EVIDENCE OF ENERGY DIFFUSION IN PURE ANHARMONIC DISORDERED CHAINS

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Abstract: We present results of large scale simulations on vibrations of anharmonic disordered chain. We find that anharmonic effects tend to counter the localisation process and lead to diffusion of the energy on the lattice. For the anharmonic ordered case the energy is concentrated in large peaks as the global energy spread linearly in time.

Keywords: Vibrations, Non-Linear Effects, Localisation, Diffusion.

Introduction

Using a massively parallel computer (Connection Machine), we have studied a chain of atoms of mass m_i, interacting by harmonic and "quartic" anharmonic interactions described by the coefficients k_2 and k_4 in the hamiltonian which is written as:

$$H = \sum_i \frac{1}{2} m_i V_i^2 + \frac{k_2}{2} \sum_{i,j,(n.n.)} (U_i - U_j)^2 + \frac{k_4}{4} \sum_{i,j,(n.n.)} (U_i - U_j)^4 \qquad (1)$$

The $U_i(t)$ are the scalar amplitudes of vibration at time t and $V_i(t) = \dot{U}_i(t)$; the last two sums run over all pairs of nearest-neighbors. Disordered systems were simulated by having the masses m_i randomly distributed. In a perfect chain, $m_i = m$ and the hamiltonian (1) is the one studied in early time by Fermi, Ulam and Pasta [1]. The nature of the stable non-linear excitations of frequencies higher than the cut-off phonon frequency is an interesting problem which was revisited recently by Sievers and Takeno [2]. They found, self-localized anharmonic modes of odd parity with frequency above the Debye cut-off frequency and dependent on the k_2 and k_4 coefficients. Recently, Page [3] has showed that the pure anharmonic hamiltonian i.e. without harmonic interaction ($k_2 = 0$), can be solved and yields two anharmonic modes of odd and even parity with frequencies above the phonon cut-off frequency.

The present study deals with this simplified pure anharmonic hamiltonian ($k_2 = 0$) in ordered and disordered chains. The main results are obtained by numerical simulation of large chains of 16000 atoms. The equation of motion are integrated numerically using either a simple leap-frog algorithm as described in reference [4] or a more sophisticated fourth order symplectic method [5]. Results were found to be independent on the

integration method. On a Connection Machine of 16384 processors with single precision hardware Weitek chips and a SUN front-end computer we reached performances of $21 \cdot 10^6$ updates/sec with the leap-frog algorithm. The symplectic solver was about 3 times slower.

Periodic boundary conditions are used and the excitation consist in an initial displacement of unit length of some chosen site (labeled 0). The time steps is 1/50 of the shortest period of vibration and averages were taken over an ensemble of 10 to 200 different samples. Whenever disordered systems were considered, the masses were distributed uniformly around the average mass $m_0 = 250$ with a relative root-mean square deviation :

$$\sigma = \left(\frac{< m_i^2 > - m_0^2}{m_0^2} \right)^{(1/2)} \tag{2}$$

with $\sigma = 11.5\%$.

The characteristic results are represented in the following figures, where the excitations has been applied at $x = 0$. We present the instantaneous energy $E_t(x)$ as a function of the space variable x for different times (in unit of the shortest period of vibration).

1 - Perfect chain

The function $E_t(x)$ is shown at a time ($t = 50$, fig. 1a) where the initial peak of energy has already split into several peaks. At time $t = 1000$ (fig. 1b), a broad packet of the peak fragments is observed. Note that well defined peaks are moving in front of the packet. It will be shown that the r.m.s. of this energy distribution varies linearly in time (cf. figure 4).

2 - Disordered chain

The same plots $E_t(x)$ for now disordered chains reveals a progressive spreading out of the energy in space. Here the energy distribution at $t = 1000$ is decreasing in space, but fluctuates largely for one given sample.

3 - Disordered chain : Ensemble average.

