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INTERPLAY OF ANDERSON LOCALIZATION AND SOLITONIC ENERGY TRANSPORT IN THE DISORDERED FERMI-PASTA-ULAM CHAIN[1]

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In this paper energy transport in a harmonically disordered chain with a regular array of quartic n.n. springs is studied. Depending on the choice of the excitation we have found two archetypes of solitary solutions (self localized soliton,ultra-debye-frequency and hypersonic kink-solitons) which respectively display constructive or destructive interplay with Anderson localization. Under certain circumstances we observe the generation of longliving subsonic solitons, which allude to the possibility of practically unhindered energy transport in disordered structures.

1. Introduction

This work is stimulated by the current debate about the role anharmonicity plays for the transport properties of nonconducting disordered materials. The discussion started with the discovery of universal anomalies in the heat conductivity of silica glasses and other materials found by Zeller and Pohl [10]. Their measurements show a T^2-law, a plateau and a further increase of the heat conductivity above the plateau region. This latter increase motivated the idea of a constructive role played by anharmonicity. On the other side numerical simulations of Allen and Feldmann [1] seem to indicate that no anharmonicity is needed to explain this increase.

Disorder and anharmonicity are the two dominant mechanisms of phonon scattering in solids. Thus on the one hand they were both supposed to reduce thermal conductivity. Especially in the fundamental paper of Peierls [5] it has been proven that in an ordered

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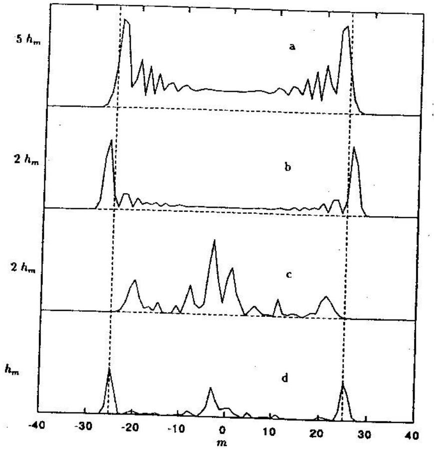

Fig. 1. Initial ($\tau = 0$) P-excitation at $m = 0$. Distribution $h_m(\tau)$ for a given instant $\tau = 50$, (a) ideal harmonic chain ($\gamma_4 = 0$, $f'/f = 1$) (b) ideal anharmonic chain ($\gamma_4 = 1$, $f'/f = 1$) (c) disturbed harmonic chain ($\gamma_4 = 0$, $f'/f = 0.5$, $c = 0.2$) (d) disturbed anharmonic chain ($\gamma_4 = 1$, $f'/f = 0.5$, $c = 0.2$) The dashed perpendicular lines mark the sound velocity edges of the undisturbed chain.

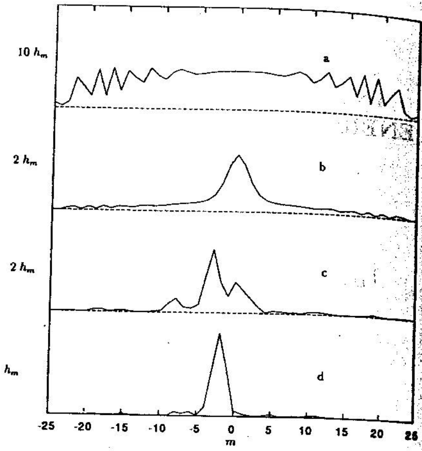

Fig. 2. Initial ($\tau = 0$) Q-excitation at $m = 0$. Distribution $h_m(\tau)$ for a given instant $\tau = 50$, (a) ideal harmonic chain ($\gamma_4 = 0$, $f'/f = 1$) (b) ideal anharmonic chain ($\gamma_4 = 1$, $f'/f = 1$) (c) disturbed harmonic chain ($\gamma_4 = 0$, $f'/f = 0.5$, $c = 0.2$) (d) disturbed anharmonic chain ($\gamma_4 = 1$, $f'/f = 0.5$, $c = 0.2$).

