Vibrational modes in aperiodic one-dimensional harmonic chains

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The present paper addresses the effect of aperiodicity in one-dimensional oscillatory systems. We study the nature of collective excitations in harmonic chains in the presence of aperiodic and pseudorandom mass distributions. Using the transfer matrix method and exact diagonalization on finite chains, we compute the localization length and the participation number of eigenmodes 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. For pseudorandom masses distribution, all eigenstates remain localized except the uniform mode ($\omega=0$). Solving numerically the Hamilton equations for momentum and displacement of the chain, we compute the spreading of an initially localized energy excitation. We show that, independent of the kind of initial excitation, an aperiodic structure of masses can induce ballistic transport of energy.

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INTRODUCTION

The simplest and almost unique class of systems for which one can perform analytic calculations is represented by harmonic chains. Even though they are characterized by a peculiar dynamics, basically because of the integrability of the motion, their behavior can help to shed some light on various aspects of heat conductivity. One of the properties of harmonic chains is the possibility to decompose the heat flux into the sum of independent contributions associated with the various eigenmodes.[1] Particularly, the heat flux in low-dimensional classical systems has been the target of recent intense investigations.[2–13] The thermal conductivity of harmonic and anharmonic chains with uncorrelated random masses,[4] as well as that of a chain of hard-point particles with alternate masses,[5] have been numerically investigated in detail. The main issue here is whether these systems display finite thermal conductivity in the thermodynamic limit, a question that remains controversial.[6]

In general, the behavior of the thermal conductivity, as well as the vibrational eigenmodes, appears to be determined by the disorder and anharmonicity.[14] When aperiodic and disordered structures are involved, the Anderson theory plays a key role in the localization properties of vibrational eigenfunctions in condensed matter physics.[15,16] The 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.[17] Further, the collective vibrational motion of one-dimensional (1D) disordered harmonic chains of N random masses can also be mapped onto a one-electron tight-binding model.[18] 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 $\sqrt{N}$.[18,19] It was shown that correlations in the mass distribution produce a new set of nonscattered modes in this system.[20] Nonscattered modes have also been found in disordered harmonic chains with dimeric correlations in the spring constants.[21] A large amount of work has been done in recent decades to understand localization behavior in randomly disordered chains.[12] Most of this work has been concentrated in uncorrelated,[15] short-range,[22] and long-range[23] correlated disorder. Among these models, chains with diluted disorder, another kind of short-range correlation, have attracted renewed interest.[24–29] In general, the model consists of two interpenetrating sub-lattices, one composed of random potentials (Anderson lattice) and the other composed of nonrandom sites of constant potential. Due to the periodicity, special resonant energies appear. Recently, the effect of this kind of local correlations in a disordered harmonic chain was studied.[29] There is another class of 1D models, the aperiodic Anderson model,[33] lying between the random Anderson model and the periodic Bloch model. They have been extensively investigated in the literature[30–34] and the localized or extended nature of their eigenstates has been related to general characteristics of the aperiodic on-site distributions. Within the line of vibration modes in classical chains, the roles played by aperiodic structure onto localizations properties and/or energy transport have not been completely studied. A very interesting study was publishied in Ref 11. The authors studied the effect of a Fibonacci-like array of masses on the thermal conductivity of a one-dimensional anharmonic lattice.

In this work, we focus on the effect of aperiodicity in one-dimensional harmonic systems. Here we will consider the mass distributions following the sequence used in Ref. 33. From this we can simulate both aperiodic and pseudorandom mass distributions. We use the transfer matrix method to obtain accurate estimates for the Lyapunov exponent. 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, the low-frequency extended vibrational modes can exist. All calculations were confirmed using an exact diagonalization procedure on a finite chain. 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, independent of the kind of

