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CONDENSED MATTER

Energy Propagation in Classical Harmonic Lattices with Diluted Disorder

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Abstract We consider the problem of a harmonic lattice in which masses' distribution is a superposition of a random and a periodic distribution. Classical equations for the mass displacement and velocities are solved using a second-order Euler formalism. Energy flow was investigated on two distinct experiments: (i) We injected an initial wave-packet with energy E_0 and analyzed the dynamics of the resulting energy pulse; (ii) we pumped one of the sides of the lattice with a external signal and then we observed the propagation of the pulse until the other side of chain. Our calculations suggest that the diluted disordered mass distribution promotes energy dynamics at high frequency limit.

Keywords Localization · Diluted disorder · Propagation · Harmonic lattice

1 Introduction

According to Anderson localization theory, extended eigenstates are absent in low-dimensional disordered systems with uncorrelated disorder [1–3]. Exceptions were demonstrated some years ago in case of correlated disorder [4–24]. The localization theory can also be applied to general phonons propagation. Most vibrational modes of one-dimensional (1D) harmonic chains with a random sequence of masses are localized [25]. It was also demonstrated that there are a few low-frequency modes not localized, whose number is of the order of $\sqrt{N}$, N being the number of masses in the chain [25–27]. Other studies about correlated disorder in classical one-dimensional harmonic lattices were made in the past. In refs. [28, 29], authors showed that short-range correlations promote the appearance of new non-scattered vibrational modes.

Among the models with short-range correlation, 1D chains with diluted disorder also support extended eigenstates [30]. The diluted disorder consists of two interpenetrating sub-lattices, one composed of random masses and the other being periodic. It was proved that special resonant energies appear, giving rise to a set of extended states. Harmonic chains with long-range correlated disorder were investigated in ref. [31]. In that case, extended states exist in the high frequency region.

Most part of literature related to vibrational modes in disordered harmonic systems, presents the dimensionality as a big problem. In general, the authors prefer investigate one-dimensional disordered chains. Two-dimensional harmonic lattices with correlated disorder is an almost unknown field. In ref. [32], the nature of the vibrational modes in a two-dimensional harmonic lattice with long-range correlation was investigated. The random masses distribution exhibited a power-law spectral density $S(k) \sim 1/k^{\alpha}$. Authors considered only longitudinal atomic displacements and computed the participation number, its fluctuations and also the local density of states. They showed numerical proof that extended vibrational modes appear when $\alpha > \alpha_c$ and that α_c depends on the magnitude of disorder.

In this work, we consider the problem of a harmonic $2D$ lattice with diluted disorder. In our model, the distribution of masses is a generalization of the $1D$ diluted model

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considered in ref. [30], i.e., a superposition of a random and a periodic mass distribution. Two distinct types of numerical simulations were performed in that system: (i) We inject an initial wave-packet with energy E_0 and then we observe energy pulse's dynamics; (ii) by pumping one of the sides of the lattice with a external signal, we analyze the propagation of this pulse until it reaches the other side of lattice. Broadly, our procedure consists of solving classical equations for masses displacements and velocities. In the end, we found evidence that intrinsic correlations which exist within the diluted mass distribution play a relevant role in the energy propagation. Our calculations also helped to predict the frequency region that propagates along the lattice.

