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Phonon localization in quasiperiodic systems

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Abstract

The effects of anharmonic interactions on the localization of phonons in quasiperiodic systems are studied by looking at the transmittance, Lyapunov exponent, participation ratio and energy-level-spacing distribution, within the rotating-wave approximation and first-order perturbation theory. For Fibonacci chains, a power-law distribution is found in the small-spacing region, since the eigenstates are critical. Even within first perturbation stages, anharmonic contributions do clearly manifest, weakening the level clustering behavior, contrary to the periodic case where the distribution is insensitive to weak anharmonic interactions. These results suggest a structural instability of the self-similar vibrational spectrum in quasiperiodic systems.

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1. Introduction

Nowadays, it is known that the eigenvalue spectrum produced by a quasiperiodic potential is singular continuous, neither absolutely continuous nor pure points. The associated eigenfunctions are critical, i.e., exhibiting intermediate localization nature between extended and exponentially localized behavior in real space [1]. However, until now this theoretically predicted critical behavior, such as multi-fractal band structures and exotic transport properties [2], has not been observed in real quasicrystals [3]. This discrepancy could be caused by the instability of the spectrum due to the presence of phasons [4], electronic correlation, and non-linear interatomic interactions. Spectral statistics has proved to be an alternative way for the study of transport properties, since there is a close relationship between the eigenfunction localization nature of a system and its eigenvalue statistics [5], e.g., for a disordered metal, the level-spacing (s) follows a Wigner distribution $P_W(s) = (\pi/2)s\exp(-\pi s^2/4)$, while for a disordered insulator it follows a Poisson's law $P_P(s) = \exp(-s)$. The essential difference between these two distributions

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arises from their small s behavior. Recently, a new kind of level statistics has been found in one-dimensional quasiperiodic systems. The level spacing distribution shows a power law behavior, revealing a level clustering mechanism [6]. The effects of anharmonic interactions have been analyzed by means of an equivalent circuit and the results show a softening of the eigenmodes [7]. In this paper, we further explore the role of anharmonic interactions on the phonon spectrum in quasiperiodic systems by looking at the transmittance, Lyapunov exponent, participation ratio, and spectral statistics.

2. The model

Let us consider a mixing Fibonacci chain (MFC), in which two kinds of atoms, A and B, are arranged following the Fibonacci sequence, i.e., if one defines the first generation $F_1 = A$ and the second one $F_2 = BA$, the subsequent generations are given by $F_n = F_{n-1} \oplus F_{n-2}$. For instance, $F_5 = BAABABAA$. In a MFC, the spring strength between atoms depends on their nature, giving two different force constants β_{AA} and $\beta_{AB} = \beta_{BA}$. Thus, the phonon dynamics of a MFC, including a quartic anharmonic term in the phonon Hamiltonian, can be described by

$$m_j \frac{\mathrm{d}^2 u_j}{\mathrm{d}t^2} = \beta_j(u_{j+1} - u_j) - \beta_{j-1}(u_j - u_{j-1}) + \eta(u_{j+1} - u_j)^3 - \eta(u_j - u_{j-1})^3,$$

where m_j can either be m_A or m_B. As we seek stationary solutions of the type $u_j = A_j \cos(\omega t)$, the well-known rotating-wave approximation [8] is used,

$$\cos^3(\omega t) = \frac{3}{4}\cos(\omega t) + \frac{1}{4}\cos(3\omega t) \approx \frac{3}{4}\cos(\omega t).$$

Thus, the equations of motion become

$$\omega^2 A_j = -\frac{\beta_j}{m_j}(A_{j+1} - A_j) + \frac{\beta_{j-1}}{m_j}(A_j - A_{j-1}) - \frac{3\eta}{4m_j} \times (A_{j+1} - A_j)^3 + \frac{3\eta}{4m_j}(A_j - A_{j-1})^3.$$

The anharmonic phonon frequencies can be determined by using a first-order perturbation theory, i.e., $E_n \approx E_n^{(0)} + E_n^{(1)}$, where $E_n = \omega^2(n)$, $E_n^{(0)}$ is the nth harmonic eigenvalue and $E_n^{(1)} = \langle \psi_n^{(0)} \mid H^{(1)}(n) \mid \psi_n^{(0)} \rangle$, being $\psi_n^{(0)}$ the harmonic eigenfunction corresponding to $E_n^{(0)}$ and $H^{(1)}(n)$ is a symmetrically tridiagonal matrix, whose elements are

$$H^{(1)}_{j,j+1}(n) = -\frac{3\eta}{4m_j}[A_{j+1}(n) - A_j(n)]^2,$$

$$H^{(1)}_{j,j}(n) = -H^{(1)}_{j,j-1}(n) - H^{(1)}_{j,j+1}(n).$$

Once the phonon eigenvalue spectrum $(\omega^2(n))$ is found, its level spacing statistics is obtained through an unfolding process [5].

