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Phonon diffusion in harmonic and anharmonic one-dimensional quasiperiodic lattices

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The phonon diffusivity in one-dimensional quasiperiodic lattices is studied using harmonic and inharmonic Hamiltonians. This study is performed by solving the equations of motion using a time discretization and the leap-frog algorithm. For the case of harmonic Hamiltonians, the results show that the variance of a wave packet in quasiperiodic systems is proportional to the time, as in a periodic lattice, but their diffusion constant is lower. This behaviour is qualitatively different from the electronic case, in which the variance increases as a power law of the time, with an exponent that depends upon the strength of the quasiperiodic potential. The difference between the electronic and phonon problems seems to be related to the localization degree of their long wavelength modes. In this limit, we present the time evolution of the phonon wave extension, showing a finite sound velocity given by averaged lattice parameters. Finally, for the inharmonic case, we found that the phonon diffusivity decreases as the nonlinear perturbation grows.

1. Introduction

The nature of transport properties in quasicrystals, which are materials with long-range order but without periodicity [1], still is not well understood [2]. For example, the electronic conductivity of quasicrystals is similar to that observed among amorphous semiconductors [3], while numerical simulations and theoretical studies predict a marginal metallic regimen due to the Conway theorem [4], since from a theoretical point of view, the wave-function resonates in a self-similar way. However, when the frustration effects of antibonding states are considered, the conductivity can be reduced by a considerable amount [5]. In one dimension (1D), it has been proved that the electron diffusivity follows a power law as a function of time, where the exponent depends upon the strength of the quasiperiodic potential [6]. Nevertheless, phonon propagation has been less studied, in spite of the fact that its spectrum is also singular continuous, where the main difference from the electronic case is that the ratio of the gap and the band width goes to zero for acoustic modes [6]. This difference can produce qualitative divergences in their behaviours

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and could be important in understanding the physical properties of quasicrystals, e.g. heat capacity, resistivity, thermal conductivity, etc. On the other hand, to get a finite thermal conductivity, it is necessary to include nonlinear effects since phonon–phonon collisions that transfer moment to the lattice (Umklapp processes) are responsible for this finite conductivity [7]. In spite of the importance of nonlinear effects in materials, there are many significant questions that are still open even for periodic and disordered systems [8], like how nonlinearity affects the localization and the transport properties [9]. In perfect periodic systems, where phonons have extended wave functions, nonlinearity produces phonon localization, usually known as intrinsic localization [10]. This effect has been observed in different kinds of physical systems such as Josephson junctions, optical waveguides arrays and laser-induced photonic crystals [8]. Thus, it is natural to expect a strong localization when both nonlinearity and disorder are present. However, several one-dimensional nonlinear models with correlated disorder exhibit delocalized states [11]. These effects have been confirmed recently using microwave waveguides [12]. An interesting question is what happens in quasiperiodic systems. For example, it has been recently found that quasiperiodic optical superlattices are useful for efficiently generating third-harmonics [13]. This fact has been corroborated using numeric simulations [14]. In this article, we study phonon propagation in a quasiperiodic system with linear and nonlinear interactions.

2. Electron and phonon diffusion

Let us consider the simplest 1D quasicrystal which consists of two kinds of atoms, A and B, arranged following the Fibonacci sequence [1], 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 order to model the behaviour of electrons and phonons in this system, for the electron case we start from a simple *s*-band tight-binding Hamiltonian, which leads to the time-dependent Schrödinger equation,

$$-i\hbar \frac{\partial u_j}{\partial t} = \varepsilon(j)u_j + Vu_{j-1} + Vu_{j+1} \tag{1}$$

where u_j is the electronic wave-function amplitude at site j and time t, $\varepsilon(j)$ is the self-energy of site j which has possible two values, ε_A and ε_B, arranged in a Fibonacci sequence, and V is the hopping integral that we take as a constant for all nearest neighbours.

