



# Vibrational modes in harmonic chains with diluted disorder

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## Abstract

We study the nature of collective excitations in harmonic chains with diluted disorder. Using a transfer matrix method, we compute the localization length of eigenmodes within the band of allowed energies in order to investigate the new extended states which appear in this model. To follow the time evolution of an initially localized energy input, we calculate the second moment  $M_2(t)$  of the energy spatial distribution. We found that for an impulse initial excitation, the super-diffusive energy spread is not affected by the presence of new resonant modes. However, the energy spread becomes faster for a displacement excitation.

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## 1. Introduction

Usually, disorder induces localization of collective excitations thus degrading transport properties. This effect is largely pronounced in low dimensions. In particular, the one-electron eigen-states in the 1D Anderson model with site-diagonal uncorrelated disorder are exponentially localized for any degree of disorder [1]. However, several 1D models with correlated disorder have been proposed which

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exhibit delocalized states [2–6]. Among these models, the diluted Anderson chain has attracted a renewed interest [7–11].

Hilke [7] introduced an Anderson model with diagonal disorder diluted by an underlying periodicity. The model consists of two interpenetrating sub-lattices, one composed of random potentials (Anderson lattice) and the other composed of non-random sites of constant potential. Due to the periodicity, special resonant energies appear. A similar model was used to study the electronic properties of semiconductor alloys [8]. The existence of an extended state at the band center was demonstrated, both analytic and numerically. The diluted Anderson model was extended to include a general diluting function which defines the on-site energies within each non-random segment [9]. Using a block decimation approach, it was demonstrated that this model displays a set of extended states, the number of which strongly depends on the length of the diluting segments and the symmetry of the diluting function. Recently, it was shown that the presence of new extended modes in the 1D diluted Anderson model promotes a sub-diffusive spread of an initially localized electron wave-packet [10]. The extension for a square lattice geometry has shown that this model can exhibit a true metal–insulator 2D transition with mobility edges delimiting a band of extended states [11].

The Anderson localization of collective excitation by a random potential is a quite general feature. It applies, for example, to the study of magnon localization in random ferromagnets [12]. Further, the collective vibrational motion of 1D disordered harmonic chains of  $N$  random masses can also be mapped onto an one-electron tight-binding model [13]. In such a case, most of the normal vibrational modes are localized. However, there are a few low-frequency modes not localized, whose number is of the order of  $\sqrt{N}$  [13,14]. It was shown that correlations in the mass distribution produce a new set of non-scattered modes in this system [15]. Also, non-scattered modes have also been found in disordered harmonic chain with dimeric correlations in the spring constants [16]. By using analytical arguments, it was also demonstrated that the transport of energy in mass-disordered harmonic chains is strongly dependent on non-scattered vibrational modes as well as on the initial excitation [17]. For impulse initial excitations, uncorrelated random chains have a super-diffusive behavior for the second moment of the energy distribution [ $M_2(t) \propto t^{1.5}$ ], while for initial displacement excitations a sub-diffusive spread takes place [ $M_2(t) \propto t^{0.5}$ ]. The dependence of the second moment spread on the initial excitation was also obtained in Ref. [18]. Recently, several studies have been employed addressing the controversial question about the thermal conductivity behavior of mass chains in the thermodynamic limit [19–21].

In this work, we study the nature of collective excitations in harmonic chains with diluted disorder. The density of vibrational states is obtained, as well as accurate estimates for the Lyapunov exponent. These are used to characterize the new extended vibrational modes which appear in this model. In order to study the time evolution of an initially localized energy input, we calculate the second moment  $M_2(t)$  of the energy spatial distribution. We show that these resonant modes are able to modify the dynamics of the energy spread.

## 2. Vibrational modes

We start by considering a disordered harmonic chain of  $N$  masses, for which the equation of motion for the displacements  $q_n = u_n \exp i\omega$  with vibrational frequency  $\omega$  is [14,15]

$$(\beta_{n-1} + \beta_n - \omega^2 m_n)u_n = \beta_{n-1}u_{n-1} + \beta_n u_{n+1}. \quad (1)$$