anharmonic solid thermal resistance may exist due to Umklapp-processes. On the other hand already in the famous paper of Fermi, Pasta and Ulam it has been demonstrated that an excited one dimensional anharmonic System (Fermi-Pasta-Ulam chain) does not merge into thermal equilibrium [3]. Later it has been verified that hypersonic solitons exist in anharmonic chains. In particular that has been shown analytically by Todá [7] for an exponential potential (Toda potential) and numerically for a fourth-order anharmonicity (Fermi-Pasta-Ulam chain) by Zavt et.al. [4].

2. System

To analyze the interplay between disorder (Anderson localization [2]) and anharmonicity we study two different classical initial excitations of a one-dimensional chain with n.n. harmonic and quartic interaction. Introducing dimensionless coordinates Q_m, the equation of motion for this system then reads:

$$\frac{d^2}{d\tau^2}Q_m(\tau) = \frac{1}{4\mu_m}\{\Phi_{m,m+1}(Q_{m+1} - Q_m) + \Phi_{m,m-1}(Q_{m-1} - Q_m) + \gamma_4\left[(Q_{m+1} - Q_m)^3 + (Q_{m-1} - Q_m)^3\right]\} \quad (1)$$

where $\mu_m = M_m/M$, and $\Phi_{m,m'} = f_2(m,m')/f$ are normalized masses and force constants respectively. M and f denote the Mass and the harmonic force constant of the undisturbed chain. $\tau = \Omega_D t = 2\sqrt{f/M}t$ is a normalized time. The parameter γ_4 characterizes the strength of the anharmonicity. An estimation of the value of γ_4 in real systems has been given in an earlier work [4]. Disorder is introduced for the harmonic part in the form of a second spring constant f' assuming to be present with concentration c and distributed at random.

To gain information about transport properties of the system, we consider the spatial evolution of the dimensionless local energy per site m, h_m which is defined as:

$$h_m = \frac{1}{2}\mu_m\left(\frac{dQ_m}{d\tau}\right)^2 + \frac{1}{16}\{\Phi_{m,m+1}(Q_{m+1} - Q_m)^2 + \Phi_{m,m-1}(Q_{m-1} - Q_m)^2 + \frac{1}{2}\gamma_4\left[(Q_{m+1} - Q_m)^4 + (Q_{m-1} - Q_m)^4\right]\} \quad (2)$$

The equation of motion has been solved with different numerical methods (fourth-order-predictor-corrector method, Runge-Kutta) in a self expanding manner.

3. Conflicting interplay

The first excitation we study (denoted as P-excitation) is of the form:

$$P_m(0) = \delta_{m,0}; \qquad Q_m(0) = 0 \quad (3)$$

In Figs. 1.a-d the energy distribution $h_m(\tau)$ at the same instant is presented. For the ideal harmonic chain (Fig. 1a) one gets a plateau region near the center which is limited by sharp peaks at the sound velocity edges ($v_{snd}\tau$). The analytical form of this evolution is discussed in more detail elsewhere [8]. If anharmonicity is introduced an additional peak beyond the sound velocity edges appears. The hypersonic peaks are solitons of kink-type, as can be seen in the Q_m representation (Fig. 3a). In the continuum limit, which corresponds to a spatially extended soliton, an analytical solution has been given by Wadati [9]. If, by contrast, disorder is introduced in the harmonic chain, we observe that the distribution of the energy splits in two components (Fig. 1c): propagating wings at the effective sound velocity edges ($v_{snd}^{eff} < v_{snd}$) and a non-propagating central part (Anderson localization [2]). Globally, energy propagation is diminished against that of Fig. 1a. If disorder and anharmonicity are combined (Fig. 1d) we observe a reduction of Anderson localization and a destabilization of the kink solitons which, however, may survive for a long time.