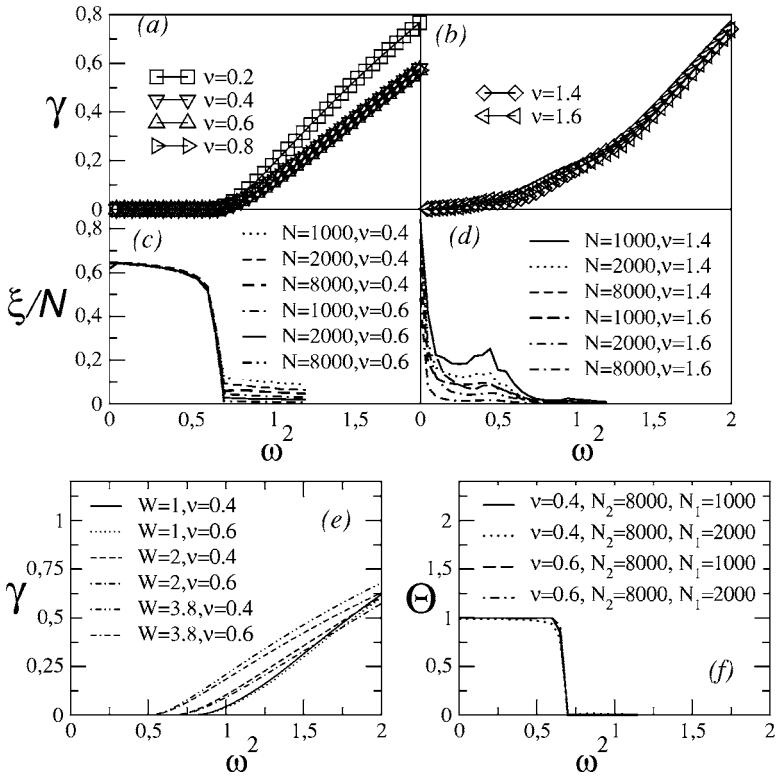

FIG. 1. (a) Lyapunov coefficient γ vs ω^2 for $\nu=0.2$ (□), 0.4 (▽), 0.6 (Δ), and 0.8 (▷); (b) the same for $\nu=1.4$ (◇) and 1.6 (◁). (c) Scaled participations number ξ/N for $\nu=0.4$ and 0.6 and distinct system size. (d) Scaled participations number ξ/N for $\nu=1.4$ and 1.6 and distinct system size. All previous calculations were done for $W=2$. These results indicate that, for $\nu<1$, there are extended vibrational modes at the low-frequency region. (e) Lyapunov coefficient γ vs ω^2 for $\nu=0.4, 0.6$ and $W=1$, 2, and 3.8. (f) The scale function for dates of (c). The critical frequency that separates extended from localized vibrational modes is independent of the ν exponent; it depends only on the width W of mass distributions, see (e). We use $m_0=4$ in all cases and $W=2$ in (a)–(d) and (f).

initial excitation, an aperiodic structure of masses can induce a ballistic energy transport. Therefore, in the thermodynamic limit the model presents extended states. This modifies the heat conduction of the harmonic chain.

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 [19,20]

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

Here, we shall consider a mass distribution given by

$$m_n=m_0+W\cos(\alpha n^\nu), \quad (2)$$

with α an arbitrary rational number and ν and W being a tunable parameter.[33] We use $m_0>W$ to avoid negative masses. In our calculations, we will use units where all elastic force couplings β_n are equivalent and equal to 1. The localization length of each vibrational mode is taken as the inverse of the Lyapunov exponent γ defined by[19,20]

$$\gamma=\lim_{N\to\infty}\frac{1}{N}\log\frac{|Q_N c(0)|}{|c(0)|}, \quad (3)$$

where $c(0)=\binom{u_1}{u_0}$ is a generic initial condition and Q_N is the product of all transfer matrices,

$$Q_N=\prod_{n=1}^{N}\begin{pmatrix}2-m_n\omega^2 & -1\\ 1 & 0\end{pmatrix}. \quad (4)$$

In addition, we compute the participation ratio P defined by $P(f^2)=\Sigma_{n=1}^N u_n^2(f^2)/\Sigma_{n=1}^N u_n^4(f^2)$,[35] where the Fourier $u_n(f^2)$ are those associated with an eigenmode f^2 of a chain of N masses and are obtained by direct diagonalization of the $N\times N$ secular matrix A defined by $A_{i,i}=2/m_i$, $A_{i,i+1}=A_{i+1,i}=1/(m_i m_{i+1})^{1/2}$, and all other $A_{i,j}=0$.[35] $P(f^2)$ displays a dependence on the chain size for extended states and is finite for exponentially localized ones. In our calculations, we compute the average participation number defined by $\xi(\omega^2)=\frac{1}{N_f}\Sigma_{f^2=\omega^2-\Delta\omega^2}^{f^2=\omega^2+\Delta\omega^2}P(f^2)$, where $\Delta\omega^2=0.05$ and N_f is the number of eigenmodes within each interval $[\omega^2-\Delta\omega^2,\omega^2+\Delta\omega^2]$. A more quantitative scaling analysis of the participation number trend can be derived by introducing the set of auxiliary functions

