DELOCALIZED VIBRATIONAL MODES IN DISORDERED HARMONIC CHAINS WITH CORRELATED SPRING CONSTANTS

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We address the question regarding the effect of correlated random spring constants in the one-dimensional harmonic model. We consider all masses to be equal but the spring constants given by a random sequence with long-range correlations. We generate the long-range correlated sequence of spring constants by using a fractional Brownian motion with a power-law spectral density $S(k) = 1/k^{\alpha}$. Using an exact diagonalization formalism, we compute the participation moments of eigenmodes within the band of allowed frequencies. We unveil a regime on which all modes below a critical frequency become extended.

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1. Introduction

The problem of heat conduction in one-dimensional classical systems of interacting particles has attracted a lot of attention in the recent years [1–19]. One of the controversial and interesting questions is whether low-dimensional classical systems displays finite thermal conductivity in the thermodynamic limite. In particular, within the framework of one-dimensional models with alternating masses, the detailed description of the thermal conductivity has a long history, starting in the eighties [7]. Within the context of disordered harmonic chains, there is the possibility to decompose the heat flux into the sum of independent contributions associated to their eigenmodes [20]. Of particular interest are the localization properties of the eigenfunctions and self-averaging properties of several observables such as the temperature profile and the heat flow. There is a large amount of works in the past decades regarding the localization behavior in randomly disordered chains [21]. Most of these works have been concentrated on uncorrelated [22] and correlated [23] disorder. In general lines, the collective vibrational motion of one-dimensional disordered harmonic chains of N random masses can be mapped onto an one-electron tight-binding model [24]. 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 $\sqrt{N}$ [24, 25]. It has been shown that short-range correlations in the mass distribution produce a new set of non-scattered modes in this system [26]. Moreover, non-scattered modes have also been found in disordered harmonic chains with dimeric correlations in the spring constants [27]. Among the models with short-range correlation, 1D chains with diluted disorder also support extended modes [28]. The model consists of two interpenetrating sub-lattices, one composed of random masses and the other being periodic. Due to the periodicity of one sub-lattice, special resonant energies appear, giving rise to a set of extended states. The problem of harmonic chains with long-range correlated random masses was investigated in Ref. [29]. It was numerically demonstrated that when the sequence of masses exhibit a power law spectral density $S(k) \sim 1/k^{\alpha}$ with $\alpha > 1$, a phase of extended modes emerges. Moreover, the vibrational modes in a two-dimensional harmonic lattice with long-range correlated random masses was investigated in Ref. [30]. The scale invariance of the fluctuations of the relative participation number and the local density of states was obtained. There were found clear signatures of extended vibrational modes when $\alpha > \alpha_c$. It was shown that α_c depends on the magnitude of disorder. To confirm this claim, the time evolution of an initially localized energy pulse was investigated. It was shown that the second moment of the spatial distribution of the energy displays a ballistic regime when $\alpha > \alpha_c$, in agreement with the presence of extended vibrational modes. We emphasize that these results demonstrating the possibility of fast transport in low-dimension systems has motivated several experimental investigations [31–37]. Therefore, the direct relation between the nature of eigenmodes and the degree of correlations within the disorder distribution represent an interesting challenger within the context of low-dimensional disordered systems.

In this work, we report further progress along the above lines by performing a numerical study of the vibrational modes in a disorder harmonic chain with the scale-free long-range correlated disorder on the spring constants. Using an exact diagonalizations formalism, we compute the participation moments of eigenmodes within the band of allowed frequencies in order to investigate the possible existence of a regime on which the system presents extended states.

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 ω is [25, 26]

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

Here, all oscillators have identical masses with $m_n = 1$ and the spring constants given by

$$\beta_n = \beta_0 + \nu_n \,, \tag{2}$$

where β_0 is a constant and ν_n is a random sequence with long-range correlations. We can generate ν_n from a fractional Brownian motion with a power-law density $S(k) = 1/k^\alpha$ [29]. Here, we chose $\langle \nu_n \rangle = 0$ and the variance $\langle (\nu_n - \langle \nu_n \rangle)^2 \rangle = 1$. $\beta_0 = 4.5$ is used to avoid negative spring constants. In order to investigate the physical properties associated with the nature of vibrational eigenstates, we numerically diagonalize the Hamiltonian and calculate the participation function $\xi(\omega^2)$ defined by [29]