2 Model and Numerical Calculations

In our model, we consider a two-dimensional harmonic lattice (see Fig. 1a). Each site (i, j) represents an atom with mass $m_{i,j}$. When the system is at rest, the x and y coordinates may be, respectively, set to $x_{i,j} = j$ e $y_{i,j} = i$ (in units of the lattice spacing $a = 1$). Masses distributions which were chosen for our studies in this paper are described as follows: i) "Random case": this kind of distribution is defined as $m_{i,j} = 1 + \eta_{i,j}$, where $m_{i,j}$ is a mass on site i, j and $\eta_{i,j}$ is a random number uniformly distributed within the interval [0, 1]; ii) "Diluted case 1": the mass distribution of case i) is modified by the following the rule: $m_{i,j} = 1$ for $i = 1, \ldots, N$ and j is odd. Therefore, the case (ii) represent a mass distribution with a line periodic (with value $m_{i,j} = 1$) alternating with random lines; iii) The "Diluted case 2" is similar to "Diluted case 1" (case ii) except that the position of periodic lines changes to : $m_{i,j} = 1$ for $i = 1, \ldots, N$ and $j = 1, 4, 7, 10, 13, 16, \ldots$. Each mass and its four neighbors are coupled through a harmonic force. $k = 1$ represents the magnitude of the spring constant. Whenever a given mass $(m_{i,j})$ has small displacement from its initial position, the four springs related with the four first nearest neighbors are deformed (see Fig. 1b a pedagogical exhibition of this phenomenon). At rest, the mean distance between each mass is 1. The distance between the site (i, j) and its four first nearest neighbors after the deformation can be measured as:

$$d_1^{i,j} = \sqrt{(x_{i,j} - x_{i+1,j})^2 - (y_{i,j} - y_{i+1,j})^2}, \tag{1}$$

$$d_2^{i,j} = \sqrt{(x_{i,j} - x_{i,j+1})^2 - (y_{i,j} - y_{i,j+1})^2}, \tag{2}$$

$$d_3^{i,j} = \sqrt{(x_{i,j} - x_{i-1,j})^2 - (y_{i,j} - y_{i-1,j})^2} \tag{3}$$

and

$$d_4^{i,j} = \sqrt{(x_{i,j} - x_{i,j-1})^2 - (y_{i,j} - y_{i,j-1})^2}. \tag{4}$$

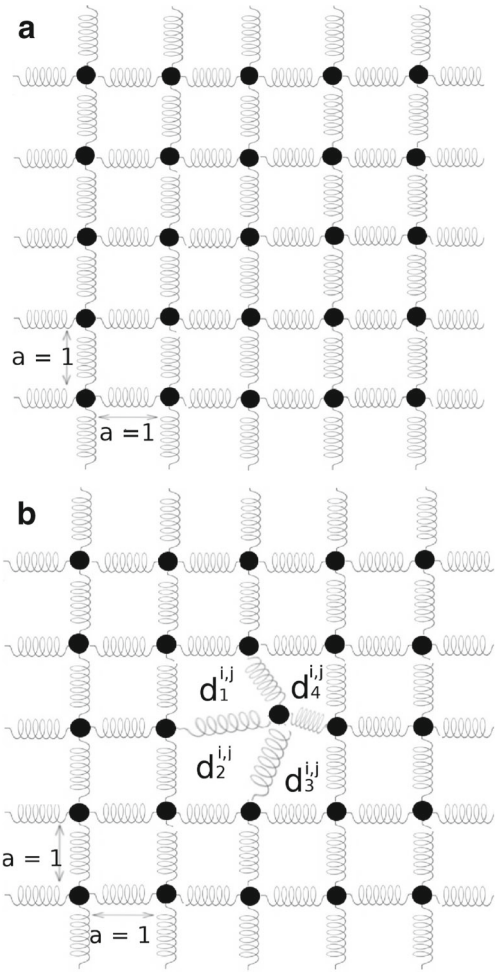

Fig. 1 **a** Two-dimensional harmonic lattice where each site (i, j) represents an atom with mass $m_{i,j}$. **b** Pedagogical exhibition of the deformed harmonic lattice after a given mass $(m_{i,j})$ is moved from its initial position