3. Results

The numerical calculations were carried out by using the transfer matrix technique [9] for a MFC of generation 17 containing $N = 2584$ atoms, with $m_A = 1$, $m_B = 1597/987$, $\beta_{AA} = 0.5$ and $\beta_{AB} = \beta_{BA} = 1$, connected to two semi-infinite leads with

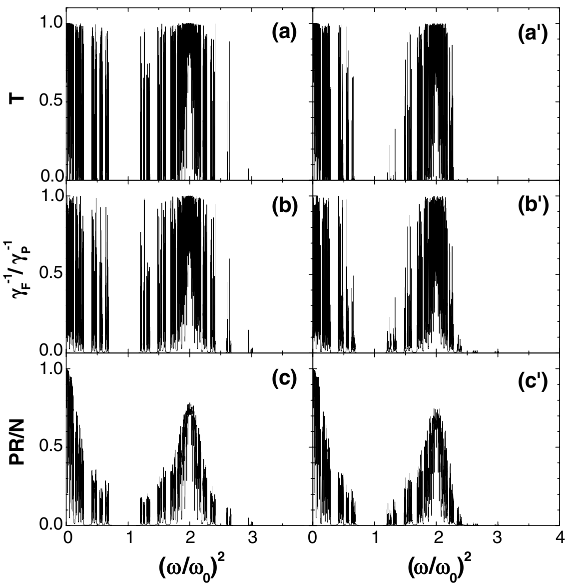

Fig. 1. (a) Transmittance (T), (b) inverse of the Lyapunov exponent (γ_F^{-1}), and (c) participation ratio (PR) versus frequency (ω) for a harmonic MFC of 2584 atoms. Figure (a′), (b′), and (c′) shows the corresponding results obtained for the same MFC with anharmonic interactions ($\eta = 0.5$).

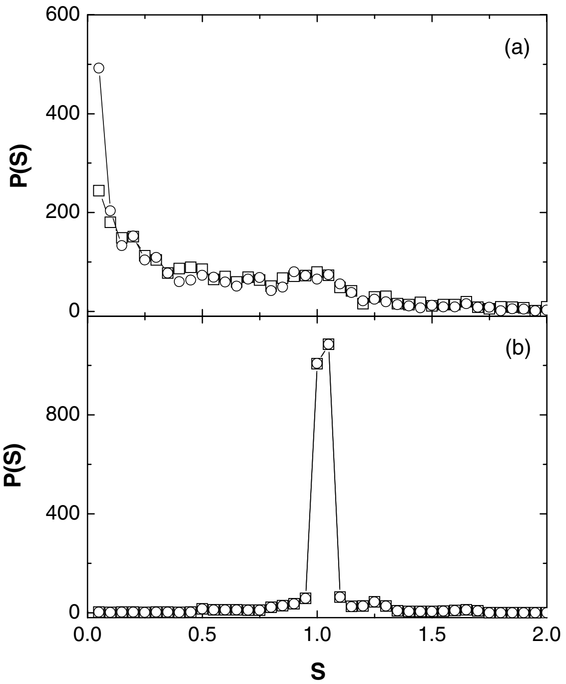

Fig. 2. Level-spacing distribution ($P(s)$) with unfolding for (a) the same MFC as in Fig. 1 and (b) a periodic chain, both containing 2584 atoms. The open circles correspond to $\eta = 0$ and open squares to $\eta = 0.5$.

$m = \beta = 1$, beginning amplitudes $C_0 = 1$ and $C_1 = e^{ika}$, where $\omega^2 = 2[1 - \cos(ka)]$. In Fig. 1(a)–(c) we show respectively the transmittance (T), Lyapunov exponent (γ_F) and participation ratio (PR), as were defined in Ref. [9], in comparison with Figs. 1(a′), (b′), and (c′) for $\eta = 0.5$, where $\omega_0^2 = \beta/m$ and γ_P is the Lyapunov exponent of a periodic chain. Additionally, we have calculated the level spacing distribution ($P(s)$) with unfolding for the same MFC as in Fig. 1 without leads, shown in Fig. 2(a), in comparison with the periodic case (Fig. 2(b)).

4. Discussion

From Fig. 1, we notice that there is a transparent state at $\omega^2 = 2\omega_0^2$ for the harmonic case [10], whose transmittance is decreased when the anharmonic interaction is introduced. Furthermore, the results show a general localization tendency of the states, although few of them become more delocalized. On the other hand, the level spacing analysis (Fig. 2) shows a Wigner-type distribution for the periodic case and its half-width becomes the standard Wigner's one if a small quantity of random disorder is introduced. For the quasiperiodic case, we observe a peak in the small level-spacing region, following a power law, which reveals a clustering nature for the quasiperiodic harmonic systems. However, this behavior is reduced toward a Poisson-like distribution by the inclusion of anharmonic interactions, contrary to what happens in periodic systems, where the distribution is insensitive to anharmonic interactions.

5. Conclusions

We have studied the effects of anharmonic interactions on the localization in quasiperiodic systems, within the rotating-wave approximation and a first-order perturbation theory. The results show a decreasing tendency of level clustering due to the anharmonicity, i.e., a deviation from the inverse power-law statistics, which is consistent with the results of the transmittance, Lyapunov exponent, and participation ratio analysis. Also, the results reveal that singular continuous spectra are more sensitive to anharmonic interactions than the continuous spectra of crystalline solids.

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