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Extended acoustic waves in a one-dimensional aperiodic system

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Abstract. We numerically study the propagation of acoustic waves in a one-dimensional system with an aperiodic pseudo-random elasticity distribution. The elasticity distribution was generated by using a sinusoidal function whose phase varies as a power-law, $\phi \propto n^{\nu}$, where n labels the positions along the media. By considering a discrete one-dimensional version of the wave equation and a matrix recursive reformulation we compute the localization length within the band of allowed frequencies. In addition, we apply a second-order finite-difference method for both the time and spatial variables and study the nature of the waves that propagate in the chain. Our numerical data indicates the presence of extended acoustic waves with non-zero frequency for sufficient degree of aperiodicity.

1 Introduction

In pure periodic systems, the electronic eigenstates are delocalized in the thermodynamic limit. This was one of the main conclusions obtained by Bloch [1,2]. However, disorder originating from lattice imperfections drastically modifies the nature of the one-electron eigenstates. The transport properties in nonperiodic systems was the main research focus of Anderson [3]. The well known Anderson localization theory predicts the absence of extended eigenstates on low-dimensional systems with uncorrelated disorder [3]. In a three-dimensional lattice, the presence of weak disorder promotes the localization of the high-energy eigenmodes [3–6]. The low-energy states with long wavelength remain extended, although acquiring a finite coherence length. Mobility edges separate the high energy localized from the low energy extended states.

Futhermore, it was realized that extended states may survive in 1D systems when correlated disorder [7–18] or deterministic nonperiodic potentials [19–28] are involved. In fact, Hamiltonian models with deterministic aperiodicity [19–28] depict features that are between those of the random Anderson model and the periodic Bloch model. The localized or extended nature of the eigenstates has been extensively investigated in the physics literature [19–24] and it has been related to general characteristics of the aperiodic on-site distribution. The effect of aperiodicity in a two-dimensional square lattice was investigated in reference [29]. By using a numerical formalism the one-electron Schrödinger equation in a square lattice with an aperiodic site potential was solved. It was numerically demonstrated that a phase of extended states emerges in the center of the band giving support to a macroscopic conductivity in the thermodynamic limit [29]. The role played by a specific aperiodic structure on the localization properties and/or energy transport in harmonic chains was studied in [30,31]. Moreover, the quantum Heisenberg ferromagnet with aperiodic exchange couplings was considered in reference [32]. The aperiodic distribution of exchange couplings was generated as a sinusoidal function whose phase ϕ varies as a power-law. By using exact diagonalization, it was shown that this ferromagnetic system displays a phase of extended spin waves in the low-energy region [32]. The great importance of aperiodicity in different domains of science was reviewed by Macia in reference [33].

The phenomenology of localization is a quite general feature. It applies, for example, to the study of acoustic waves in nonperiodic media [34–44]. In fact, the propagation of acoustic waves has attracted both theoretical [34–42] and experimental [43,44] interest. In general lines, it was shown that such waves may be localized in media with uncorrelated disorder. However, recents works point out the drastic effect of correlations within the acoustic waves context [38–42]. In reference [38] the propagation of acoustic waves in the random-dimer chain was studied using the transfer-matrix method, exact analytical analysis, and direct numerical solution of the scalar wave equation. The results indicated that there exists a resonance frequency at which the localization length of the acoustic waves diverges [38]. It was also shown that only the resonance frequency can propagate through the 1d media. Moreover, the wave propagation in random system with a power-law correlation function was investigated by using renormalization group formalism as well as numerical methods [39–42]. Calculations indicate that there can be a disorder-induced transition from delocalized to localized states of acoustic waves in any spatial dimension.

In this work, we numerically study the propagation of acoustic waves in a one-dimensional system with an aperiodic pseudo-random elasticity distribution. We follow reference [38] considering a discrete one-dimensional version

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of the wave equation. Therefore, the elasticity distribution appears as an effective spring constant. The kind of elasticity used here was generated by using a sinusoidal function whose phase varies as a power-law, $\phi \propto n^{\nu}$, where n labels the positions along the media. We will solve the discrete form of the wave equation by applying a transfer matrix formalism and compute the localization length associated with the acoustic waves. In addition, we will apply a second-order finite-difference method for both the time and spatial variables to study the nature of the waves that propagate in the chain. Our numerical data indicates the presence of extended acoustic waves with non-zero frequency for sufficient degree of aperiodicity.