Therefore, the effective force on mass $(m_{i,j})$ can be computed as $\mathbf{F}^{i,j} = \mathbf{F}_1^{i,j} + \mathbf{F}_2^{i,j} + \mathbf{F}_3^{i,j} + \mathbf{F}_4^{i,j}$ where $\mathbf{F}_z^{i,j} = k|d_z^{i,j} - 1|\hat{r}_z$ with $z = 1, 2, 3, 4$. $\hat{r}_z$ is a unity vector along the spring z. We emphasize that the direction of $\hat{r}_z$ depends on the distance $d_z^{i,j}$: if $d_z^{i,j} > 1$ the vector $\hat{r}_z$ points to the direction of mass i, j; on the contrary, if $d_z^{i,j} < 1$, then $\hat{r}_z$ points to the opposite direction of mass i, j. The vibrational energy dynamics is obtained by solving the classical equations :

$$[\mathbf{F}^{i,j}]_x = m_{i,j} \frac{d^2 x_{i,j}}{dt^2} \tag{5}$$

and

$$[\mathbf{F}^{i,j}]_y = m_{i,j} \frac{d^2 y_{i,j}}{dt^2} \tag{6}$$

In general, (5) and (6) can be solved as follows: each second order equation can be separated in two first order equations (e.g. the (5) is written as : $[\mathbf{F}^{i,j}]_x = m_{i,j} \frac{dv_x^{i,j}}{dt}$ and $v_x^{i,j} =$

$\frac{dx_{i,j}}{dt}$; the same is done for the (6)). Therefore, we have a set of four equations for each mass (i, j) which can be solved using a second order Euler method (2EM).

In order to explain the (2EM) method, we will use, as example, the first-order equations for the x direction. Considering we know the initial value of $x_{i,j}(t = 0)$ and $v_x^{i,j}(t = 0)$, we find a first-order estimation for these quantities at time dt as: $x_{i,j}(t = dt)^1 = x_{i,j}(t = 0) + dt * v_x^{i,j}(t = 0)$ and $v_x^{i,j}(t = dt)^1 = v_x^{i,j}(t = 0) + dt * [\mathbf{F}^{i,j}(t = 0)]_x / m_{i,j}$. The second-order formula for these quantities is written as: $x_{i,j}(t = dt)^2 = x_{i,j}(t = 0) + (dt/2) * (v_x^{i,j}(t = 0) + v_x^{i,j}(t = dt)^1)$ and $v_x^{i,j}(t = dt)^2 = v_x^{i,j}(t = 0) + (dt/2) * ([\mathbf{F}^{i,j}(t = 0)]_x + [\mathbf{F}^{i,j}(t = dt)]_x)/m_{i,j}$. The same second-order procedure may be used for the y direction. In our calculations, we use $dt \approx 5 \times 10^{-3}$ along the entire time interval. We also check numerical accuracy of our procedure. It was done by monitoring the temporal evolution of the total energy contained within the lattice. If an initial localized wave-packet with energy E_0 was injected into the lattice, the time-dependent total energy $E(t)$ should be constant along the time; we find that $|1 - E(t)/E_0| < 10^{-10}$ within the entire interval. The time-dependent energy may be computed as $E(t) = \sum_{i,j} h_{i,j}(t)$ where

$$h_{i,j}(t) = \frac{m_{i,j} * [(v_x^{i,j})^2 + (v_y^{i,j})^2]}{2} + \sum_{z=1}^{4} \frac{k|d_z^{i,j} - 1|^2}{4} \quad (7)$$

Our first analysis consists of injecting an initial wave-packet with energy E_0 close to the center of the lattice and then calculate its spread with time. The fraction of the initial energy on the mass (i, j) (i.e., $f^{i,j} = h_{i,j}/E_0$) is used to estimate the spread of energy within the lattice.

$$\Sigma(t) = \sqrt{\sum_{i,j} [(x_{i,j} - x_{i_0,j_0})^2 + (y_{i,j} - y_{i_0,j_0})^2] f^{i,j}} \quad (8)$$

The quantity Σ has the same status of the root-mean-square displacement of the wave packet of an electron in a solid. Here, x_{i_0,j_0} and y_{i_0,j_0} represent the coordinates of the site in which energy is initially injected into the lattice. The time-dependent behavior of $\Sigma(t)$ provides a description of the energy flow within this model and its relationship with the type of correlated disorder that we are dealing with. We emphasize that $\Sigma(t)$ is measured in units of the lattice spacing $a = 1$.

