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LETTER TO THE EDITOR

Localization length scaling in binary harmonic chains with correlations controlled by thermal annealing

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Abstract. We investigate the nature of the vibrational modes of a random binary harmonic chain with site correlation for which an annealing temperature T is used as a disorder controlling parameter. In the low-temperature regime one finds that the localization length L_c does not scale with T like the mean cluster size $\xi_a \propto e^{a/T}$ but follows a power law scaling. Furthermore, the power law exponent varies continuously with the mode frequency. As a function of both the frequency and temperature, the localization length curves can all be collapsed down to a universal function of the frequency, namely $f(\omega) = L_c(\omega, T)T^{(\mu_1 + \mu_2\omega^2)}$, with $\mu_1 = 2.1 \pm 0.1$ and $\mu_2 = 1.1 \pm 0.1$.

The effect of disorder in an otherwise crystalline system has been the subject of extensive studies since Anderson's [1] seminal work on localization in 1958. For intermediate disorder a three-dimensional (3D) system may undergo a metal–insulator transition (MIT) at a critical energy called the mobility edge [2] which separates a metal from an insulator. More recently it has been shown [3] that close to the MIT the electronic wave functions show spatial multifractal behaviour. In this case the singularity spectrum does not depend either on the energy or on the disorder.

The interest in the transport properties of 1D systems exhibiting correlated disorder has also grown in the last few years [4–9]. Such systems basically consist of a distribution of defects placed randomly amongst an otherwise crystalline host system in such a way that the distribution exhibits some kind of spatial correlation. The very existence of extended states violates Anderson's [1, 10] rule, according to which the electron states for 1D on-site disordered systems should be localized even for an infinitesimal amount of disorder.

Correlation seems to be an essential key for electronic delocalization in 1D. In practice one usually randomly distributes the parameters amongst the lattice sites in such a way that, for a given site, their values depend on the corresponding neighbouring values to within a correlation length. In a binary tight-binding model for example, one can assign the on-site energies randomly to pairs of sites forming the so called random dimer model (RDM). The correlation is then implicit in the internal symmetry of the structure of the dimers with the delocalized states appearing as the resonant modes of such structures. However, as recently shown [11], the internal symmetry of the clusters is not a necessary condition to produce near-resonant non-scattered modes. Another point is that delocalization is not only associated with correlated on-site energies. Disordered chains with correlated off-diagonal interactions [8, 9] and a nonlinear random binary alloy modelled by a discrete nonlinear Schrödinger equation [12] have also been reported to display delocalized states. In the RDM model \sqrt{N} of the electronic stationary states are extended throughout the whole lattice. The large number of extended electronic states associated to these systems, may alter its transport

properties, possibly leading to the discovery of new materials with significant technological applications.

Since the 1D harmonic chain can be mapped onto a tight-binding model of an electronic system almost all normal vibrational modes are localized in the 1D disordered harmonic chain [13]. These systems have been shown [14, 15] to behave like a pure chain at the frequency $\omega = 0$ once this mode represents the uniform translational motion of the entire chain. Matsuda and Ishii [14] showed that in such systems a few low-frequency modes are not localized and that the number of such modes is of the order of \sqrt{N} . Correlations are generally introduced in the masses which are distributed randomly except by the fact that a given mass value only appears in pairs. One could also consider all the masses equal and let the spring constants take on two values, one of which is distributed in pairs, i.e. in a dimer-like fashion. The cluster distribution, however, is usually considered to be completely uncorrelated.

In this work we introduce thermally controlled correlations amongst the sites of a random binary harmonic chain and carry out a numerical study of the nature of its normal vibrational modes. This is done by allowing for a short-range interaction between the sites with the thermal equilibrium achieved at an annealing temperature T . This is the parameter that controls the correlation, allowing us to continuously move from a completely uncorrelated site distribution to a correlated one. Thermally controlled correlations reduce the degree of disorder thus leaving room for more delocalized modes to appear. A characteristic length suitable for determining the degree of localization is the inverse participation number L_c , defined below. Unexpectedly one finds that, in the regime of small temperatures, L_c does not follow the same exponential scaling law with temperature as the mean cluster size. It actually displays a power law behaviour with frequency-dependent exponents. As a matter of fact, one finds that all L_c versus ω^2 curves can be collapsed down to a universal function of the frequency, namely $L_c(\omega, T)T^{(\mu_1 + \mu_2\omega^2)}$, with $\mu_1 = 2.1 \pm 0.1$ and $\mu_2 = 1.1 \pm 0.1$.