On the other hand, the phonon dynamics, including a quartic inharmonic term in the spring–mass Hamiltonian, can be described by the following equation of motion,

$$m_j \frac{d^2u_j}{dt^2} = \beta(u_{j+1} - u_j) - \beta(u_j - u_{j-1}) + \eta(u_{j+1} - u_j)^3 - \eta(u_j - u_{j-1})^3 \tag{2}$$

where m_j is the mass of atom j and can be either m_A or m_B following the Fibonacci sequence, and u_j is the displacement of atom j at time t. The distance and spring strength between all nearest-neighbour atoms are constants, given by

a and β, respectively. The strength of the nonlinear effects are controlled by the parameter η. It is widely accepted that within the tight-binding model, electron and phonon behaviours are essentially the same, as revealed by a direct comparison of equations (1) and (2), where the inharmonic terms would correspond to the electron–electron correlation in equation (1). However, in this work we will demonstrate that their dynamical behaviour in quasiperiodic systems could be very different.

In the absence of electron–electron correlations in equation (1), or inharmonic terms in equation (2), the solutions of these equations are given by a superposition of the corresponding time-dependent eigenfunctions. These eigenfunctions can be obtained from the diagonalization of the Hamiltonian or by using the transfer matrix method [6]. For $\eta \neq 0$ these methods do not work, and some approximations are needed. In a previous paper we used the transfer method in conjunction with a perturbative approach and the rotating wave-approximation, which predicts a shift of the original frequencies [15]. To go beyond this approach, in this paper we solve the equations of motion using a discrete time $\Delta t = 0.001\hbar/V$ for electrons and $\Delta t = 0.001\sqrt{m/\beta}$ for phonons. To solve equation (1), two coupled equations for the real and imaginary parts of the wave function are used. For the case of phonons, at each time the force, velocity and acceleration of each particle in the chain are calculated using the leap-frog integration method [16]. Periodic boundary conditions were used in all cases for $N = 10\,946$ sites. As initial conditions, we always chose a delta function at the middle of the chain, $u_j(t) = a\delta_{j,N/2}$, and zero velocity at all sites, $\mathrm{d}u_j/\mathrm{d}t = 0$.

Once the chains are excited, the systems are allowed to evolve until they reach a certain number of time steps $t_{\max} = 2^l$, where l is an integer that usually has the value of 18, determined in such a way that boundary effects are avoided. To obtain the diffusivity, we evaluate the spreading of the wave packet as time evolves with the square root of the second-moment probability distribution defined as

$$\sigma(t) = \sqrt{\frac{1}{N}\sum_{j=1}^{N}\left(j - \frac{N}{2}\right)^2 |u_j|^2}. \tag{3}$$

In figure 1a we show $\sigma(t)$ for the electron case as a function of time using different strengths of the quasiperiodic potential, measured by the parameter $\lambda = \varepsilon_A - \varepsilon_B$. A log–log plot of the data reveals that $\sigma(t) \propto t^{\alpha}$, where α depends upon λ as shown in the inset figure 1a′. These results are similar to those obtained by other groups with the transfer matrix [17, 18]. For the harmonic phonon case ($\eta = 0$), figure 2a shows a plot of $\sigma(t)$ for different values of the parameter $\gamma = m_A/m_B$. The first interesting observation is that $\sigma(t) = At$ where A is a constant that depends on γ. It would be worth mentioning that A is related to the diffusivity constant (D) as $A = \sqrt{D/2}$ [17]. The inset of figure 2a shows the dependence of A with γ. Notice that for both cases the periodic results, $\alpha = 1$ and $A = 1/2$, are recovered when $\lambda = 0$ or $\gamma = 1$, as proved analytically [19].