2 Model and formalism

We consider here the acoustic wave equation in nonperiodic media (see. Ref. [38]):

$$\frac{\partial^2}{\partial t^2}\psi(x,t) = \frac{\partial}{\partial x}\left[\eta(x)\frac{\partial \psi(x,t)}{\partial x}\right]. \quad (1)$$

Here, $\psi(x,t)$ is the wave amplitude, t is the time, and $\eta(x) = e(x)/m$ is the ratio of the stiffness $e(x)$ and the medium's mean density m. Following reference [38] we will use $m = 1$ and consider a discrete one-dimensional version of the wave equation ($\Delta x = 1$)

$$\eta_i(\psi_{i+1} - \psi_i) - \eta_{i-1}(\psi_i - \psi_{i-1}) + \omega^2\psi_i = 0. \quad (2)$$

The elastic constants η_i will be considered to follow a deterministic rule given by

$$\eta_i = V_0 + [\cos(\alpha i^{\nu})], \quad (3)$$

with α being an arbitrary rational number ($\alpha = 0.1$ here) and ν being a tunable parameter [19,20]. From this sinusoidal form, one can control the degree of aperiodicity in the sequence of hopping couplings. In what follows, $V_0 = 2$ will be taken in order to avoid negative or null elastic constants. The main motivation for considering the specific model we study in this manuscript is that from the sinusoidal form we can control the degree of aperiodicity in the hopping distribution. Within the context of on-site diagonal terms, the regime $\nu > 1$ was called "pseudorandom" at reference [22]. It was shown that one electron eigenstates become localized at the presence of an aperiodic potential at this regime.

Equation (2) can be solved by using the transfer matrix formalism (TMF) [28,38]. The TMF is obtained by using a matrix recursive reformulation of equation (2). The matricial equation is

$$\begin{pmatrix}\psi_{i+1}\\ \psi_i\end{pmatrix} = \begin{pmatrix}\frac{-\omega^2+\eta_i+\eta_{i-1}}{\eta_i} & -\frac{\eta_{i-1}}{\eta_i}\\ 1 & 0\end{pmatrix}\begin{pmatrix}\psi_i\\ \psi_{i-1}\end{pmatrix} = T_i\begin{pmatrix}\psi_i\\ \psi_{i-1}\end{pmatrix}. \quad (4)$$

The wave amplitude of the complete 1D system is given by the product of the transfer matrices $Q_N = \prod_{i=1}^{N} T_i$. The logarithm of the smallest eigenvalue of the limiting matrix $\Gamma = \lim_{N\to\infty}(Q_N^{\dagger}Q_N)^{1/2N}$ define the Lyapunov exponent γ (inverse of localization length $\lambda = 1/\gamma$). Further details about the computation of this parameter can be found in [4–6]. Tipically, we use up to $N = 2^{21}$ transfer matrices to compute the localization length. For extended states $\lambda/N \approx$ const. and goes to zero for localized waves. In our calculations we compute also the average localization length defined as $\langle\lambda\rangle = \frac{1}{N_f}\sum_{\omega=0.5}^{\omega=1.5}\lambda(\omega)$ where N_f is the number of acoustic modes within the interval $[0.5, 1.5]$. In our calculations we have used $N_f = 500$. Let us stress that the bottom of the band was avoided in this sum because the localization length of a low-frequency acoustic wave is large even in the presence of strong uncorrelated disorder [38]. We are interested in the existence of extended states apart the bottom of the band. Therefore, $\langle\lambda\rangle/N$ does not depend of N for extended modes and goes to zero for localized ones. In addition, we apply the finite-difference method with second-order discretization for both the time and spatial variables proposed in reference [38]. Thus, in discretized form, $\psi(x,t)$ is written as ψ_i^n, where n denotes the time step number and i is the grid point number [38]. Therefore, the second time derivative in equation (1) is given by [38]

$$\frac{\partial^2}{\partial t^2}\psi(x,t) \approx \frac{\psi_i^{n+1} - 2\psi_i^n + \psi_i^{n-1}}{\Delta t^2}, \quad (5)$$

where Δt is the size of the time step. The spatial derivative will be written as

$$\frac{\partial}{\partial x}\left[\eta(x)\frac{\partial\psi(x,t)}{\partial x}\right] \approx \frac{1}{\Delta x^2}\Big[\eta_i(\psi_{i+1}^n - \psi_i^n) - \eta_{i-1}(\psi_i^n - \psi_{i-1}^n)\Big]. \quad (6)$$

In our calculations the spacing Δx between two neighboring grid points was set $\Delta x = 1$. In order to ensure the stability of the discretized equations we will use $\Delta t < \Delta x/100$. We carry our dynamical analysis by sending a wave from one side of the chain ($L = 0$) and recording the transmitted wave close to the other side (position $L = 20\,000$). We calculate the intensity spectrum of the transmitted wave at the end of chain defined as

$$A(\omega) = (1/2)|\psi_L(\omega)|^2 \quad (7)$$

where $\psi_L(\omega)$ if the Fourier transform of the transmitted wave $\psi_L(t)$ at position $L = 20\,000$. For transmitted acoustic modes, $A(\omega) > 0$ and goes to zero for filtered ones. In our dynamical calculations the chain length was $N = 2^{15}$.

