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Vibrational modes in a two-dimensional aperiodic harmonic lattice

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Abstract

We study the nature of collective excitations in classical harmonic lattices with aperiodic and pseudo-random mass distributions. Using a matrix recursive reformulation of the mass displacement equation, we compute the localization length within the band of allowed frequencies. Our numerical calculations indicate that, for aperiodic arrays of masses, a new phase of extended states appears in this model. Solving numerically the Hamilton equations for momentum and displacement along the chain, we compute the spreading of an initially localized energy excitation. We find that for sufficient aperiodicity, there is a ballistic propagation of the energy pulse.

1. Introduction

The transport properties in nonperiodic lattices are a very important issue which has attracted scientific interest for several decades. The problem of electronic transport in disordered lattices was investigated by Anderson [1–3]. In one-dimensional (1D) and two-dimensional (2D) electronic systems, the scaling theory [2] predicts the absence of a disorder-driven metal–insulator transition (MIT) for any degree of uncorrelated disorder. In a three-dimensional lattice, the presence of weak disorder promotes the localization of the high-energy eigenmodes. The low-energy states with long wavelength remain extended, although acquiring a finite coherence length. A mobility edge separates the high energy localized from the low-energy extended states. The localization of collective excitation in random low-dimensional lattices is a quite general feature. It applies, for example, to the study of magnon localization in random ferromagnets [4] and collective vibrational motion of 1D disordered harmonic chains [5]. Within the disordered harmonic chain context, it was shown there are about $\sqrt{N}$ low-frequency non-localized modes, where N is the number of masses in the chain [5, 6]. Besides these low-frequency extended modes, short or long-range correlations in the disorder distribution (spring constants or masses) lead to a new set of non-scattered modes [7–11].

Among models with disordered geometry or composition, Hamiltonian models with aperiodicity have attracted renewed interest. For example, the well known aperiodic Anderson model [12] lies between the random Anderson model and the periodic Bloch model. It was shown that the localized or extended nature of their eigenstates is related to general characteristics of the aperiodic on-site distributions [12–16]. The effect of aperiodicity on the electronic dynamics in 2D lattices was studied in [17]. The one-electron Schrödinger equation in a 2D square lattice with an aperiodic site potential was solved numerically. 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 [17]. The role played by a specific aperiodic structure on the localization properties and/or energy transport in harmonic chains was studied in [18, 19]. Moreover, the quantum Heisenberg ferromagnet with aperiodic exchange couplings was considered in [20]. 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 [20]. The great importance of aperiodicity in different domains of science was showed by Macia in [21].

In this work, we study 2D harmonic lattices with masses following a distribution similar to that used in [12] that simulate both aperiodic and pseudo-random mass distributions. We focus on the Lyapunov exponent, estimated using a transfer matrix method. These results are used to characterize the nature of vibrational modes in this model. We show that, due to the aperiodicity of the mass array, low-frequency extended vibrational modes can exist. The dynamics of an initially localized excitation is also studied by computing the energy distribution. We find that, associated with the emergence of a phase of delocalized modes, a ballistic regime takes place.

2. Model and formalism

We consider a 2D harmonic lattice of $N \times M$ masses, for which the classical Hamiltonian can be written as $H = \sum_{n,m} h_{n,m}(t)$, where the energy $h_{n,m}(t)$ of the mass at site (n, m) is given by

$$h_{n,m}(t) = \frac{P_{n,m}^2}{2m_{n,m}} + \frac{1}{4}[(Q_{n+1,m} - Q_{n,m})^2 + (Q_{n,m} - Q_{n-1,m})^2 + (Q_{n,m+1} - Q_{n,m})^2 + (Q_{n,m} - Q_{n,m-1})^2]. \quad (1)$$

Here $P_{n,m}$ and $Q_{n,m}$ define the momentum and displacement of the mass at site (n, m). The 2D aperiodic mass distribution will be take to be aperiodic in the form:

$$m_{n,m} = m_0 + W * \cos(\alpha n^{\nu_x}) \cos(\alpha m^{\nu_y}), \quad (2)$$

where m_0, $W < m_0$, α, ν_x and ν_y are variable parameters. Calculations will done by using all elastic couplings equal to unity, $m_0 = 4$ and $\alpha = 0.5$. By considering displacements along the N-direction (longitudinal displacements) and inserting a solution of the form $Q_{n,m} = u_{n,m} \exp(\mathrm{i}\omega t)$ we obtain the following equation of motion

$$(4 - \omega^2 m_{n,m}) u_{n,m} = u_{n-1,m} + u_{n+1,m} + u_{n,m+1} + u_{n,m-1}. \quad (3)$$