The difference between the phonon and electron diffusions observed in figures 1a and 2a can be understood by considering that the diffusivity is related to the fractal dimension of the spectra [20] and this dimension decays with the frequency in the acoustic region for the phonon spectra [6]. On the other hand, the fractal dimension

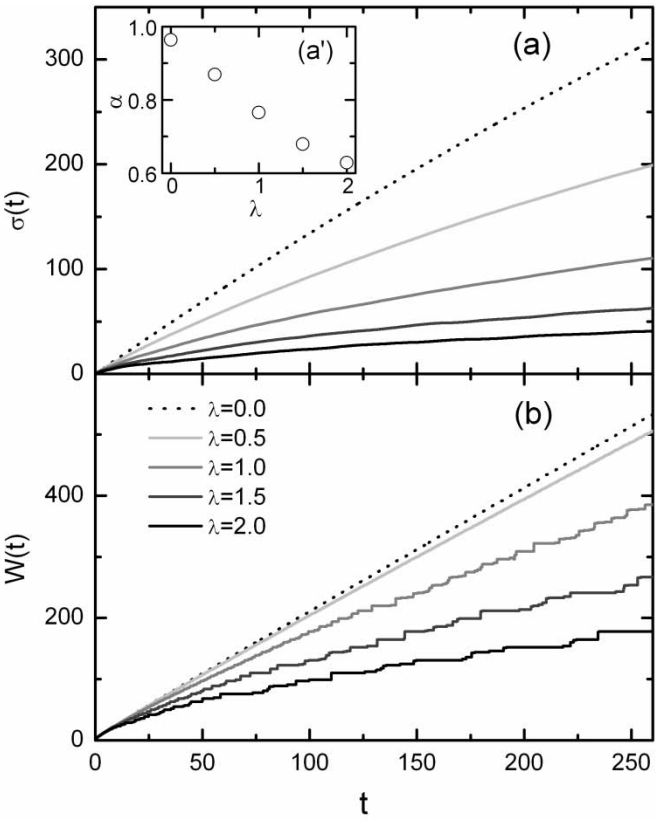

Figure 1. (a) Time evolution of the wave-packet variance for electrons in a chain of 10 946 sites, with different quasiperiodic strengths given by $\lambda = \varepsilon_A - \varepsilon_B$. The data follow a power law as $\sigma(t) \propto t^{\alpha}$. Inset (a′): values of the exponent α for different value of λ. (b) Electronic wave extension [$W(t)$] versus time for the same values of λ as in (a).

is directly associated with the localization nature of the eigenstates [21], i.e. a bigger bandwidth means that its states are less localized, as observed in figure 2b, where a plot of the wave extension $W(t)$ is shown. In this work the wave extension is quantified by looking at the number of sites whose wave amplitude is larger than a certain cut-off. From figure 2b, we observe that $W(t) = v_s t$, where v_s is the speed of the wave front propagation. In the inset figure 2b′ we show the variation of v_s as a function of γ, which is very well approximated by

$$\langle v_s \rangle = \sqrt{\frac{\beta}{\langle m \rangle}} \tag{4}$$

represented by a solid line in figure 2b′, where $\langle m \rangle = m_A/\tau + m_B/\tau^2$ is the averaged mass and τ the golden mean. Thus, the acoustic modes only "feel" an average periodic lattice [22]. It is important to stress that the apparent increasing of v_s with γ is mainly due to the reduction of $\langle m \rangle$, instead of an effect of quasiperiodicity.