Disorder is introduced on the masses  $m_n$  which are uncorrelated random numbers chosen from a previously defined distribution. In our calculations, we will use units such that all elastic force couplings  $\beta_n = 1$  and the random site masses will be taken uniformly from a given interval. It is interesting to notice that the above motion equation has the same form exhibited by the Schroedinger equation for the eigenfunction amplitudes  $c_n$  of a tight-binding Hamiltonian describing one-electron of energy  $E$  moving in a potential  $\varepsilon_n$  coupled by hopping transfer terms  $t_n$ . Mapping the harmonic chain model into the tight-binding Hamiltonian is done by the replacements  $c_n \rightarrow m_n^{1/2}u_n$ ,  $E \rightarrow \omega^2$ ,  $\varepsilon_n \rightarrow (\beta_{n-1} + \beta_n)/m_n$  and  $t_n \rightarrow -\beta_n/\sqrt{m_n m_{n+1}}$  [22]. Therefore, the harmonic chain with uncorrelated random masses is mapped into a tight-binding model with correlated diagonal and off-diagonal terms. These effective correlations are responsible for new features presented by the vibrational modes, in particular, the weak sensitivity of the low-energy modes to the underlying disorder.

The diluted harmonic chain is constructed by introducing a new site between each original pair of neighboring masses. These sites have identical masses  $m_0$ . Eq. (1) can be rewritten as

$$\begin{pmatrix} u_{n+1} \\ u_n \end{pmatrix} = \begin{pmatrix} 2 - m_n \omega^2 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u_n \\ u_{n-1} \end{pmatrix}. \quad (2)$$

For a specific frequency  $\omega$ , a  $2 \times 2$  transfer matrix  $T_n$  connects the displacements at the sites  $n - 1$  and  $n$  to those at the site  $n + 1$ :

$$T_n = \begin{pmatrix} 2 - m_n \omega^2 & -1 \\ 1 & 0 \end{pmatrix}. \quad (3)$$

Once the initial values for  $u_0$  and  $u_1$  are known, the value of  $u_n$  can be obtained by repeated iterations along the chain, as described by the product of transfer matrices

$$Q_N = \prod_{n=1}^N T_n. \quad (4)$$

The localization length of each vibrational mode is taken as the inverse of the Lyapunov exponent  $\gamma$  defined by [14,15]

$$\gamma = \lim_{N \rightarrow \infty} \frac{1}{N} \log \frac{|Q_N c(0)|}{|c(0)|}, \quad (5)$$

where  $c(0) = \begin{pmatrix} u_1 \\ u_0 \end{pmatrix}$  is a generic initial condition. Typically,  $5 \times 10^6$  matrix products were used to calculate the Lyapunov exponents.

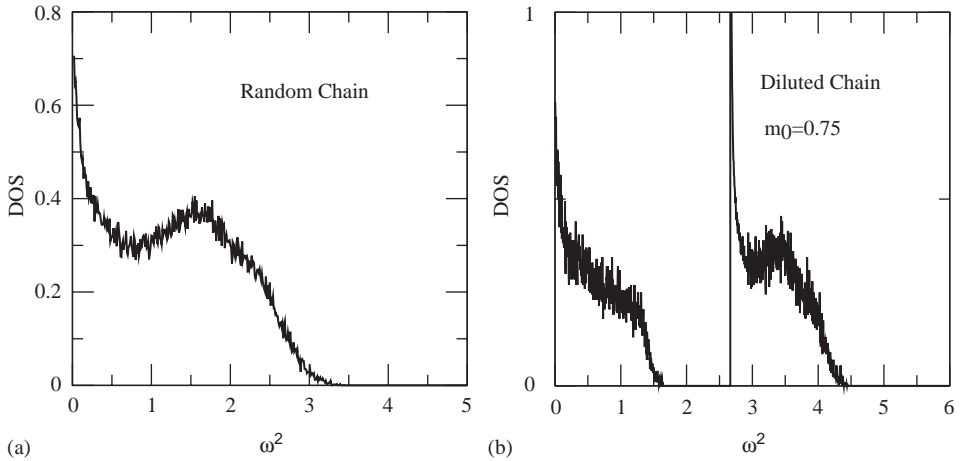


Fig. 1. Normalized density of states (DOS) as a function of energy  $E$  obtained using Dean's method for a chain with  $N = 10^5$  sites: (a) random harmonic chain with masses taken uniformly from the interval  $[1, 3]$ ; (b) diluted 1D harmonic chain with  $m_0 = 0.75$ . The DOS displays a pseudo-gap for  $m_0 \neq \langle m_n \rangle$ , which is reminiscent of the gap appearing in the DOS of the corresponding pure chain.