After defining $u_{n,m} = c_{n,m}/\sqrt{m_{n,m}}$ we get

$$\left(\frac{4}{m_{n,m}} - \omega^2\right) c_{n,m} = \frac{c_{n-1,m}}{\sqrt{m_{n,m} m_{n-1,m}}} + \frac{c_{n+1,m}}{\sqrt{m_{n,m} m_{n+1,m}}} + \frac{c_{n,m+1}}{\sqrt{m_{n,m} m_{n,m+1}}} + \frac{c_{n,m-1}}{\sqrt{m_{n,m} m_{n,m-1}}}. \quad (4)$$

2.1. Localization properties

A very standard quantity used to reveal the degree of localization is the Lyapunov exponent γ (which is the inverse of the localization length λ). The better numerical method for accurately computing localization lengths in nonperiodic systems is the transfer matrix method (TMM). The TMM is obtained by using a matrix recursive reformulation of the scaled displacement equation (equation (4)) in a 2D strip of width M ($N \times M$ with $N \gg M$). The matricial equation is

$$\begin{pmatrix} \vec{C}_{i+1} \\ \vec{C}_i \end{pmatrix} = \begin{pmatrix} \frac{1}{\mathbf{t}_{i,i+1}}(\mathbf{H}_i + \mathbf{J}_i - \omega^2 \mathbf{I}) & -\frac{\mathbf{t}_{i-1,i}}{\mathbf{t}_{i,i+1}} \\ \mathbf{I} & 0 \end{pmatrix} \begin{pmatrix} \vec{C}_i \\ \vec{C}_{i-1} \end{pmatrix} = T_i \cdot \begin{pmatrix} \vec{C}_i \\ \vec{C}_{i-1} \end{pmatrix} \quad (5)$$

where $C_{i+1} = (c_{i+1,1}, \ldots, c_{i+1,M})^{\mathrm{T}}$ represents the scaled displacements along the i th slice, $\mathbf{H}_i$ is a square $M \times M$ diagonal matrix with $[\mathbf{H}_i]_{k,k} = 4/m_{i,k}$, $\mathbf{J}_i$ is a square $M \times M$ Hermitian matrix with null elements except $[\mathbf{J}_i]_{k,k+1} = 1/\sqrt{m_{i,k} m_{i,k+1}}$ and $\mathbf{t}_{i,i+1}$ denotes a diagonal matrix with $[\mathbf{t}_{i,i+1}]_{k,k} = 1/\sqrt{m_{i,k} m_{i+1,k}}$. The scaled displacements of the complete 2D strip are given by the product of the transfer matrices $Q_N = \prod_{i=1}^{N} T_i$. The logarithm of the smallest eigenvalues of the limiting matrix $\Gamma = \lim_{N\to\infty}(Q_N^{\dagger} Q_N)^{1/2N}$ define the Lyapunov exponent γ. Further details about the computation of this parameter can be found in [22].

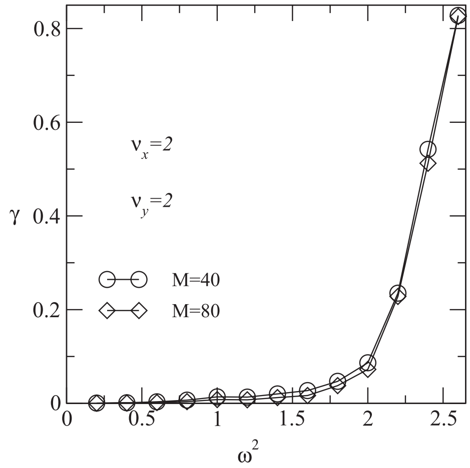

Figure 1. Lyapunov exponent γ as a function of frequency ω^2 for $\nu_x = \nu_y = 2$, $W = 1.8$, $M = 40$ and 80. The Lyapunov exponent vanishes close to the low-frequency region ($\omega \to 0$) as expected for low-dimensional harmonic systems. In the high-frequency region, $\gamma > 0$ corroborating previous results that indicate localization in nonperiodic square lattices.