Beyond previous analysis, we also perform a direct measure of the energy pulse propagation along the system. We consider that one of the sides of the lattice is coupled to some oscillators. These oscillators inject a pulse into the lattice such as:

$$x_{i,0} = \sum_{\omega_n} Z \cos(\omega_n t) \quad (9)$$

where Z is a small amplitude and ω_n is a set of frequencies within the interval $[0.05, 5]$. We use about 100 frequency values separated by $\delta\omega = 0.05$ in order to calculate $x_{i,0}$. Formally, the amplitude Z could be any value less than one. However, as Z is increased, the discretization in time (dt) needs to decrease then, the computational time diverges. So, we choose $Z = 0.001$ and $dt = 5 \times 10^{-3}$. We stress that, within this experiment, we are interested to study the energy propagation along one direction; thus we can solve the equations in a rectangular geometry $L \times N$ (with $N > L$ representing the propagation axis). In order to analyze the energy propagation along the system, we follow the time-evolution of energy pulse by monitoring the mass position x_{i_0,d_0}. In our calculations, $i_0 \approx L/2$ and d_0 is close to N. Hence, x_{i_0,d_0} represent the position of a mass far from the lattice's side that received the energy pumping. We calculate the displacement of mass (i_0, d_0) relative to the initial condition i.e. $D_{i_0,d_0}(t) = x_{i_0,d_0}(t) - x_{i_0,d_0}(t = 0)$ (in units of the lattice spacing $a = 1$). Using this quantity, we compute $I(\omega) = |FT(D_{i_0,d_0}(t))|$, where $FT(A)$ represent the Fourier transform of function A. $I(\omega)$ reveals some information about the frequencies that propagate along the chain. When $I(\omega) = 0$, it advocates that frequency ω does not reach the end of lattice (position d_0). If $I(\omega) > 0$, our calculations indicate that the frequency ω crossed the lattice from one side to another. In other words, $I(\omega) > 0$ suggests propagation and a possible existence of extended modes.

3 Results and Discussion

We emphasize that we investigated vibrational dynamics in a two-dimensional disordered harmonic lattice. We considered three distinct types of distribution of masses: (i) "Random case": the masses distribution is defined as $m_{i,j} = 1 + \eta_{i,j}$ where $\eta_{i,j}$ is a random number uniformly distributed within the interval $[0, 1]$; (ii) "Diluted case 1": the mass distribution of case (i) is modified by following the rule: $m_{i,j} = 1$ for $i = 1, \ldots, N$ and j is odd. (iii) The "Diluted case 2" is similar to "Diluted case 1" (case ii) except that the position of periodic lines changes to: $m_{i,j} = 1$ for $i = 1, \ldots, N$ and $j = 1, 4, 7, 10, 13, 16, \ldots$. In Fig. 2, we plot a summary of our main results for the spread of the energy distribution (8) versus time t. We stress that initial vibrational energy input was injected on site i_0, j_0 according to two quite distinct classes: (A) *Impulse* excitations corresponding to $v_x^{i,j}(t = 0) = v_y^{i,j}(t = 0) = \delta_{i,i_0}\delta_{j,j_0}$ and $x_{i,j}(t = 0) = j$ and $y_{i,j}(t = 0) = i$. (B) *displacement* excitations, i.e., $x_{i,j}(t = 0) = j + \Delta\delta_{i,i_0}\delta_{j,j_0}$, $y_{i,j}(t = 0) = i + \Delta\delta_{i,i_0}\delta_{j,j_0}$ and $v_x^{i,j}(t = 0) = v_y^{i,j}(t = 0) = 0$ (in our calculations, we used $\Delta = 0.1$, however, for $\Delta < 1$, calculations did not exhibit any qualitative difference). Also, for all numerical calculations related to the random case (case i),