In total the sequence of Figs. 1 demonstrates the conflicting interplay of Anderson localization and solitary energy transport. With respect to energy propagation we realize the phenomenon that indeed anharmonicity may favour energy transport. Additional details are discussed in the paper of Zavt et.al. [4].

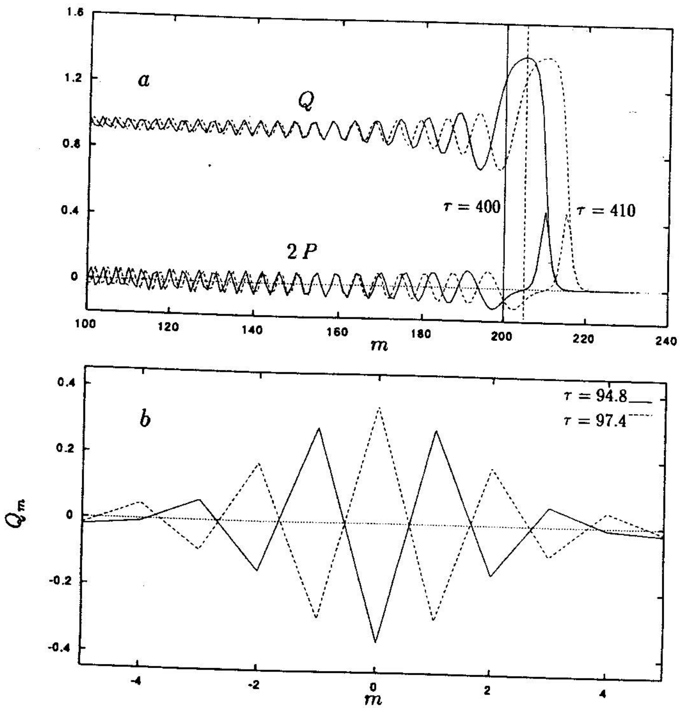

Fig. 3. Solitons in the ideal anharmonic chain ($\gamma_4 = 1$, $f'/f = 1$) . (a) Kink soliton (P-excitation). The sound velocity edge $m = v_{snd}\tau$ is marked by perpendicular lines. Residual "harmonic" space oscillations below this edge. (b) Oscillating self localized soliton (Q-excitation) ($\gamma_4 = 1$, $f'/f = 1$).

4. Enhanced localization

In this section we consider an alternate archetype of initial excitation ("Q - excitation")

$$Q_m(0) = \delta_{m,0}; \quad P_m(0) = 0 \tag{4}$$

In Figs 2a-d the energy distribution $h_m(\tau)$ at the same given instant is presented. For the ideal harmonic chain (Fig. 2a) we observe that more energy remains in the central region as compared to P-excitation (Fig. 1a), whereas near the sound velocity edge the wings play a less pronounced role. This has been discussed analytically by Vazquez-Marquez et al [8].

In the ordered anharmonic chain (Fig. 2b) we note the upgrow of a strong selflocalized oscillating soliton at site $m = 0$ (see also (Fig. 3b). This selflocalized mode is of the type considered in the group of Sievers [6].

