DELOCALIZATION INDUCED BY NONLINEARITIES OF ANDERSON LOCALIZED LINEAR MODES IN A RANDOM MEDIUM

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It is known for many decades that in some very particular models, there are exact solutions which correspond to spatially localized time periodic vibrations ("breathers"). About a decade ago, it has been realized that in classical systems which are both *nonlinear* and *discrete,* such solutions generically exist, that is no special potential forms are required[1].

In principle, *discrete breathers* may exist in any periodic nonlinear model at any dimension taking into account the whole complexity of real systems, and moreover they are robust against model perturbations.

The existence of these *discrete breathers* is a consequence of the facts that on one hand the vibration frequency of an oscillation in a nonlinear system depends on its amplitude and on the other hand, the linear phonon spectrum is bounded in frequency because the system is discrete. Then, when the frequency and the harmonics of the *discrete breathers* are in the phonon gaps, no energy radiation is possible so that this localized vibration persists forever as an exact solution[2].

These discrete breather solutions are often linearly stable, that is the small fluctuations do not grow exponentially[3]. This result implies physically that in the presence of moderate fluctuations, for example the thermal fluctuations at low temperature, their life time will be much longer that those predicted by standard models of relaxation. Thus, it is not by chance that these classical excitations were first found numerically by molecular dynamics in a series of model with increasing complexity. It has been found that they appear spontaneously in some conditions out of thermodynamical equilibrium, for example under the effect of a thermal shock.

Otherwise, it is well-known since the pioneering works of Anderson[4] in the fifties that the linear modes of a random medium may be spatially localized. In that case, disorder detunes in some sense, all the resonances which would exist between the vibrations which are localized at different spots of the system, which forbids any propagation of vibrational energy over long distance. This theory was also very successful for explaining the insulating properties of some random metallic alloys (e.g. $Nb_x V_{1-x}$) or of semiconductors.

Thus, it seems natural to expect that when both nonlinearity and disorder are involved in the same system, the localization effect of vibrational excitations will be enhanced. Indeed, since the localized phonons of the linearized system cannot propagate any energy, the energy of a localized excitation cannot be dissipated through the system even if its frequency belongs to the phonon spectrum, and then it should persist indefinetely.

Actually, the phenomenon is more complex than one could believe, because nonlinearities play a "*double-game* ". On one hand, disorder and nonlinearity may cooperate for generating discrete breathers which then are exact well localized solutions. On the other hand, for other time periodic solutions, disorder and nonlinearity conflict. Nonlinearity may restore resonances between sites which are far apart, and then generate unexpectedly spatially extended modes which can propagate some flux of energy.

We analysed in detail this effect on a very simple model which consists into a one dimensional chain of quartic oscillators coupled by harmonic springs. For that purpose, we improved and developed several original and reliable techniques for calculating very accurately both localized and the extended modes in large systems (which could become possibly very complex such as macromolecules)[5].

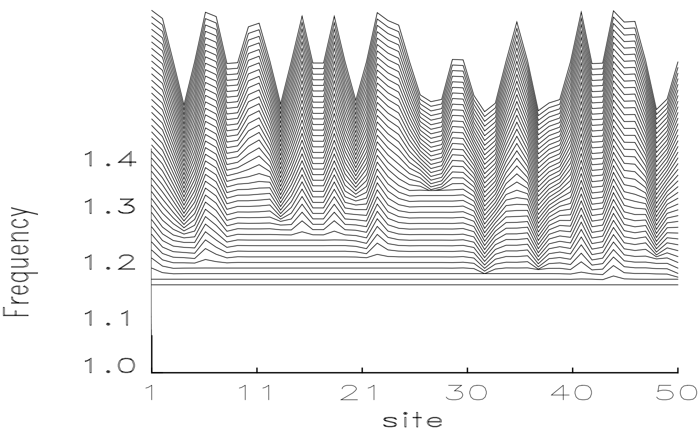

Figure: Profile of the initial positions for an exact time periodic and time reversible solution at different amplitudes which is initially a localized linear mode (on site 44) at zero amplitude for the hamiltonian

$$H = \sum_i \left(\frac{1}{2}\dot{u}_i^2 + \frac{1}{2}\omega_{i,0}^2 u_i^2 + \frac{1}{4}u_i^4 + \frac{C}{2}(u_{i+1} - u_i)^2\right)$$

ω_{0i}^2 *is uniformly random in the interval* [0.5,1.5] *in a finite system with 50 sites. Each line corresponds to a given frequency and amplitude of the initial localized mode, increasing from lower to upper line.*

With these methods, we can follow continuously the evolution of a time periodic solution as a function of its frequency (or amplitude of the initially localized linear mode) when model nonlinearities are present. The figure shows an example of such an evolution, for a solution which is initially a localized linear mode (on site 44) at amplitude zero. It is first observed as expected that the frequency of this solution increases as a function of its amplitude because of nonlinearities. However, it is clear that extra oscillations grow at spots which are possibly very far from the initial excited spot. These new oscillations start to develop precisely at the location of linear localized modes the frequency of which becomes resonant with those of the solution. Thus for an infinite system with a dense phonon spectrum, an infinite number of resonant frequencies are crossed for any small variation of the amplitude (or equivalently the frequency). As a result, the initial solution immediately delocalizes with small peaks at the corresponding resonant spots. However, while the solution is still small, the distribution of these spots is sparse which only allows a tiny transport of energy which nevertheless is not zero. When the amplitude becomes larger, the amount of energy which can be propagated by such a solution increases and becomes comparable to those of a nonlinear phonon in a similar but non random system.

We are also able to calculate accurately localized discrete breathers in the same systems, but with other methods[6]. Our numerical results agree with a theorem of Albanèse and Fröhlich[7] proven on a similar model, which states that there is a "quasicontinuum" of solutions with frequency in a fat Cantor set (that is with a finite measure). The gaps in this Cantor set are the consequences of the resonances with the linear modes which destroy the localized character of the solution and must be avoided. Since there are infinitely many possible resonances, there are infinitely many gaps but however the widths of these gaps, decay as an exponential function of the distance between the breather to the resonant localized linear mode. Because of that, the frequency Cantor set is not void and keeps a finite measure.

These original results open new perspectives for a better understanding of glasses and other amorphous materials, which is non phenomenologic. On one hand, we predict that nonlinearities even very small imply that a nonvanishing residual thermal conductivity persists at low temperature but drops very fast to zero at zero K. On the other hand, a substantial part of the vibrational energy of the system may be spontaneously trapped as localized discrete breathers for very long times, which become macroscopic at very low temperature. This effect, which can be easily checked by molecular dynamics test, provides an alternative interpretation for the slow relaxation processes in glasses usually described by the old phenomenological two-level model of Anderson. Our interpretation only requires some nonlinearity in the model, which may be very weak and thus which should always exist. On contrary, the Anderson model requires the existence of double wells which actually has never been confirmed by direct structural observations (at least in most materials).

References
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