Averages of energy profiles from 200 samples are plotted at different times (fig. 3a). As time increases the energy spreads on the lattice. In fig. 3b we plotted $E_t(x) \cdot \sqrt{t}$ vs. $x/\sqrt{t}$. As time increase the distribution function becomes increasingly well approximated by a gaussian function. For t=10000 data we found that we could express $E_t(x)$ (solid line in fig. 3b) as :

$$E_t(x) = \frac{4.72 \cdot 10^{-2}}{\sqrt{(t)}} exp(-2.18 \cdot 10^{-2} (\frac{x}{\sqrt{(t)}})^2) \tag{3}$$

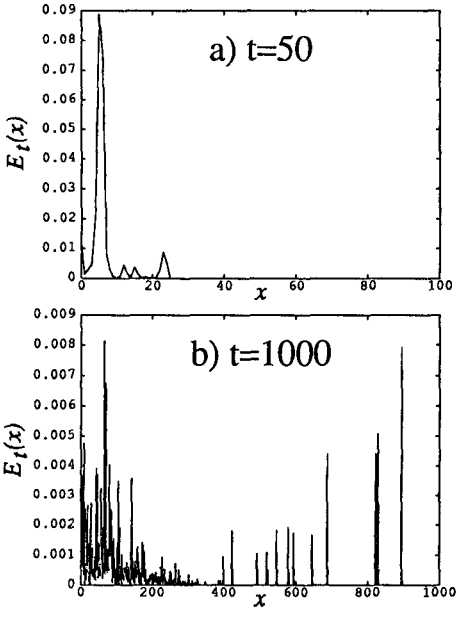

Figure 1. Energy distribution function $E_t(x)$ in the ordered case for a) $t = 50$ and b) $t = 1000$. The horizontal axis is in lattice units, the vertical scale is arbitrary units. The excited sites is site 0. The energy also spread in the negative direction (not shown).

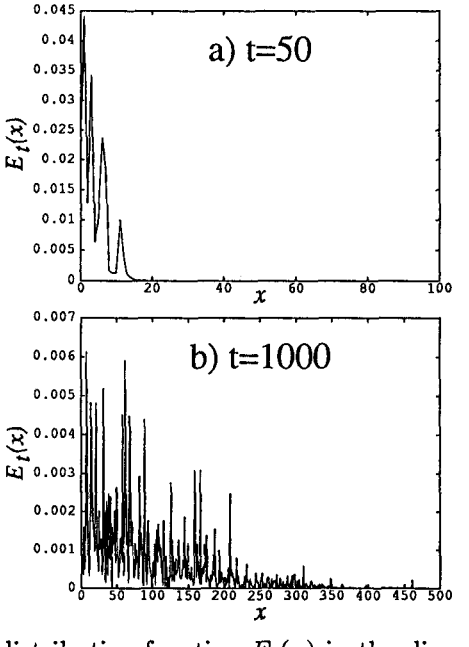

Figure 2. Energy distribution function $E_t(x)$ in the disordered case for a) $t = 50$ and b) $t = 1000$. The energy present large fluctuations with a general tendency to decrease. The characteristic length of decrease grows with time as does the number of peaks.