The equation of motion for a one-dimensional array of atoms with masses $\{m_i\}$ coupled by harmonic springs with the frequency ω is written as

$$(\beta_{i-1} + \beta_i - \omega^2 m_i)u_i = \beta_{i-1}u_{i-1} + \beta_i u_{i+1}. \quad (1)$$

Here β_i is the spring constant of the i th spring that couples together the two masses m_i and m_{i+1} . u_i is the Fourier transform of the amplitude of vibration of the i th mass. In what follows we shall consider $\beta_i = 1$ and assume that the masses can take on only two values, namely m_a and m_b . The chain is then composed of type A sites containing one atom of mass m_a and type B sites containing one atom of mass m_b . This is called the binary harmonic chain model.

In order to introduce a correlated site distribution we allow for a site interaction through a first-neighbour symmetric pair potential such that the energy of a given pair configuration is given by

$$E(AA) = E(BB) = -\epsilon_0 \quad (2)$$

$$E(AB) = E(BA) = \epsilon_0. \quad (3)$$

The distribution of sites A and B over the chain is then obtained by following an annealing process. We start by randomly classifying the sites in types A and B with a fixed concentration ρ of sites B . The thermal equilibrium at temperature T is achieved by letting the site distribution evolve under the following dynamical rules: (a) if a given site is between two different types of sites it will remain as it is since, according to equations (2) and (3), $E(AAB) = E(ABB) = 0$; (b) the probability p of a given site being between like

sites obeys a Boltzmann distribution

$$p = p(AAA) = p(BBB) = e^{1/T} / (e^{1/T} + e^{-1/T}) \quad (4)$$

where T is the temperature measured in units of $2\epsilon_0/k_B$. In order to satisfy the above probability distribution a given site with two equal neighbours becomes a like site with probability p . In practice one must allow the concentration ρ to fluctuate between $\rho \pm \Delta\rho$ with $\Delta\rho \ll \rho$, and the last step is realized only if this constraint is not violated. The random initial site distribution is then allowed to evolve over a large time interval under the above dynamical rules and the distribution is quenched once thermal equilibrium is achieved. The annealing temperature can then be used as a disorder controlling parameter. As a matter of fact one gets a completely random site distribution for large T whereas phase separation is observed as T approaches zero ($\epsilon_0 > 0$). For the sake of completeness we checked that the mean cluster size ξ_a scales with the temperature as $\log \xi_a \propto 1/T$ for very low temperature. The degree of localization of the vibrational modes can be measured by computing the inverse participation number defined as

$$L_c(\omega^2, T) = \frac{\sum_{i=1}^N u_i^2}{\sum_{i=1}^N u_i^4} \quad (5)$$

for the range of frequencies lying inside the common band of the constituent atoms.

In what follows we give the results obtained for the particular case $m_a = 1$ and $m_b = 2$, with $\rho = 0.30$. In this case the common band is in the range $0 \leq \omega^2 \leq 2$ [16, 17]. The total number of sites used in our simulation was $N = 5000$, and we performed 5000 runs over the entire chain in order to achieve thermal equilibrium. The localization length was obtained by averaging over 100 configurations of the final quenched site distribution.

Figure 1 shows the localization length as a function of the squared frequency for several values of the annealing temperature. One observes the existence of the delocalized pure mode at the $\omega = 0$ resonant frequency and a general increase of L_c with decreasing correlation (increasing temperature), as expected. One also notices that the thermal correlations do not lead to the emergence of any new resonant frequency, contrary to the behaviour of models in which correlations are introduced by allowing the sites to have an fixed internal structure [8, 9, 14, 15]. At the upper band edge the localization length becomes small, and above this frequency the vibrational modes exhibit an exponential decay in the large mass sites.