2.2. Energy transport

The fraction of the total energy H_0 at site (n, m) is given by $f_{n,m}(t) = h_{n,m}(t)/H_0$ where $h_{n,m}(t)$ is defined by equation (1). By considering a uniform energy packet spread on a pure $N \times N$ harmonic square lattice ($m_{n,m}$ = constant), we have $f_{n,m} \approx 1/N^2$. Therefore, we can define the following time dependent quantity

$$\xi(t) = \frac{1}{\sum_{n,m=1}^{N} f_{n,m}^2}. \quad (6)$$

For a uniform energy packet we have $\sum_{n,m=1}^{N} f_{n,m}^2 = (1/N^4)\sum_{n,m=1}^{N}(1) = (1/N^2)$. Therefore, $\xi \propto N^2$ for a uniform energy packet spread on a square harmonic lattice with $N \times N$ masses. In a periodic square harmonic lattice ($m_{n,m}$ = constant), the second moment of the energy distribution defined as [9, 19]

$$M_2 = \sqrt{\sum_{n,m}[(n - n_0)^2 + (m - m_0)^2] f_{n,m}}, \quad (7)$$

displays a ballistic dynamics [$M_2(t) \propto t$]. Therefore we conclude that $\xi(t) \propto t^2$ for the energy transport in a periodic harmonic square lattice [9, 19]. The function ξ measures the number of masses that participate in the energy transport. This function is similar to the participation number for electrons [11]. In our calculations an initial excitation is introduced at site (n_0, m_0). We solved the Hamilton equations for $Q_{n,m}$ and $P_{n,m}$ by using a Dormand–Prince eighth-order Runge–Kutta method with monitoring of local truncation error [23] and then computing $\xi(t)$.

3. Results and discussion

In order to calculate the typical localization length of the eigenmodes, we use the transfer matrix technique for a long

