave as solitary waves propagating at speeds larger than the harmonic wave speed; also the spectrum of those excitations involves frequencies higher than the cutoff frequency. Two kinds of peaks have been observed: progressive and immobile. The immobile mode pattern has an amplitude profile very similar to the one predicted recently by Takeno, Kisoda, and Sievers.[7] In one dimension, this amplitude profile corresponds approximately to the sequence $\{\ldots,0,-\frac{1}{2},1,-\frac{1}{2},0,\ldots\}$. We have also observed propagating modes with the profile $\{\ldots,0,-1,1,0,\ldots\}$, which have never been considered before. During the motion of those peaks on a finite linear chain and square lattices we have observed interactions between them. The collision of two peaks propagating in opposite directions can produce either their "fragmentation" in which new peaks of smaller intensity are created or "immobilization" in which one resulting peak becomes localized on the lattice. Our preliminary results indicate that these interactions can be responsible for the evolution of the system toward an ergodic state.

The tentative conclusion of this study is that the localization regime of vibrations is unstable versus anharmonicity, as small as it may be: *the modes are delocalized by anharmonicity and are responsible for an "anomalous diffusion regime" for the energy transport.* Hence when both anharmonicity and disorder are present the diffusion regime then appears to be the most universal situation.

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