$$\xi\left(\omega^2\right) = \frac{\sum_n \left|u_n\left(\omega^2\right)\right|^2}{\sum_n \left|u_n\left(\omega^2\right)\right|^4} \,, \tag{3}$$

where the Fourier components $u_n(\omega^2)$ are those associated with an eigenmode ω^2 of a chain with N masses and are obtained by direct diagonalization of the $N \times N$ secular matrix A defined as $A_{n,n} = (\beta_n + \beta_{n+1})$, $A_{n,n+1} = A_{n+1,n} = \beta_n$, and all other $A_{n,m} = 0$ [29]. In general, the participation number is a good estimate of the number of masses that participate in the vibrational state. For extended states, ξ is proportional to the total number of masses ($\xi \propto N$). On the other hand, wave-functions presenting power-law decaying tails may display an anomalous scaling of the participation number $\xi \propto N^{D_2}$, with $D_2 < d = 1$ [38]. We averaged ξ in a small window $\Delta\omega^2$ around ω^2

$$\left\langle \xi\left(\omega^2\right)\right\rangle = \left[\sum_{y=\omega^2-\Delta\omega^2/2}^{y=\omega^2+\Delta\omega^2/2} \xi(y)\right] \Big/ N_{\omega^2} \,. \tag{4}$$

We use $\Delta\omega^2 \approx 0.1$ and a large number of samples such that the number of eigenmodes at each window (N_{ω^2}) is close to 10^5 in order to obtain a good accuracy of the statistically averaged quantities. Here, we will be particularly interested in computing the relative fluctuation of the participation number given by

$$\Delta\xi\left(\omega^2\right) = \frac{\sqrt{\left\langle \xi\left(\omega^2\right)^2\right\rangle - \left\langle \xi\left(\omega^2\right)\right\rangle^2}}{\left\langle \xi\left(\omega^2\right)\right\rangle} \,, \tag{5}$$

where $\langle\xi(\omega^2)^2\rangle$ can be computed as in Eq. (4). Within the framework of random and non-random long-range hopping models, it was demonstrated rigorously that the relative fluctuation of the participation number goes to zero for extended eigenmodes [39, 40].

3. Results

In our calculations, the eigenmodes and eigenfrequencies were obtained by direct diagonalization of the equation for the amplitudes u_n, using lattices up to $N = 1600$ sites with open boundary conditions. From them, the participation number and its relative fluctuation were calculated. Results were obtained after averaging over 1000 realizations of the random sequence of spring constants. The error bars obtained were smaller than the symbols size. Figure 1 (a) shows the re-scaled participation number ξ/N *versus* ω^2 for $\alpha = 0$ *i.e.*, the uncorrelated random case. We have considered $N = 200$, 400, 800, 1600. Note that the re-scaled participation number ξ/N for ω^2 remains finite in the thermodynamic limit. However, for any nonzero frequency, the vibrational modes become localized since ξ/N goes to zero. This result reflects the localization of the eigenstates with finite frequency in the presence of disorder, either in the masses or spring constants, and the delocalization of the uniform mode ($\omega^2 = 0$). In order to investigate the effects of long-range correlations in random spring distribution, we compute the participation number for $\alpha > 0$. Figure 1 (b) shows the re-scaled participation number ξ/N *versus* ω^2 for $\alpha = 1.5$ and $N = 200$, 400, 800, 1600. We can see again that the re-scaled participation number ξ/N for $\omega^2 > 0$ vanishes

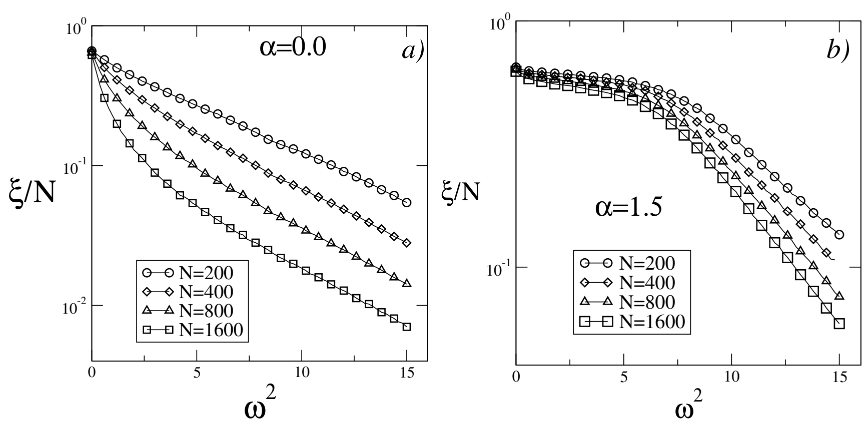

Fig. 1. The re-scaled participation number ξ/N *versus* ω^2 for $N = 200$, 400, 800, 1600 and (a) $\alpha = 0$ and (b) $\alpha = 1.5$. For all values of the correlation parameter $\alpha \leq 2$, we have found that the uniform mode ($\omega = 0$) is extended and all modes with $\omega > 0$ are localized.

