ac conductivity of the transparent states in Fibonacci chains

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The electrical transport in quasiperiodic systems at zero temperature is studied by means of the Kubo-Greenwood formula within a tight-binding model. Their dc conductivity is compared with that obtained from the Landauer formula. Special attention is paid to the transparent states, whose transmittance is unity. The ac conductivity of these states shows a rapid diminution as a function of the frequency, in comparison with that of periodic systems. Minima in these conduction spectra are observed, which are located at $(N-1)\hbar\omega=4n\pi|t|$ for the periodic case. Finally, the localization of the eigenstates is analyzed by looking at the Lyapunov exponent and the participation ratio. The latter is shown to be an inappropriate quantity to characterize the critically localized states.

I. INTRODUCTION

The quantum transport in aperiodic systems is an open and interesting problem. In particular, the relationship between the exotic localization of states and the anomalous transport phenomena is not fully understood.[1] Since the discovery of the quasicrystals, considerable effort has been expended in the study of their localization properties.[2] It has been established that both electronic and phonon spectra of Fibonacci chains or Fibonacci superlattices are of Cantor set with zero Lebesgue measure and the corresponding eigenstates are critical.[3–7] Thus, the electronic conduction in quasiperiodic structures is not expected to be ballistic as in a periodic lattice neither diffusive as in a disordered one.[6] The hopping conductivity in Fibonacci chains has been addressed by using the Miller-Abrahams equations[8,9] and by the dc Kubo-Greenwood conductivity.[10] Recently, transparent states with unity transmission coefficient have been reported for mixing Fibonacci systems (MFS) of N atoms.[11] However, their localization nature is still controversial. It is observed that the eigenfunctions of these transparent states, with energies satisfying $E=\alpha(1+\gamma^2)/(1-\gamma^2)$ and $E^2-\alpha^2=4\,t^2\cos^2(K\pi/N)$, are periodiclike wave functions,[12] where $+\alpha(-\alpha)$ are the on-site energies of atoms $A(B)$, $\gamma=t_{AA}/t_{AB}$ is the ratio of the hopping parameters, K and N/K are integer numbers. On the other hand, the ac conductivity of these transparent states is an unclear issue. In general, the ac electrical conductivity at zero temperature is a good probe of the nature of the electronic eigenvalue spectrum and the localization of wave functions, since it depends not only on the states at the Fermi level but also on the global structure of the spectrum.

A general quantum mechanical expression, within the linear response approximation, for calculating the real part of the electrical conductivity for finite temperature (T) and frequency (ω) is given by the Kubo-Greenwood formula[13]

$$\sigma(\mu,\omega,T)=\lim_{\Omega\to\infty}\frac{2e^2\hbar}{\pi\Omega m^2}\int_{-\infty}^{\infty}dE\,\frac{f(E)-f(E+\hbar\omega)}{\hbar\omega}\times\mathrm{Tr}[p\,\mathrm{Im}\,G^+(E+\hbar\omega)p\,\mathrm{Im}\,G^+(E)],\quad(1)$$

where Ω is the volume of the system, p is the projection of the momentum operator along the applied electric-field direction, $G^+(E)$ is the retarded one-particle Green's function, and $f(E)$ is the Fermi-Dirac distribution with Fermi energy μ and temperature T. In this paper, the ac conductivity of the transparent states at zero temperature is addressed by evaluating Eq. (1).

The present paper is organized as follows. Section II defines the system and the Hamiltonian. An analytical solution of the Kubo conductivity for a periodic linear chain is also given. In Sec. III, the dc-conductivity numerical results for quasiperiodic systems are compared with the transmittance and the localization spectra. In Sec. IV, the frequency dependence of the transparent-state conductivity is reported. Particularly, the ac conductivity in the low-frequency regime is analyzed in detail. Finally, some conclusions and possible extensions of the model are given in Sec. V.

II. THE MIXING FIBONACCI SYSTEM

There are several ways to generate a Fibonacci system, for example, by using two hopping strengths (bond problem) or two sorts of atoms (site problem). In this paper, we consider a MFS, 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 generation $F_2=BA$, the next generations are given by $F_n=F_{n-1}\oplus F_{n-2}$. For instance, $F_5=BAABABAA$. In particular, this sequence is chosen in order to obtain the transparent states reported in Refs. 11,12. In the MFS, the hopping integrals between atoms depends on the nature of them, contrary to the same hopping in the site problem, giving rise to the existence of two different parameters t_{AA} and $t_{AB}=t_{BA}$. For the sake of simplicity, a uniform bond length (a) is considered.