3 Results

The calculations of the typical localization length were done by using the transfer-matrix technique for a chain of size very large ($N \approx 2 \times 10^6$). In this method, the self-averaging effect automatically takes care of statistical fluctuations. We estimate and control these fluctuations following the deviations of the calculated eigenvalues of

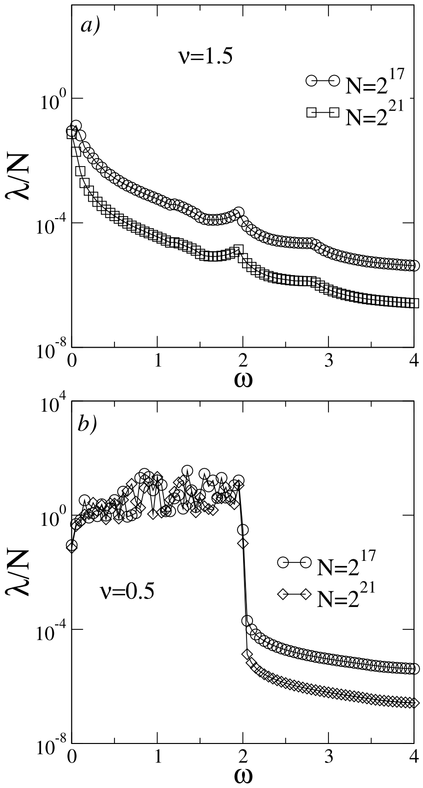

Fig. 1. The scaled localization length λ/N versus ω computed for $\alpha = 0.1$, $V_0 = 2$, distinct system size ($N = 2^{17}$ and 2^{21}), and (a) $\nu = 1.5$, (b) $\nu = 0.5$. For $\nu = 1.5$ we obtain the same physical properties of a 1D random media, only for $\omega = 0$ the localization lenght scales proportional to the system size. For $\nu = 0.5$ a rough data collapse in a wide region of low frequencies is obtained with $\lambda \propto N$ thus suggesting extended acoustic modes in this low-frequency region.

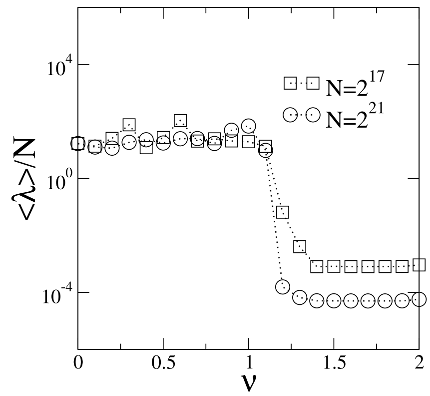

Fig. 2. Scaled average localization length $\langle\lambda\rangle/N$ versus the degree of aperiodicity ν. As it can be noticed, we obtain extended states with $\lambda \propto N$ for $\nu < 1$.

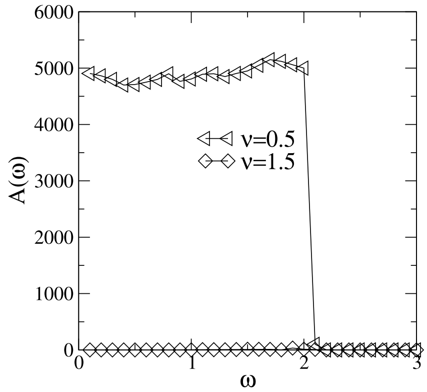

Fig. 3. The intensity spectrum $A(\omega)$ versus ω obtained from the dynamics formalism. We have used the incident wave as a superposition of harmonic waves with frequencies $\omega_n < 3$ ($\Psi_0(t) = \sum_{\omega_n<3} \cos(\omega_n t)$). The second order finite-difference method was carried using $N = 2^{15}$ points, $\Delta t < 1/100$, $t = 5\,000\,000\Delta t$, $\nu = 0.5(\triangleleft)$ and $\nu = 1.5(\diamond)$. For $\nu = 0.5$, the medium behaves as a filter to transmit only the modes below frequency $\omega_c \approx 2.0(1)$. For $\nu = 1.5$, all modes with $\omega > 0.0$ decay.