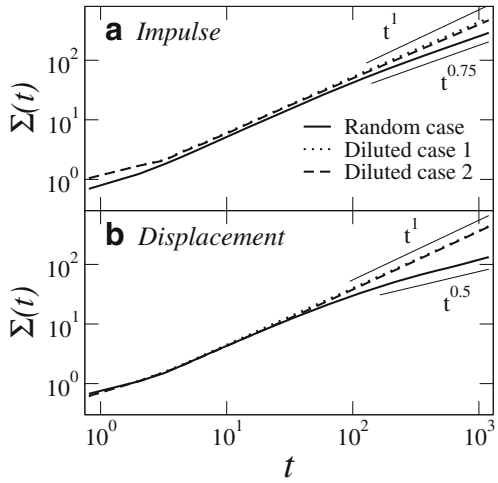

Fig. 2 Energy spread distribution $\Sigma(t)$ versus time t for (**a**) *Impulse* excitations that correspond to $v_x^{i,j}(t=0) = v_y^{i,j}(t=0) = \delta_{i,i_0}\delta_{j,j_0}$ and $x_{i,j}(t=0) = j$ and $y_{i,j}(t=0) = i$ and (**b**) *displacement* excitations that correspond to $x_{i,j}(t=0) = j + \Delta\delta_{i,i_0}\delta_{j,j_0}$, $y_{i,j}(t=0) = i + \Delta\delta_{i,i_0}\delta_{j,j_0}$ and $v_x^{i,j}(t=0) = v_y^{i,j}(t=0) = 0$ (here we used $\Delta = 0.1$). The initial wave-packet was localized on a site (i_0, j_0) close to the center of lattice with $m_{i_0,j_0} = 1$. We observe that, for the random case, standard deviation of energy follows a super diffusive dynamics ($\Sigma(t) \propto t^{3/4}$) in (**a**) and a diffusive one ($\Sigma(t) \propto \sqrt{t}$) in (**b**). Moreover, for this kind of initial condition, the diluted disorder promotes a ballistic dynamics ($\Sigma(t) \propto t^1$)

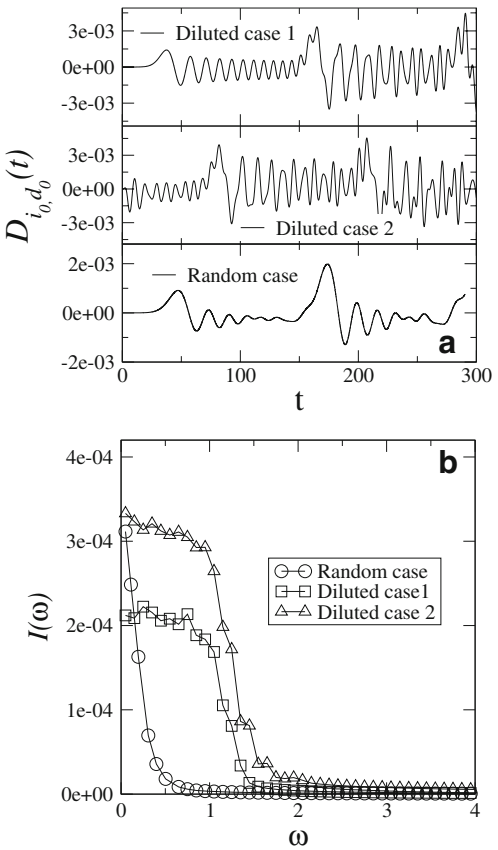

Fig. 3 **a** D_{i_0,d_0} versus t for the random case and for both types of diluted disorder. Calculations were done in a rectangular $(L \times N)$ harmonic lattice with $N = 1500$ and $L = 360$. In our calculations $i_0 \approx L/2$ and $d_0 \approx 1200$. We emphasize that we consider $t = 0$ the time in which that $|D_{i_0,d_0}| > 10^{-10}$. B) $I(\omega) = |FT(D_{i_0,d_0}(t))|$ where $FT(D_{i_0,d_0}(t))$ represent the Fourier transform of $D_{i_0,d_0}(t)$ for the data in (**a**). For the random case, the function $I(\omega)$ is null for $\omega > 0$ and it is nonvanishing for $\omega \approx 0$. For both types of diluted disorder, $I(\omega)$ exhibits a plateau that suggests the existence of a band of extended vibrational modes