as the system size N is increased. Therefore, all modes with nonzero frequency remain localized. The uniform mode ($\omega^2 = 0$) remains extended in the thermodynamic limit. For all values of the correlation parameter $\alpha \leq 2$, we have found similar results: The uniform mode ($\omega = 0$) is extended, while all modes with $\omega > 0$ are localized. When the correlation parameter becomes larger than 2 ($\alpha > 2$), the characteristics of the vibrational modes change dramatically. The re-scaled participation number ξ/N for $\alpha = 2.5$ (see Fig. 2) exhibits a well defined collapse of all curves in a finite frequency range. This result is a clear signature of extended states. In Fig. 3, we plot

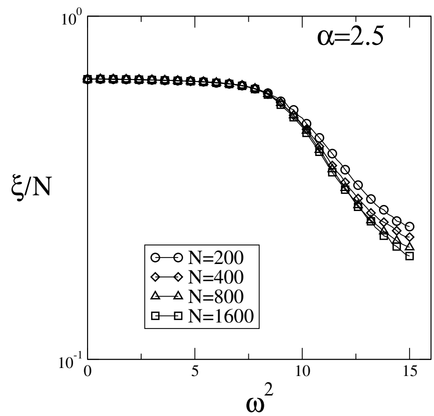

Fig. 2. ξ/N for $\alpha = 2.5$ and $N = 200$, 400, 800, 1600. We observe a well defined collapse of all curves in a finite frequency range. This result suggests the existence of a band of extended states in this regime.

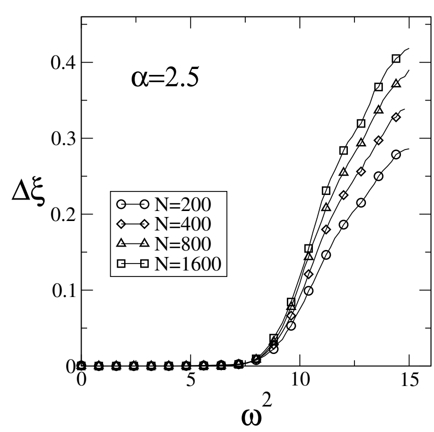

Fig. 3. The relative fluctuation of the participation number ($\Delta\xi$) *versus* ω^2 for $\alpha = 2.5$ and $N = 200$, 400, 800, 1600. For $\omega < \omega_c$, we observe that the relative fluctuation goes to zero thus indicating extended states within this frequency range.

the relative fluctuation of the participation number *versus* ω^2. We can see that the relative fluctuation goes to zero in a finite range of nonzero frequencies. We can also observe that the region in which the relative fluctuation vanishes is in good agreement with the frequency range where we found the collapse of the re-scaled participation number (see Fig. 2).

4. Summary and conclusions

In summary, we studied the nature of collective excitations in harmonic chains with correlated random spring constants. We considered the spring constants to be given by a random sequence with long-range correlations. The long-range correlated sequence of spring constants was generated by using a fractional Brownian motion with a power-law spectral density $S(k) = 1/k^\alpha$. Using an exact diagonalization technique, we computed the participation moments of eigenmodes within the band of allowed frequencies. Our results suggest that for weak correlations all eigenmodes with $\omega > 0$ are localized. The uniform mode ($\omega = 0$) remains extended in the thermodynamic limit. For strong correlations ($\alpha > 2$), our calculations suggest the existence of a localization–delocalization transition. The numeral results indicate the presence of a finite region of frequencies $\omega < \omega_c$ in which the participation number diverges and the relative fluctuation of the participation vanishes. Therefore, linear chains with strong enough long-range correlated spring constants allow the transport of low-frequency harmonic components, while exponentially damps those with frequencies above a well defined threshold. This feature can be used to design new devices that are able to filter high-frequency components of acoustic waves. We hope the present results may stimulate future experimental works aiming to probe the here proposed phenomenology.

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