$$\Theta(\omega^2,N_1,N_2)=\exp\left[-\left|\frac{N_2}{\xi(\omega^2,N_2)}-\frac{N_1}{\xi(\omega^2,N_1)}\right|\right], \quad (5)$$

which is a measure of the difference between data from two consecutive chain sizes investigated. For extended states, $\Theta\approx 1$ for large chain sizes. For localized states, $\Theta\to 0$ in the thermodynamic limit.

In Fig. 1(a), we show the Lyapunov exponent γ as a function of ω^2 obtained from the transfer matrix method for $\nu=0.2$ (□), 0.4 (▽), 0.6 (Δ), and 0.8 (▷). Here we use $m_0=4$ in all cases and $W=2$ in Figs. 1(a)–1(d) and 1(f). One can see that this exponent vanishes in the low-frequency region $[\omega^2<\omega_c^2\approx 0.6(1)]$. This feature is a clean signature of extended vibrational modes. In Fig. 1(b), we show the Lyapunov exponent γ as a function of ω^2 for $\nu=1.4$ (◇), and 1.6 (◁). As this coefficient does not vanish for $\omega^2>0$, for $\nu\geq 1$ all eigenstates are localized for $\omega>0$. In Fig. 1(c), we show data for the scaled participation number for $\nu=0.4, 0.6$ and $N=1000$, 2000, and 8000. The well-defined

data collapse in the low-frequency region confirms the extended nature of these vibrational modes. For $\nu>1$ [see Fig. 1(d)], only for $\omega=0$ are the participation number scales proportional to the system size. The critical frequency ω_c^2 that appears in Figs. 1(a)–1(c) separating extended from localized vibrational modes does not depend on the ν exponent. In Fig. 1(e), one can see that it depends only on the width W of the mass distributions. Both results for participation number [Figs. 1(c) and 1(d)] are in perfect agreement with the calculated Lyapunov exponents [Figs. 1(a) and 1(b)]. In Fig. 1(f), the Θ versus ω^2 data suggest that the phase of extended low-frequency vibrational modes is stable in the thermodynamic limit and that the critical frequency ω_c^2 does not depend on the ν exponent for $\nu<1$. We use distinct system sizes ($N=5\times10^6$, 10^7, 2×10^7, and 4×10^7) to verify if our results are due to a finite-size effect. For all studied system sizes, we obtain a linear vanishing exponent ($\gamma\propto 1/N$, not shown here) that signs for true extended states in the thermodynamics limit ($N\to\infty$). This behavior does not completely assure the existence of extended states, as in the case of a vibrational wave envelope displaying a power-law decaying,[15,19] thus we further study the dynamics of an initially localized excitation in the chain to understand energy spread in this system.

ENERGY TRANSPORT

In order to study the time evolution of a localized energy pulse, we calculate the second moment of the energy distribution.[3,36] This quantity is related to the thermal conductivity by Kubo's formula.[3] The classical Hamiltonian H for a harmonic chain can be written as

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

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

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

Here P_n and Q_n define the momentum and displacement of the nth site mass.

The fraction of the total energy H at site n is given by $h_n(t)/H$ and the second moment of the energy distribution, $M_2(t)$, is defined by[3]

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

where $\langle n(t)\rangle=\Sigma_{n=1}^{N} n[h_n(t)/H]$.

An initial excitation is introduced at the site n_0 at $t=0$. Using the fourth-order Runge-Kutta method, we solve the Hamilton equations for $P_n(t)$ and $Q_n(t)$ to calculate $M_2(t)$. In harmonic chains, the energy spreads faster for an initial impulse excitation than for an initial displacement excitation,[3,36] in such a way that the behavior is strongly dependent on the initial conditions. We have performed calculations for both kinds of initial excitation.