In order to isolate the quasicrystalline effects on the physical properties of the system, we consider a simple s-band tight-binding Hamiltonian, which can be written as

$$H=\sum_j\{\epsilon_j\;|j\rangle\langle j|+t_{j,j+1}\;|j\rangle\langle j+1|+t_{j,j-1}\;|j\rangle\langle j-1|\},\quad(2)$$

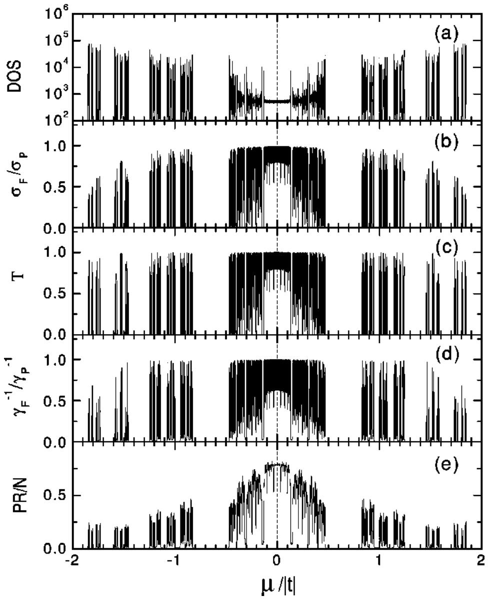

FIG. 1. (a) Density of states (DOS), (b) Kubo conductivity (σ_F), (c) transmittance (T), (d) Inverse of the Lyapunov exponent (γ_F^{-1}), and (e) participation ratio (PR) for a mixing Fibonacci system of 2584 atoms with $\epsilon_A=\epsilon_B=0$, $t_{AB}=t_{BA}=t$, and $t_{AA}=(\sqrt{5}-1)t/2$. The system is saturated by two semi-infinite periodic linear chains with $\epsilon=0$ and hopping integrals t. σ_F and γ_F^{-1} are normalized by their respective σ_P and γ_P^{-1} of a periodic chain. The transparent state ($\mu=0$) is indicated by a dashed line.

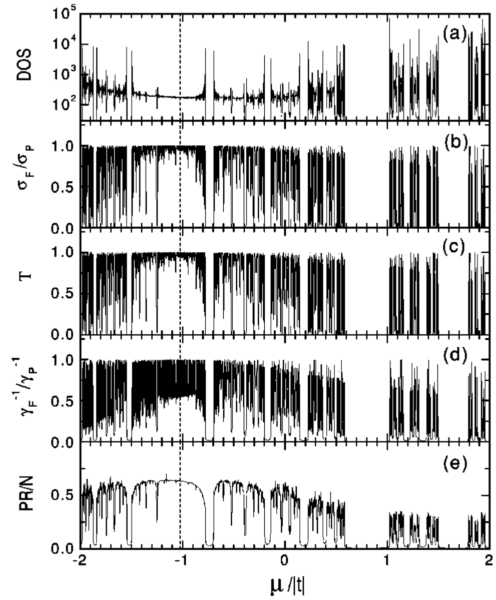

FIG. 2. (a) Density of states (DOS), (b) Kubo conductivity (σ_F), (c) transmittance (T), (d) Inverse of the Lyapunov exponent (γ_F^{-1}), and (e) participation ratio (PR) for a mixing Fibonacci system of 987 atoms with $\epsilon_A=-\epsilon_B=0.225|t|$, $t_{AA}=1.25t$, and $t_{AB}=t_{BA}=t$. The system is also connected to two semi-infinite periodic linear chains with $\epsilon=0$ and hopping integrals t. In this case, the transparent state is located at $\mu=-1.025|t|$, and indicated by a dashed line. σ_F and γ_F^{-1} are normalized by their respective σ_P and γ_P^{-1} of a periodic chain.

where ϵ_i denote the on-site energies ϵ_A (ϵ_B) and $t_{i,j}$ are the corresponding hopping parameters. To evaluate the Kubo-Greenwood formula, Eq. (1), one needs the Green's function[14] and the momentum operator (p). The latter can be determined by using the relations $p=(im/\hbar)[H,x]$ and $x=\Sigma_j ja|j\rangle\langle j|$. Thus, in the Wannier representation, we have

$$p=\frac{ima}{\hbar}\sum_j \{t_{j,j+1}|j\rangle\langle j+1|-t_{j,j-1}|j\rangle\langle j-1|\}. \tag{3}$$

For instance, in the case of an infinite periodic linear chain with on-site energy ϵ_0 and hopping parameter t, the one-particle retarded Green's function is given by[14]

$$G^+_{l,m}(E)=\frac{ie^{i\theta|l-m|}}{2|t|\sin\theta}, \tag{4}$$

where $\cos\theta=(E-\epsilon_0)/2|t|$. Substituting this expression into Eq. (1) and defining $\cos\theta'=(E+\hbar\omega-\epsilon_0)/2|t|$, $s(n)=\sin n\theta\sin n\theta'$, and $\nu(n)=1-\cos n\theta\cos n\theta'$, we can write, after some algebra, the following general expression for a system of N identical sites saturated by two semi-infinite periodic linear chains