We obtain the density of states (DOS) using the numerical Dean's method [22]. Strong fluctuations in the DOS are related to the presence of localized states, whereas a smooth DOS is usually connected to the emergence of delocalized states [6,15]. In Fig. 1 we show the normalized DOS as a function of  $\omega^2$  obtained using Dean's method for a chain with  $N = 10^5$  sites of the (a) random harmonic chain with masses taken uniformly from the interval  $[1, 3]$  and (b) diluted 1D harmonic chain with  $m_0 = 0.75$ . One notices that the DOS for the diluted chain displays a pseudo-gap. We found that this gap is always present whenever  $m_0 \neq \langle m_n \rangle$ , which is reminiscent of the gap present in the DOS of the corresponding pure chain. At the upper gap edge the DOS presents a diverging singularity, while the lower one is rounded by the underlying disorder.

In Fig. 2 we show the Lyapunov exponent  $\gamma$  as a function of  $\omega^2$  obtained from the transfer matrix method for exactly the same cases as in Fig. 1. We can see that, due to the diluted disorder, the system displays a new extended state at  $\omega_c > 0$ . Close to the critical frequency,  $\gamma$  vanishes as  $\gamma \propto (\omega - \omega_c)$ . The frequency of this extended vibrational mode is exactly at the DOS singularity. This mode can be viewed as an extended harmonic mode which has null displacements at the sites with random masses.

### 3. Energy transport

In order to study the time evolution of an initially localized energy pulse, we calculate the second moment of the energy distribution [17,18]. This quantity is

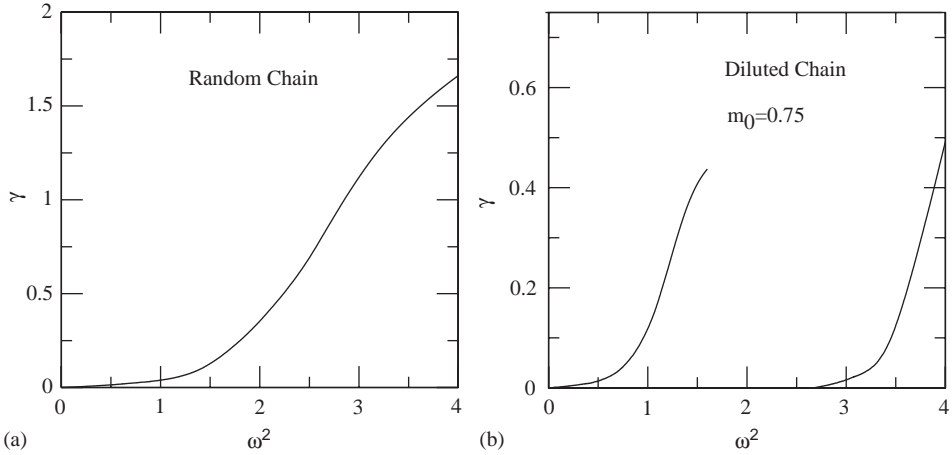


Fig. 2. Lyapunov exponent  $\gamma$  as a function of  $\omega^2$  obtained from the transfer matrix method for a chain with  $N = 5 \times 10^6$  sites: (a) random harmonic chain with masses taken uniformly from the interval  $[1, 3]$ ; (b) diluted 1D harmonic chain with  $m_0 = 0.75$ . It shows clearly the new resonant state at  $\omega_c > 0$  induced by the dilution of the disorder distribution.

related to the thermal conductivity by Kubo’s formula [17]. The classical Hamiltonian  $H$  for an harmonic chain can be written as

$$H = \sum_{n=1}^N h_n(t), \tag{6}$$

where the energy  $h_n(t)$  at the site  $n$  is given by

$$h_n(t) = \frac{P_n^2}{2m_n} + \frac{\beta_n}{4} [(Q_{n+1} - Q_n)^2 + (Q_n - Q_{n-1})^2]. \tag{7}$$

Here  $P_n$  and  $Q_n$  define the momentum and displacement of the mass at the  $n$ th site. The fraction of the total energy  $H$  at the site  $n$  is given by  $h_n(t)/H$  and the second moment of the energy distribution,  $M_2(t)$ , is defined by [17]

$$M_2(t) = \sum_{n=1}^N (n - n_0)^2 [h_n(t)/H], \tag{8}$$

where an initial excitation is introduced at the site  $n_0$  at  $t = 0$ . Using the fourth-order Runge–Kutta method, we solve the Hamilton’s equations for  $P_n(t)$  and  $Q_n(t)$  and calculate  $M_2(t)$ . The second moment of the energy distribution  $M_2(t)$  has the same status of the mean-square displacement of the wave-packet of an electron in a solid [17]. In random harmonic chains with an initial impulse excitation, the energy spread is super-diffusive ( $M_2(t) \propto t^{3/2}$ ) in contrast with the slower sub-diffusive spread of an initial displacement excitation ( $M_2(t) \propto t^{1/2}$ ) [17,18]. The origin of these distinct asymptotic dynamics was shown to originate on the way modes are populated by these two different kinds of excitations. In the case of impulse excitations, the modes