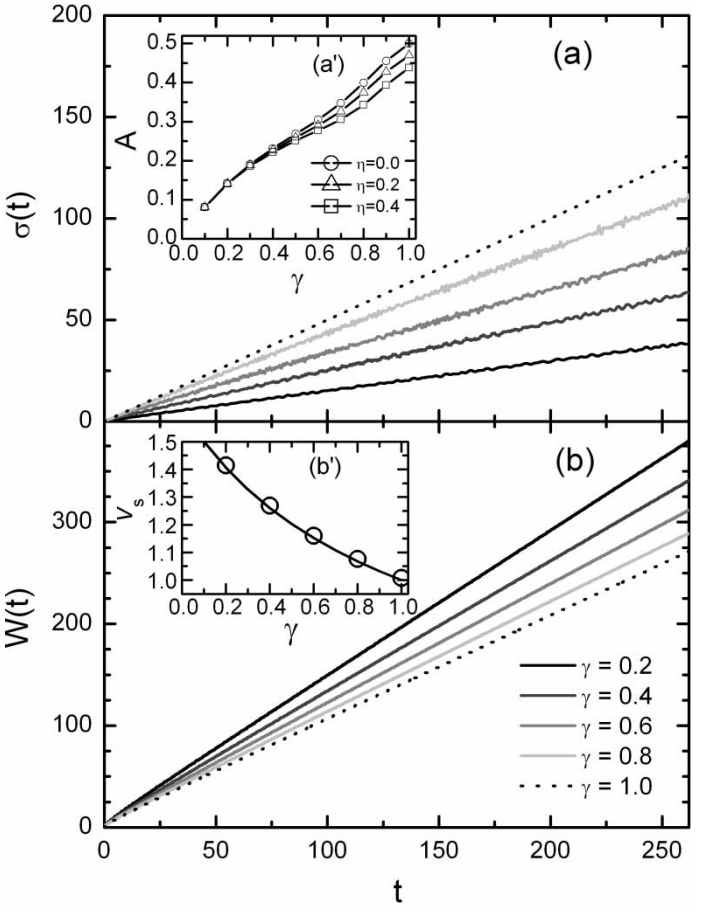

Figure 2. (a) Time evolution of the wave-packet variance for phonons in a chain of 10 946 sites without inharmonic interactions, for different values of the quasiperiodic strength characterized by the mass ratio $\gamma = m_A/m_B$. The data follow a linear relation of the type $\sigma(t) = At$. Inset (a′): values of the constant A as a function of γ for different values of the nonlinear perturbation, η. (b) Wave extension $[W(t)]$ for phonons versus time for the same values of γ as in (a). All these data can be fitted with $W(t) = v_s t$. Inset (b′): v_s for different values of γ (open circles), in comparison with the averaged sound velocity $\langle v_s \rangle$ (solid line) defined in equation (4).

In contrast, for the electron case, $W(t)$ does not grow linearly with t and it diminishes with the quasiperiodicity strength, as shown in figure 1b.

Finally, we study the effects of nonlinear perturbations (η) on the phonon dynamics. For this case, the linear dependence of $\sigma(t)$ on time persists, where the slope A decreases as the non-linearity grows, as illustrated in the inset figure 2a′. This fact can be understood as a consequence of intrinsic localization induced by the presence of quartic terms [8], i.e. it leads to a larger effective spring constant and a decreased transmittance, as obtained within the rotating wave approximation [15]. In general, the presence of nonlinear interactions produces a transfer of vibrational energy towards higher frequency modes which usually

are more localized in systems with disorder. Recently, we have observed that this tendency is enhanced in quasiperiodic systems [14].

3. Conclusions

We have studied the electron and phonon diffusion in harmonic and inharmonic 1D quasiperiodic systems. For harmonic Hamiltonians, our results show that there are clear differences between the electron and phonon cases. In the latter, the diffusivity scales linearly with time, whose slope depends upon the strength of the quasiperiodicity. On the other hand, the electronic diffusivity follows a power law. We propose that this qualitative difference in diffusion behaviours is caused by the fractal dimension of the spectrum in the low frequency region. For the case of small nonlinearities, phonon diffusion still scales linearly with time, although the corresponding diffusivity is smaller than in the harmonic case. Finally, it would be worth mentioning that for systems with two possible nearest-neighbour distances, arranged following the Fibonacci sequence, there are in consequence two different spring constants and the results are essentially the same as those presented in this paper, i.e. the nature of diffusion is dominated by acoustic modes, in spite of the differences in the details of their band structures.

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