two adjacent iterations [4–6,28,38]. The finally obtained data have statistical errors less than 5%. In Figure 1 we show the scaled localization length λ/N versus ω computed for $\alpha = 0.1$, $V_0 = 2$, $\nu = 1.5$ (Fig. 1a), 0.5 (Fig. 1b) and distinct system sizes ($N = 2^{17}$ and 2^{21}). For $\nu = 1.5$ the localization lenght scales proportional to the system size only for $\omega = 0$. For high-frequencies, the absence of periodicity induce the localization of acoustic waves and a nonzero Lyapunov exponent. Therefore, for $\omega > 0$ there are no truly delocalized states in this regime of aperiodicity. Within the 1d acoustic waves propagation context, the $\nu > 1$ limit showed the same physical properties of a 1D random media [4–6,38]. However, for $\nu = 0.5$ a rough data collapse in a wide region of low frequencies is obtained with $\lambda \propto N$. Accordingly, our results suggest that for this degree of aperiodicity, extended acoustic modes appear in a finite frequency range. In Figure 2 we collect data of the scaled average localization length $\langle\lambda\rangle/N$ versus the degree of aperiodicity ν. The scaled average localization length $\langle\lambda\rangle/N$ was computed within interval $[0.5, 1.5]$, i.e, avoiding the bottom of the band, because the localization length of low-frequency acoustic waves is large even in the presence of strong uncorrelated disorder [38]. As it can be noticed, there is a well defined data colapse for ($\nu < 1$). For all system sizes studied here, we obtain $\lambda \propto N$ that indicates extended modes in the thermodynamic limite. Then, our results suggest that when $\nu < 1$, extended acoustic modes in a finite frequency range. However, this behavior does not guarantee the existence of extended states, as in the case of a vibrational wave envelope displaying a power-law decay [4–6]. Therefore we further study the dynamics of an initially localized excitation in the chain to better characterize the transport properties in this system. In Figure 3 we plot the resulting frequency dependence of the intensity spectrum $A(\omega)$ obtained from the dynamics simulation. The incident wave was a superposition of harmonic waves with frequencies $\omega_n < 3$ ($\Psi_0(t) = \sum_{\omega_n<3} \cos(\omega_n t)$). Calculations were done using $N = 2^{15}$ points, $\nu = 0.5(\triangleleft)$ and $\nu = 1.5(\diamond)$. As shown in Figure 3 for $\nu = 0.5$, all modes with $\omega > 2.0$ decay, and the medium behaves as a filter to transmit only the modes below frequency $\omega_c \approx 2.0(1)$. For the pseudo-random limit ($\nu = 1.5$), all the modes with $\omega > 0.0$ decay. We observe that for $\nu = 0.5$ the incident wave displays a free propagation through the aperiodic media. These results confirm those obtained by the numerical analysis based on the TMF method described before. Futhermore, we observe that both formalisms are in good agreement about the mobility edge position ($\omega_c = 2.0(1)$). Therefore the numerical evidences reported here shows that the low-frequencies modes in a 1d aperiodic media are in fact delocalized.

4 Summary and conclusions

In this work we studied the propagation of acoustic waves in 1d media with an aperiodic pseudo-random elasticity distribution. By using a discretized form of the acoustic wave equation the ratio of the stiffness $e(x)$ and the medium's mean density m behaves as an elastic constant. To produce an aperiodic distribution of elastic constants, we used a sinusoidal function whose phase varies as a power-law, $\phi \propto n^{\nu}$, where n labels the grid positions along the 1d media. Using a transfer matrix formalism we computed the localization length of acoustic modes within the band of allowed frequencies. We observed that, for $\nu < 1$, the localization length diverges with N in the low-frequency region ($\omega < \omega_c$). Therefore there is a new phase of extended acoustic waves in these aperiodic media. In addition we showed that the presence of these non-scattered acoustic modes can modify the propagation of an incident wave. We solved directly the scalar wave equation and showed that the chain filters all frequencies except those in the frequency range below ω_c. Within our numerical precision, both formalisms provide the critical frequency $\omega_c = 2$. Therefore, we numerically reported the existence of extended acoustic modes with frequency $\omega > 0$ in a 1d model with an aperiodic defect distribution. We expect that the present work will stimulate further theoretical and experimental investigations along this line.

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