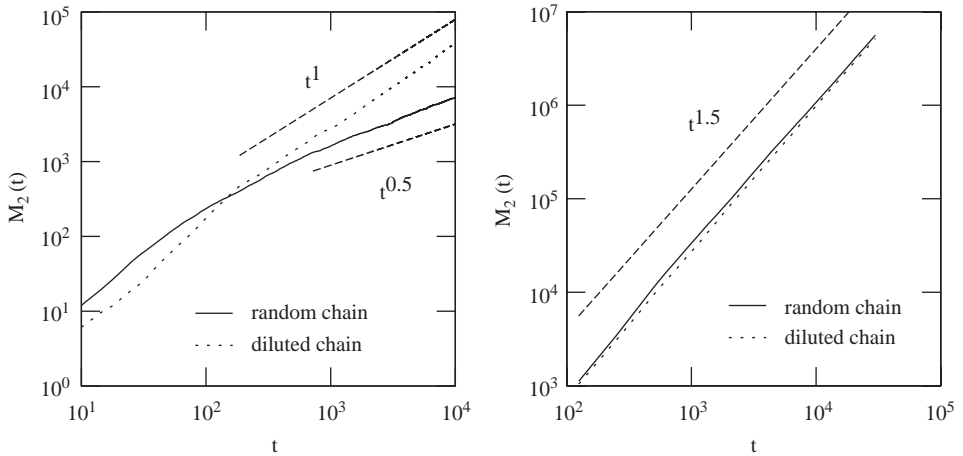


Fig. 3. The second moment of the energy distribution,  $M_2(t)$  versus time  $t$  for a diluted 1D harmonic chain with  $m_0 = 1.0$  and  $N = 1.5 \times 10^4$  sites. The random masses were chosen within  $[0.5, 3.5]$ . We considered two kinds of initial conditions: (a) displacement excitations and (b) impulse excitation. The solid lines correspond to the excitation spread in the non-diluted random chain.

are populated uniformly. On the other hand, the contribution of a vibrational mode of frequency  $\omega$  is proportional  $\omega^2$  for a displacement excitation [17]. Therefore, the effectively extended low-energy modes play distinct roles in these two cases and their weak contribution to a displacement excitation results in the slower energy spread. In Fig. 3 we show the second moment of the energy distribution,  $M_2(t)$  versus time  $t$  for a diluted 1D harmonic chain with  $m_0 = 1$  and  $N = 1.5 \times 10^4$  sites. The random masses were chosen within  $[0.5, 3.5]$ . We consider *displacement initial excitations* in (a) and *impulse initial excitation* in (b). Here, we put the initial excitation in a diluting site  $n_0$  close to the chain center. The asymptotic dynamics in the case of *impulse initial excitation* [ $M_2(t) \propto t^{1.5}$ ] has the same super-diffusive spread presented by the usual random chain with uncorrelated masses. However, for the case of *displacement initial excitation*, the energy spread in the diluted chain becomes diffusive, i.e., [ $M_2(t) \propto t^1$ ]. This shall be contrasted with the slower sub-diffusive spread [ $M_2(t) \propto t^{0.5}$ ] that takes place for uncorrelated random mass chains.

#### 4. Conclusions

In summary, we studied the nature of collective excitations in harmonic chains with diluted disorder. In this model system, sites of constant mass  $m_0$  intercalate random masses taken from an uniform distribution. This model presents an extended harmonic state at frequency  $\omega_c$  with null displacement at the random masses. The Lyapunov exponent vanishes linearly as the resonance frequency is approached. Further, the DOS presents a diverging singularity at the resonance

frequency. We showed that the presence of this resonant mode can modify the energy spread of an initially localized excitation. By calculating the second moment  $M_2(t)$  of the energy spatial distribution, we found that an initial impulse excitation spreads super-diffusively [ $M_2(t) \propto t^{1.5}$ ] irrespective to the presence of dilution. On the other hand, the spread of an initial displacement excitation is strongly affected by the dilution changing from a sub-diffusive behavior [ $M_2(t) \propto t^{0.5}$ ] in the absence of dilution to a faster diffusive spread [ $M_2(t) \propto t^1$ ]. Therefore, the presence of new extended modes and the faster energy spread can be relevant to the thermal conductivity of harmonic chains with diluted disorder. It would be interesting to see this point being addressed in future contributions to this subject.

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