we considered $(i_0, j_0) = (N/2, N/2)$. For the diluted cases (case ii and iii), the site (i_0, j_0) represents a site close to the center of lattice $((N/2, N/2))$ such that $m_{i_0,j_0} = 1$. Calculations of the spread $\Sigma(t)$ were done for a square lattice with $N \times N = 3000 \times 3000$. By analyzing Fig. 2, we observed that, for the random case, the spread of energy showed a super diffusive dynamics ($\Sigma(t) \propto t^{3/4}$) in Fig. 2a and a diffusive one ($\Sigma(t) \propto \sqrt{t}$) in Fig. 2b. The dependence of $\Sigma(t)$ with the type of initial condition (impulse or displacement) it was also obtained in disordered one-dimensional harmonic chains [31, 32]. The main physical explanations for this phenomena is the amount of low-frequency modes that exist within the initial conditions [31]. In the case with an initial impulse excitation, the amount of low-frequency states is larger than the case with initial displacement, hence the dynamics is faster. In both cases with diluted disorder, the mean square displacement exhibits a ballistic behavior ($\Sigma(t) \propto t$), thus indicating the presence of extended vibrational modes within this two-dimensional disordered harmonic model. Our calculations indicate that types 1 and 2 of diluted disorder promotes the ballistic dynamics. The fast dynamics found in the case with diluted disorder suggest the presence of extended vibrational eigenstates. We investigated this point using the numerical calculations of quantity $I(\omega)$. In Fig. 3a, we plot D_{i_0,d_0} versus t for the random case and both types of diluted disorder. Calculations were done in a rectangular $(L \times N)$ harmonic lattice with $N = 1500$ and $L = 360$. In our calculations $i_0 \approx L/2$ and $d_0 \approx 1200$. We emphasize that, in Fig. 3a, we consider $t = 0$ the time in which that $|D_{i_0,d_0}| > 10^{-10}$. By using the time-evolution of D_{i_0,d_0}, we calculated the quantity $I(\omega)$ as $I(\omega) = |FT(D_{i_0,d_0}(t))|$, where $FT(D_{i_0,d_0}(t))$ represents the Fourier transform of $D_{i_0,d_0}(t)$. The results of $I(\omega)$ for the random case and also the diluted case types 1 and 2 can be found in Fig. 3b. Our calculations are summarized as follows: The function $I(\omega)$ for the random case is almost null for $\omega > 0$ and exhibits a pronounced peak around $\omega = 0$. This is a clear signature that only the modes around the uniform mode ($\omega = 0$) propagates along the lattice. This result is in good agreement with the previous calculations for a one-dimensional disordered harmonic chain [25, 29]. The uniform mode ($\omega = 0$) in a $1d$ harmonic disordered chain represents a mode without spring deformation, so it has

divergent wave-length and, also, it is not affected by the disorder propagating through the system [25, 29]. Conversely, harmonic modes with $\omega > 0$ cannot propagate along disordered harmonic chain. It happens due to the intrinsic disorder distribution. Our calculations of $I(\omega)$ suggest the same behavior occurs for the $2d$ disordered harmonic case. The diluted disorder 1 and 2 exhibit a new and interesting framework. There is a plateau in the low-frequency region. It suggests that nonzero frequencies propagate along the disordered harmonic lattice and that, for both types of diluted disorder, a band of extended vibrational modes arises. It is a new and interesting result. Within our numerical calculations, we observed that the aforementioned band lies roughly within the interval of frequencies [0,1.2]. Therefore, this type of correlated disorder might promote the appearance of a localization-delocalization transition. Data shown in Fig. 3a, b are in a good agreement with the ballistic dynamics found in Fig. 2. In general, both diluted case 1 and 2 exhibiting fast energy propagation. Our spectral calculations suggests that at the diluted case (2), the intensity of the lattice deformation displays a extremely tiny increasing in comparison to the case (1). These small changes are observed in the calculations of $D_{i_0,d_0}(t)$ as well as at the difference between the plateau of the $I(\omega)$ curves for the diluted cases. We also observed a very slight increasing of the width of the region in which that $I(\omega) > 0$ (i.e., bandwidth of extended vibrational modes). However, those discrepancies do not change qualitatively the energy dynamics, neither the diffusion coefficient in both types of diluted disorder. We believe that if we increased the periodicity of the lines with $m_{i,j} = 1$ we would not find any qualitative change in our results.