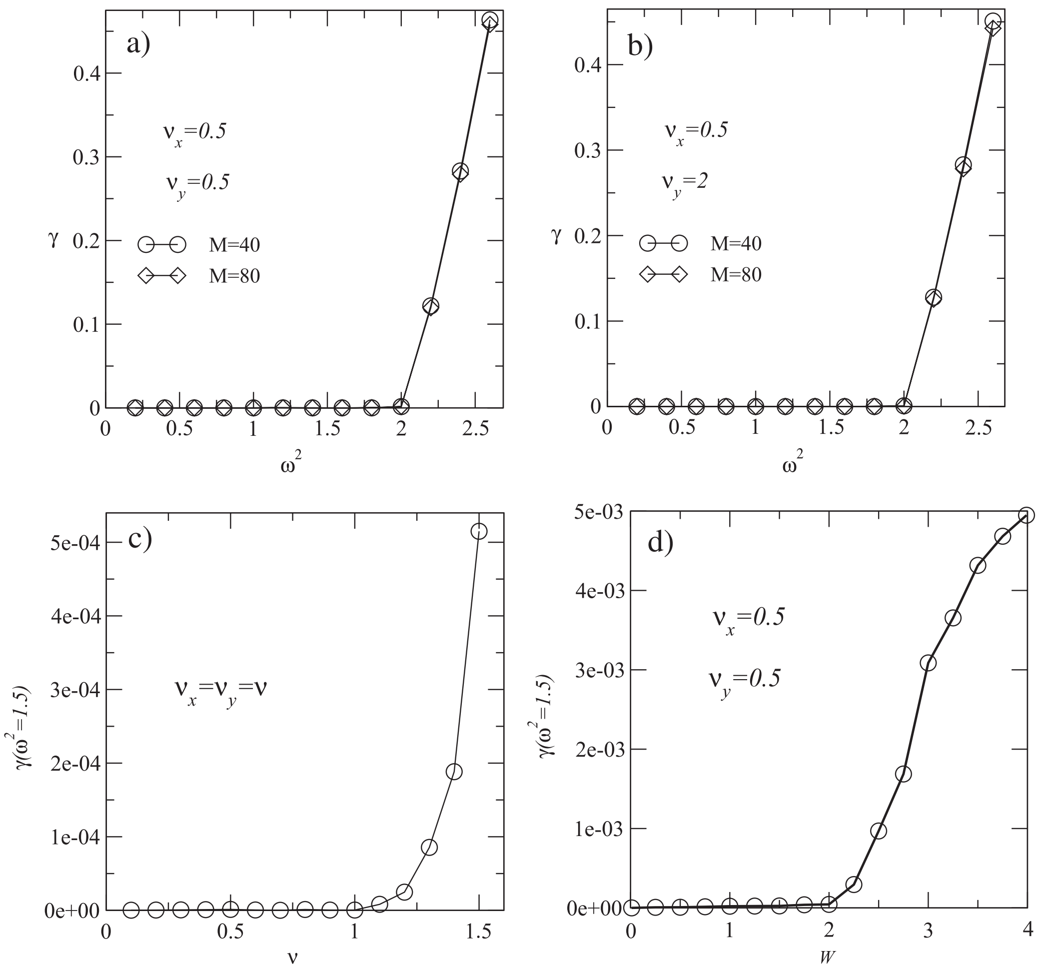

Figure 2. (a) Lyapunov exponent γ as a function of squared frequency ω^2 for $\nu_x = \nu_y = 0.5$, $W = 1.8$, $M = 40$ and 80. (b) The same as (a) for $\nu_x = 0.5$, $\nu_y = 2.0$, $M = 40$ and 80. (c) Lyapunov exponent γ computed at frequency $\omega^2 \approx 1.5$ versus $\nu = \nu_x = \nu_y$ for $W = 1.8$, $M = 40$ and 80. (d) Lyapunov exponent γ computed at frequency $\omega^2 \approx 1.5$ versus W for $\nu_x = \nu_y = 0.5$. Calculations indicate that, for $W < 2$, γ vanishes in the frequency region ($\omega^2 < \omega_c^2 \approx 2.0(1)$) when at least one of the degrees of exponents characterizing aperiodicity is smaller than unity ($\nu_x < 1$ or $\nu_y < 1$).

strip of size $N \times M$ with N being extremely large ($N \approx 3 \times 10^6$). 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 two adjacent iterations. The finally obtained data have statistical errors less 5%. In figure 1 we show data for the Lyapunov exponent γ versus frequency ω^2 for aperiodic harmonic lattices with $\nu_x = \nu_y = 2$, $M = 40$ and 80. In low-dimensional nonperiodic lattices the zero-frequency mode is a uniform mode with $\gamma = 0$. For high-frequencies, the absence of periodicity induces the localization of eigenmodes and a nonzero Lyapunov exponent should be obtained [6, 9, 19, 11]. Our results agree reasonably with this main picture. The Lyapunov exponent vanishes close to the low-frequency region ($\omega \to 0$) and it is nonzero in the high-frequency region. For both ν_x and ν_y larger than 1.0, the aperiodic mass distribution promotes non-scattered (extended) modes only for frequencies very close to zero. Within the 1D aperiodic harmonic chain context, the $\nu > 1$ limit showed the same physical properties as a 1D random harmonic chain [19] and was called the pseudo-random limit. In 2D our calculations indicate that the aperiodic mass distribution in the regime $\nu_x > 1$ and $\nu_y > 1$ displays a similar pseudo-random character. In figures 2(a) and (b) we show the Lyapunov exponent γ as a function of frequency ω^2 for (a) $W = 1.8$, $\nu_x = \nu_y = 0.5$, $M = 40$ and 80 and (b) $W = 1.8$, $\nu_x = 0.5$, $\nu_y = 2.0$, $M = 40$ and 80. Both calculations indicate that γ vanishes in the low-frequency region ($\omega^2 < \omega_c^2 \approx 2.0(1)$). In figure 2(c) we collect data of the Lyapunov exponent γ computed at frequency $\omega^2 \approx 1.5$ versus $\nu = \nu_x = \nu_y$ for $W = 1.8$, $M = 40$ and 80. Therefore, our results suggest that when at least one of the exponents characterizing degree of aperiodicity is smaller than 1 ($\nu_x < 1$ or $\nu_y < 1$), extended vibrational modes appear in the high-frequency region. In figure 2(d) we report the dependence of the Lyapunov exponent with width W. We plot the Lyapunov exponent γ computed at frequency $\omega^2 \approx 1.5$ versus W for $\nu_x = \nu_y = 0.5$. For $W > 2$ there are no extended vibrational eigenmodes. For all studied system sizes, we obtain $\gamma \propto 1/N$ (not shown here) which indicates the true extended vibrational modes in the thermodynamics limit ($N \to \infty$). This behavior does not guarantee the existence of extended states, as in the case of a vibrational wave envelope displaying a power-