We investigated the behaviour of L_c with temperature for several values of the mode frequency. It was found that L_c exhibits a power law increase in the low-temperature regime of the form $L_c \propto T^{-\nu}$, with the exponent showing a roughly linear dependence on ω^2 . In figure 2 we plot $L_c(\omega^2, T)T^{(\mu_1 + \mu_2\omega^2)}$ versus ω^2 in a linear-log scale for several values of the annealing temperature. According to our numerical estimates the temperature exponent that better characterizes the curve collapsing occurs for $\mu_1 = 2.1 \pm 0.1$ and $\mu_2 = 1.1 \pm 0.1$. This shows that, as a function of both the frequency and temperature, L_c follows a universal curve of the frequency, apart from a slight deviation at the edges of the common band. Therefore the localization length does not follow an exponential scaling law with the temperature as would be expected from the scaling behaviour of the correlation length $\xi_a \propto e^{a/T}$.

In conclusion, we studied the nature of the normal vibrational modes of a random binary harmonic chain with site correlations introduced through an annealing process. We showed that the localization length exhibits the expected trend, i.e. it generally increases with decreasing annealing temperature. However, we obtained that the mean cluster size and the localization length increase with decreasing temperature following quite distinct laws, with the latter exhibiting a power law increase with frequency-dependent critical exponents.

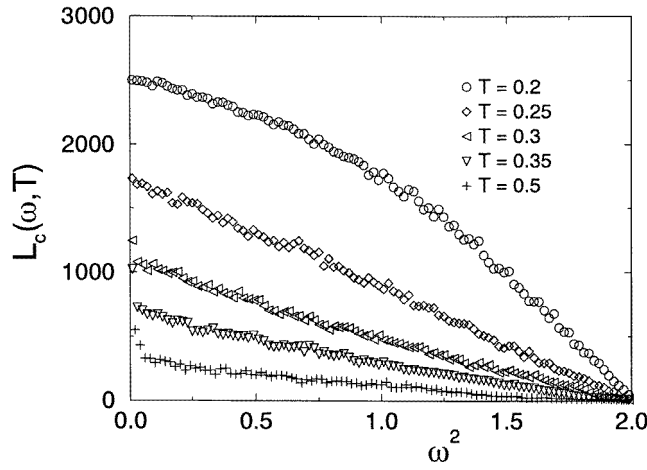


Figure 1. Localization length $L_c(\omega^2, T)$ versus ω^2 for $T = 0.2$, $T = 0.25$, $T = 0.3$, $T = 0.35$ and $T = 0.5$. Notice that the localization length generally increases with decreasing disorder, i.e. decreasing temperature.

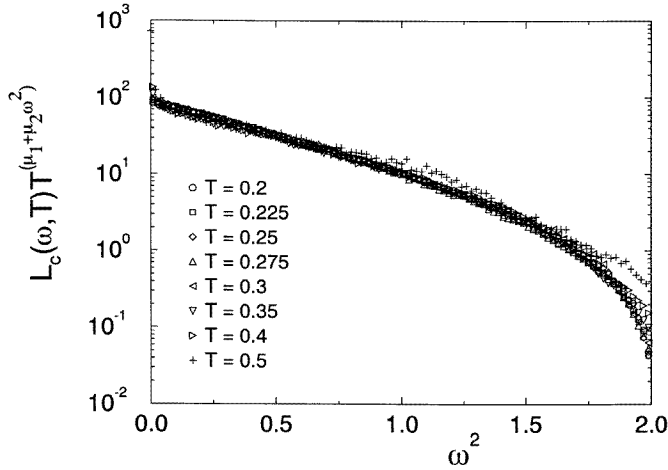


Figure 2. Linear-log plot of $L_c(\omega^2, T)T^{(\mu_1 + \mu_2 \omega^2)}$ versus ω^2 for several values of the annealing temperature. The temperature exponent used for the curve collapsing was $\mu_1 = 2.1 \pm 0.1$ and $\mu_2 = 1.1 \pm 0.1$. Notice that the collapsing breaks down at the common band edges and higher temperatures.

This result is quite intriguing and it would be interesting to obtain it on analytical grounds. An extension of a recently proposed local functional integral approach to the problem of diffusion and localization in random media can possibly be used to obtain the scaling laws in systems with correlated disorder [18]. Further investigation must be pursued in order to determine the role played by the system parameters, such as the concentration and mass relation, in the above scaling law. Work in this direction is currently in progress.

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