Before our concluding statements, we briefly discuss the dependence of our results for the spread Σ with the type of initial condition. We emphasize that, in order to compute Σ we injected the energy in an initial site (i_0, j_0) close to center of the lattice. The condition for choosing this position (i_0, j_0) was that its mass $m_{i_0,j_0} = 1$. Therefore, all previous investigations about Σ were done considering the initial energy injected into the periodic sub-lattice. We show some results of Σ by considering the initial energy put on a site i_0, j_0 belonging to the random sub-lattice. In Fig. 4, we plot Σ versus time for both types of diluted disorder and also (A) impulse excitation and (B) displacement excitation. Dynamics is apparently slower than those in the previous cases (see Fig. 2). We got $\Sigma(t) \propto t^{0.9}$ for the case with an initial impulse excitation (Fig. 4a) and $\Sigma(t) \propto t^{0.75}$ for the case with an initial displacement excitation (Fig. 4b). Therefore, our results suggest that the type of dynamics in harmonic lattices with diluted disorder depends on the nature of the initial excitation (impulse or displacement) and also of the initial site (i_0, j_0). When we started the dynamics by injecting the energy into the periodic

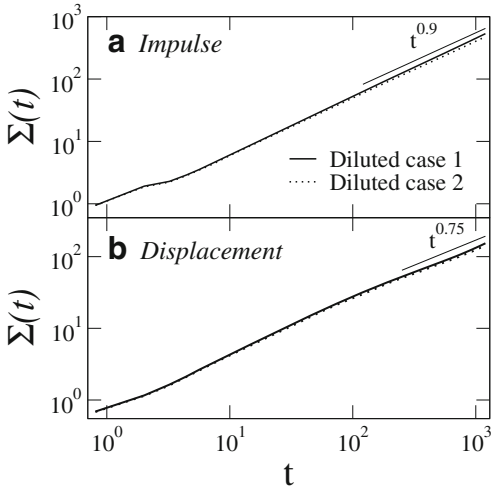

Fig. 4 Σ versus t considering the initial energy put on a site i_0, j_0 belonging to the random sub-lattice (i.e.: the initial site (i_0, j_0) is a site close to the center of chain with $m_{i_0,j_0} \neq 1$). Calculations were done for **a** impulse excitation and **b** displacement excitation

sub-lattice, we obtained a fast ballistic dynamics (for both impulse and displacement excitation). However, if the initial energy pulse were injected into the random sub lattice, the energy flow within the lattice became slower. This phenomena was also observed in one-dimensional systems with diluted disorder [30, 33]. The extended vibrational modes of the models with diluted disorder were localized at periodic sub lattice [33]. Thus, an energy wave-packet initially localized within the random sub lattice has a small contribution from those frequencies with large localization lengths. Consequently, that turns energy dynamics slower.

4 Summary and Conclusions

We studied the energy flow in a harmonic lattice with diluted disorder. Here, the distribution of masses was obtained as a superposition of a random and a periodic mass distribution. By using numerical methods, we solved the classical equations for mass displacement and velocity. We analyzed the energy flow by considering two types numerical tools: (i) the spread of an initially localized energy pulse around the center of lattice and (ii) the evolution of a pulse that is pumping at one side of the lattice. Our calculations suggest that the type of diluted disorder used here promotes the appearance of new extended vibrational modes. We demonstrate numerically that the velocity of energy flow depends on the type of initial energy pulse (impulse or displacement excitation) and also on the initial position of the pulse. Results indicate that if the initial energy pulse is localized at the periodic sub lattice, the dynamics is ballistic. However, if

the initial excitation is fully restricted to the random sub lattice our calculations point to a super diffusive spread.

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