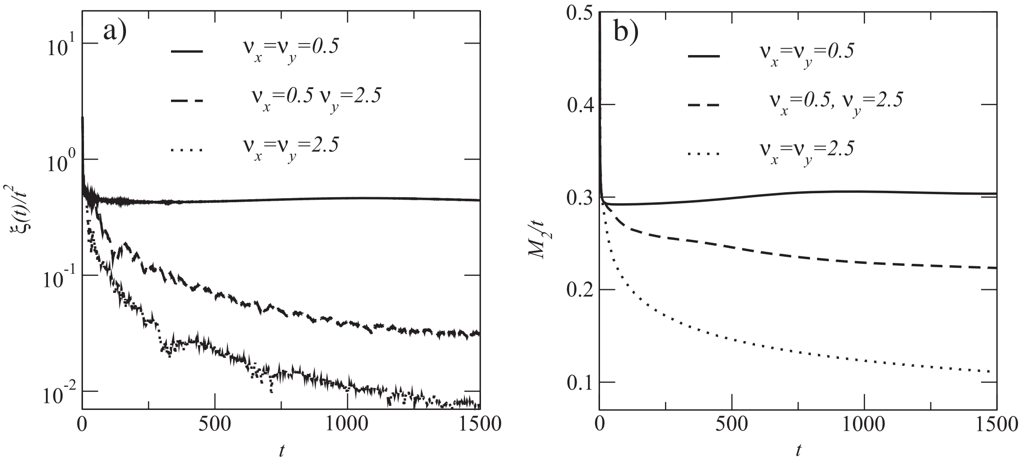

Figure 3. (a) The timescaled function $\xi(t)/t^2$ and (b) the scaled second moment $M_2(t)/t$ as a function of time for a square $N \times N$ aperiodic harmonic lattice with $W = 1.8$, $\nu_x = \nu_y = 0.5$ (solid line), $\nu_x = 0.5$ and $\nu_y = 2.5$ (dashed line) and $\nu_x = \nu_y = 2.5$ (dotted line). For both ν_x and ν_y smaller than unity, a ballistic energy spread with $M_2(t) \propto t$ and $\xi \propto t^2$ was obtained. However, when at least one of the degrees of aperiodicity exceeds unity a slower energy transport takes place.

law decay [6, 22]. Therefore we further study the dynamics of an initially localized excitation in the lattice to better characterize the energy spread in this system. To do this, we solve the Hamilton equations for $Q_{n,m}$ and $P_{n,m}$ by using an initial energy impulse excitation ($P_{n,m} = \delta_{n=N/2,m=N/2} P_0$ and $Q_{n,m} = 0$). In figure 3 we plot the timescaled function $\xi(t)/t^2$ and scaled second moment $M_2(t)/t$ as a function of time for a square $N \times N$ aperiodic harmonic lattice with $\nu_x = \nu_y = 0.5$ (solid line), $\nu_x = 0.5$ and $\nu_y = 2.5$ (dashed line) and $\nu_x = \nu_y = 2.5$ (dotted line). Calculations were done by using $N \times N = 2500 \times 2500$ and an eighth-order Runge–Kutta method with time step $\Delta t = 0.005$. The energy conservation was checked to ensure numerical precision. For both ν_x and ν_y smaller than unity a ballistic energy spread with $M_2(t) \propto t$ and $\xi \propto t^2$ was obtained. However, when at least one of the degrees of aperiodicity exceeds unity a slower energy transport takes place. We have performed calculations for an initial displacement excitation and the results are similar, a ballistic energy transport when both ν_x and ν_y are smaller than unity. Let us stress that the Lyapunov exponent calculation predicted extended states if at least one of the degrees of aperiodicity is smaller than unity ($\nu_x < 1$ or $\nu_y < 1$). By following the time evolution of an initially localized energy pulse we add valuable information about the localization–delocalization transition found here. In fact, the dynamical analyses indicate that extended states only appear when both ν_x and ν_y are smaller than unity. Therefore, to promote free energy transport we need to impose sufficient aperiodicity on both directions of the square lattice.

4. Summary and conclusions

In this paper we have studied the nature of collective excitations in 2D harmonic lattices with aperiodic and pseudo-random mass distributions. To produce an aperiodic distribution of masses, sinusoidal functions were used the phases of which vary as a power-law, $\phi_x \propto n^{\nu_x}$ and $\phi_y \propto m^{\nu_y}$, where n, m labels the positions along the square lattice. Using a transfer matrix formalism we compute the localization length of eigenmodes within the band of allowed frequencies. We observed that, for both $\nu_x < 1$ and $\nu_x < 1$, the localization length diverges with N in the low-frequency region. Therefore there is a new phase of extended vibrational modes in these aperiodic harmonic square lattices. In addition, we showed that the presence of these non-scattered vibrational modes can modify the spreading of an initially localized energy pulse. By calculating the energy spatial distribution, we found the existence of a ballistic propagation of the energy pulse. For at least one of the degrees of aperiodicity (ν_x or ν_y) larger than unity the pseudo-random character of masses induces a similar behavior to that found in 2D harmonic lattices with uncorrelated random mass distributions [9, 19, 11]. The thermal conductivity can be strongly influenced by the presence of new extended modes at low-frequencies [24]. We expect that the present work will stimulate further studies along this direction.

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