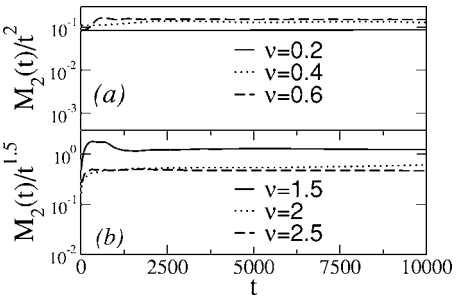

FIG. 2. The time-scaled second moment $M_2(t)/t^a$ vs time t obtained by using initial *impulse* excitation. (a) For $m_0=4$, $W=2$, and $\nu=0.2$, 0.4, and 0.6, the system displays ballistic spreading [$M_2(t)\propto t^2$]. (b) The same for $\nu=1.5$, 2.0, and 2.5; in this case the system is in a *superdiffusive* regime [$M_2(t)\propto t^{1.5}$]. For $\nu<1.0$, the frequencies below ω_c are extended over the lattice. This causes the ballistic energy spread of the pulse.

In Figs. 2 and 3 we plot, for *impulse* and *displacement* initial excitations, respectively, the time-scaled second moment $M_2(t)/t^a$ as a function of time for a 1D aperiodic harmonic chain with $\nu<1.0$ (a) and $\nu>1.0$ (b), using $N=1.6\times10^4$. For $\nu<1.0$, the extended modes for frequencies below ω_c induce ballistic energy spread of the pulse, i.e., $a=2$ independent of the kind of initial excitation. For $\nu>1.0$, the pseudorandom character of the mass chain induces nonscattered (extended) modes only for frequencies very close to zero. Therefore, we obtain a dynamic behavior similar to those found on the uncorrelated random harmonic chain: $a=1.5$ for *impulse* initial excitation and $a=0.5$ for *displacement* initial excitation.[3]

SUMMARY AND CONCLUSIONS

We study the nature of collective excitations in harmonic chains with aperiodic and pseudorandom mass distributions given by Eq. (2). Using a transfer matrix method and exact diagonalization on finite chains, we compute the localization length and the participation number of eigenmodes within the band of allowed frequencies. We observe that, for $\nu<1$,

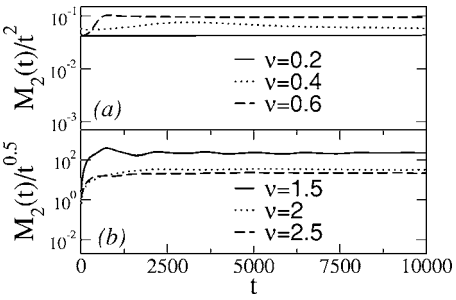

FIG. 3. The time-scaled second moment $M_2(t)/t^a$ vs time t obtained by using initial *displacement* excitation. (a) For $m_0=4$, $W=2$, and $\nu=0.2$, 0.4, and 0.6, as in Fig. 2(a), ballistic energy spreading is observed ($a=2$) associated with the low-frequency extended vibrational eigenstates. (b) For $\nu=1.5$, 2.0, and 2.5 the pseudorandom character of random masses induces a subdiffusive behavior ($a=0.5$).

the Lyapunov exponent vanishes and the participation number diverges with N in the low-frequency region; therefore, there is a new phase of extended vibrational modes in these aperiodic-mass chains. We also show that the presence of these nonscattered vibrational modes can modify the energy spreading of an initially localized excitation. By calculating the second moment $M_2(t)$ of the energy spatial distribution, we find that, associated with the emergence of a phase of low-energy extended collective excitations, $M_2(t)$ displays ballistic propagation of the energy pulse independent of the kind of initial excitation. For $\nu > 1$, the pseudorandom character of mass array induces a similar behavior to those found in harmonic chains with uncorrelated random mass distributions, sub- or superdiffusive depending on the kind of initial excitation, impulse or displacement-like, respectively.[3] The authors of Ref. 11 found that the thermal conductivity at low temperatures of a one-dimensional nonlinear lattice is strongly dependent on the nature of the harmonic eigenstates. They found constant flux for a periodic lattice and normal heat flux for disordered system; this scenario happens due to the extended and localized behavior of the eigenstates, respectively. For the aperiodic kind of system that they studied, the heat flux appears to be power law divergent, and the strength of divergence is strongly related to the specific structure of the model and, clearly, to the degree of localizations of their eigenstates. In light of these previous results, the presence of a finite phase of extended harmonic modes at low frequencies and the anomalous energy spreading found in our model also suggests an abnormal thermal conductivity in agreement with Ref. 11. We expect that the present work will stimulate further studies along this direction.

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