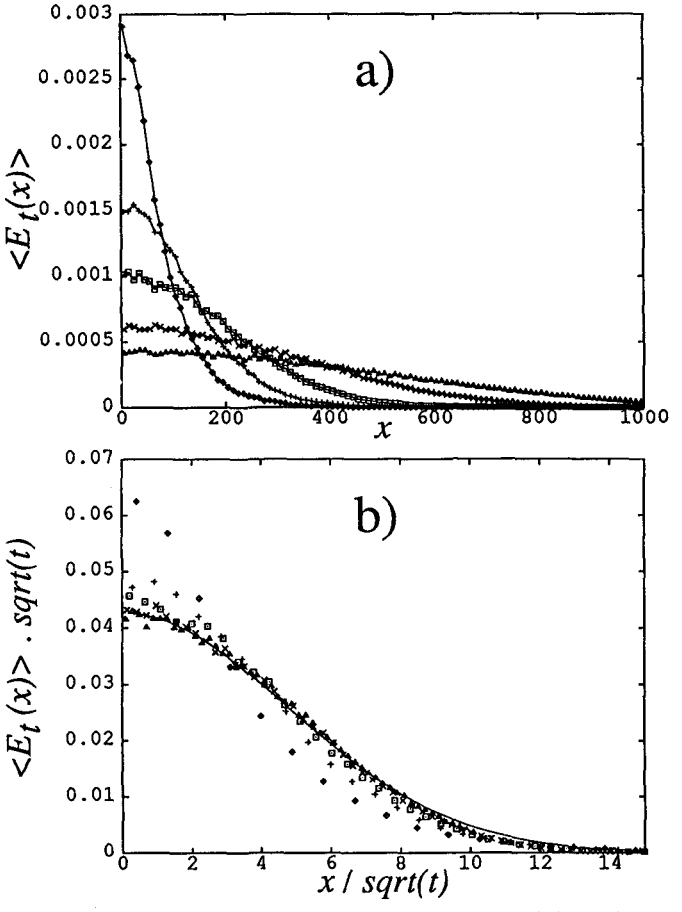

Figure 3. Average energy distribution function $< E_t(x) >$ (a) in the disordered case for $t = 500(\diamond), 1000(+), 2000(\square), 5000(\times)$ and $10000(\triangle)$. Over 200 samples were averaged. In (b) we have plotted $< E_t(x) > \cdot\sqrt{t}$ vs. $x/\sqrt{t}$ and eq. (3) (solid line). As time increase the curves converge toward a gaussian.

4 - Evolution of the energy distribution

The second moment of the energy distribution $< x^2 >$ is plotted as a function of time for three different situations : - the losanges for the perfect chain exhibiting a t^2 variation at large times, - the crosses for an ensemble of 10 disordered chain show a law proportional to time for about two decades, - the square for a pure harmonic disordered chain ($k_4 = 0$) where the localization phenomenon is revealed by the saturation of

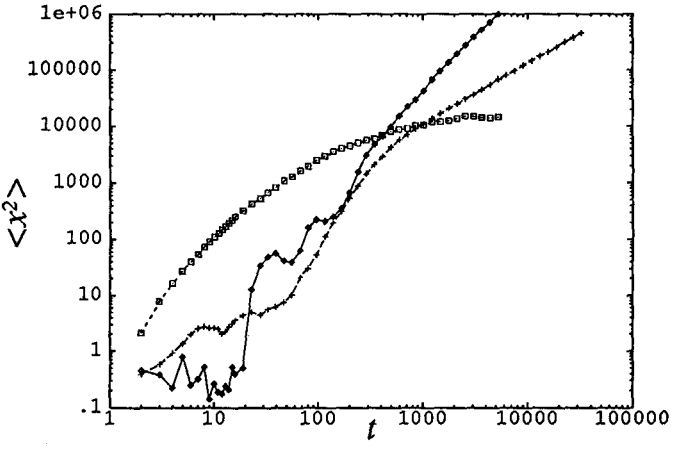

Figure 4. Second moment of the energy distribution function $< x^2 >$ for the harmonic disordered case (□), the anharmonic disordered case (+) and the anharmonic ordered case (◇). The first curve shows how the energy becomes localized due to the disorder in harmonic systems. With anharmonicity the second moment increases linearly with time for ($t > 1000$) as in a diffusion process. In the anharmonic *ordered* case the moment increases as t^2.

$< x^2 >$ at long time. The estimated localization length is obtained from this asymptotic value: $x_0 \approx 100$.

5- Analysis

A preliminary analysis of the observed phenomenon can be formulated in the following terms:

- the energy peaks of the perfect and pure anharmonic chain are basically instable. One observes a spontaneous desintegration a big peaks in fragments of smaller energy. At longer times the packet of fragments moves uniformly in time. This uniform motion reveals an underlying conservation law during the fragmentation of the type "conservation of momentum". This relation comes from the translational invariance property of the perfect chain.

- The apparent "normal diffusion" would come from the fragmentation of the peak excitation on the mass impurity. Let us call R_i, T_i and L_i the fraction of the incident energy which is reflected, transmitted of localized on the mass m_i. The energy conservation law gives : $R_i + T_i + L_i = 1$.

The problem of random fragmentation can be changed into the more conventional problem of random walk of a fictive particle which is reflected, transmitted or immobilized with probability R_i, T_i and L_i. It is not difficult to show [6] that the particle obeys a diffusive law characterized by a diffusion constant $D \propto (R_i/T_i)^{-1}$. Hence, this diffusive motion leads to a well known law $< x^2 > \sim 2Dt$. Since this law is well observed in the simulations, the model of random fragmentation on the impurities is validated. This conceptual frame, in addition to the expected characteristic lengths present in

the problem like the interatomic distance and the soliton or peak width, provides us a new length l : the average distance between two random fragmentations. The previous regime of normal diffusion is hence obtained when $l >> \Lambda \sim a$. (Λ is the soliton width). Other interesting regimes could be also considered, particularly when the harmonicity is restored, where an additional characteristic length : the localization length must be taken into account. This more complex regime exhibits anomalous diffusion [4].

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