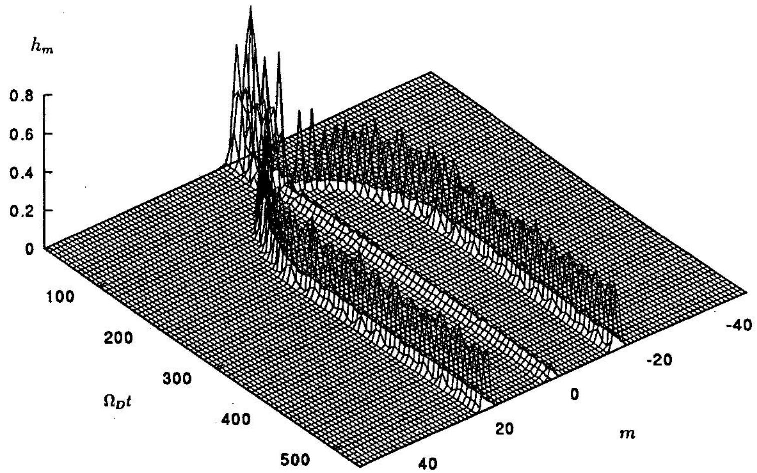

Fig. 4. Spatiotemporal evolution of the site energy $h_m(\tau)$ in the ordered anharmonic chain ($\gamma_4 = 10$, $f'/f = 1$). Initial ($\tau = 0$) Q-excitation at $m = 0$.

Introducing spring-disorder in the harmonic chain (Fig. 2b) we find a much larger Anderson localization than in the corresponding P case (Fig. 1c)

Finally again combining disorder and anharmonicity we notice a strong enhancement of the central localized energy portion which demonstrates the constructive interplay between Anderson localization and solitary selflocalization.

5. Unexpected propagation paths

¿From the foregoing sections we have learned that neither of the two archetypical excitations seems to allow for a free ballistic transport of energy in the disturbed anharmonic chain. But by further increasing the value of γ_4 our computer simulation hints at the possibility of ballistic transport pathways.

In Fig. 4 again a Q-excitation in an ordered anharmonic FPU-chain is shown in its space-time development. After some time the energy packet splits up in three stable selflocalized solitons, where the central one is of odd-parity [6] whereas the other two are of even parity. If spring disorder is turned on, already a rather small amount of it suffices to prevent the splitting in three peaks (Fig. 5). But in addition to this effect a much more interesting phenomenon with respect to energy transport is observed. As noted, a pulse like longliving excitation moving with subsonic velocity separates from the selflocalized part in the central region.

Now, it could be argued that in the considered example the anharmonicity parameter γ_4 is unrealistically high. But the same situation can be realized by a smaller γ_4 value, if

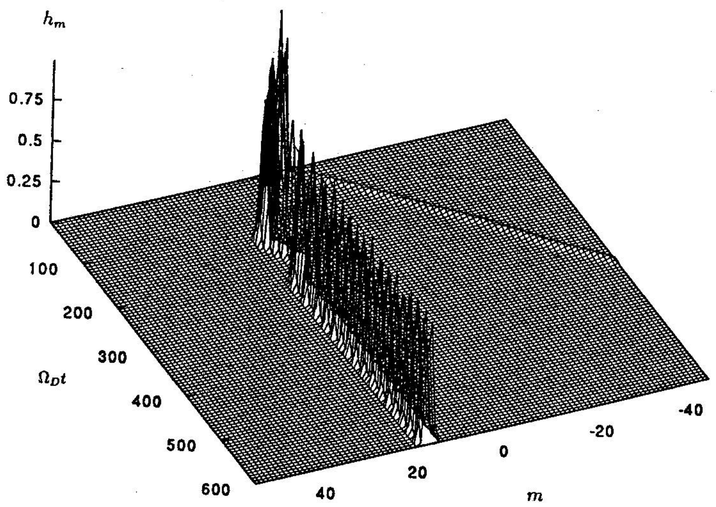

Fig. 5. Spatiotemporal evolution of the site energy $h_m(\tau)$ in the disordered anharmonic chain ($\gamma_4 = 10, \quad c = 0.5, \quad f'/f = 0.95$). Initial ($\tau = 0$) Q-excitation at $m = 0$.

the measure of the initial excitation $Q_m(0)$ is appropriately increased. Thus, the ballistic packet of Fig. 5 may appear also in systems without excessively high anharmonicity. Although the localized energy in the central region may be non-realistically high, the moving soliton carries much less energy, and since it is found to be an individual object apart from the central one, it can be considered just as a possible solution of the equation of motion irrespective of the generation process. In particular it is conceivable to generate it directly by a suitably chosen initial excitation.

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