$$\sigma(\mu,\omega,T)=\frac{8e^2t^2a}{\pi(N-1)\hbar^3\omega^2}\int_{-\infty}^{\infty}dE\,\frac{f(E)-f(E+\hbar\omega)}{\hbar\omega}\times\left\{\frac{1}{2}\nu(N-1)\left(\frac{\nu^2(1)}{s(1)}+s(1)\right)-s(N-1)\nu(1)\right\}, \tag{5}$$

where we have taken the system length $\Omega=(N-1)a$. In the limit of T and $\omega\rightarrow 0$, the factor $[f(E)-f(E+\hbar\omega)]/\hbar\omega$ becomes to $\delta(E-\mu)$, where μ is the Fermi energy. Therefore, the dc conductivity of a periodic linear chain within the energy band is

$$\sigma_p=\frac{e^2a}{\pi\hbar}(N-1). \tag{6}$$

Notice that this conductivity is not dependent on the Fermi energy. Moreover, in the thermodynamic limit the dc conductivity of a periodic linear chain at zero temperature diverges, because in this case the electrical conduction is ballistic and then the mean free path is as large as the size of the system.[15] However, for quasiperiodic systems the mean free path is bounded, except for the transparent states, which have a transmission coefficient of unity and their Landauer scatterer resistance of the system becomes zero.[15] In the next section, some characteristic quantities of the localization and the dc electrical conductivity of these transparent states are comparatively investigated.

III. dc CONDUCTIVITY

Let us consider a finite MFS, connected to two semi-infinite periodic linear chains with hopping integrals t and null on-site energies. Its electrical conductivity can be studied by means of the Kubo-Greenwood formula, in which the Green's function is calculated with the mentioned boundary conditions and the trace in Eq. (1) is taken over the Fibonacci system. Figure 1(a) shows the density of states (DOS), in logarithmic scale, of a MFS of generation $n=17$

with 2584 atoms, in which $\epsilon_A=\epsilon_B=0$, $t_{AA}=(\sqrt{5}-1)t/2$, and $t_{AB}=t_{BA}=t$. Observe that this spectrum shows many fine structures, since it contains 100 000 data and the imaginary part of the energy in the Green's function is $10^{-7}|t|$. The zero-temperature dc Kubo conductivity of the same Fibonacci system as Fig. 1(a) (σ_F) is calculated by means of Eq. (1) and presented in Fig. 1(b) in units of that for a periodic linear chain (σ_p) given by Eq. (6). Notice that there are many states having an electrical conductivity very close to that of a periodic system, and a more detailed analysis reveals that the normalized Kubo conductivity (σ_F/σ_p) of the state at $\mu=0$ is exactly unity, which confirms that it is a transparent state as reported by Maciá and Domínguez-Adame.[11] It is worth mentioning that the double-precision numerical results do not show any other transparent states, despite that the normalized Kubo conductivity of many eigenstates is larger than 0.99999.

On the other hand, the transmittance of the system (T) can be written as[1,16]

$$T(E)=\frac{4-(E/t)^2}{[\tau_{21}-\tau_{12}+(\tau_{22}-\tau_{11})E/2t]^2+(\tau_{22}+\tau_{11})^2(1-E^2/4t^2)}, \tag{7}$$

in which

$$\begin{pmatrix} c_{N+1} \\ c_N \end{pmatrix}=\begin{pmatrix} \tau_{11} & \tau_{12} \\ \tau_{21} & \tau_{22} \end{pmatrix}\begin{pmatrix} c_1 \\ c_0 \end{pmatrix}=\prod_{i=1}^{N}\begin{pmatrix} \dfrac{E-\epsilon_i}{t_{i,i+1}} & -\dfrac{t_{i,i-1}}{t_{i,i+1}} \\ 1 & 0 \end{pmatrix}\begin{pmatrix} c_1 \\ c_0 \end{pmatrix}, \tag{8}$$

where c_i are the normalized amplitudes of the wave function (Ψ), i.e., $\Psi=\Sigma_{i=1}^{N}c_i|i\rangle$ and $\Sigma_{i=1}^{N}|c_i|^2=1$. Figure 1(c) shows the transmittance (T) calculated for a MFS as in Fig. 1(a). Observe that there is a remarkable similarity between Figs. 1(b) and 1(c), since the electrical conductance is proportional to the transmission coefficient via the Landauer formula.[17] The difference between these two spectra seems to be originated from the small imaginary part ($10^{-7}|t|$) included in the calculation of the Kubo conductivity through the Green's function.

The localization of the eigenstates is studied by looking at the Lyapunov exponent (γ) and the participation ratio (PR), which can be written, respectively, as[13]

$$\gamma=\frac{1}{N}\ln\sqrt{\tau_{11}^2+\tau_{12}^2+\tau_{21}^2+\tau_{22}^2} \quad \text{and} \quad PR=\left(\sum_{i=1}^{N}|c_i|^4\right)^{-1}. \tag{9}$$

The inverse of the Lyapunov exponent, calculated for a MFS as in Fig. 1(a) and normalized with respect to that of a periodic chain, is presented in Fig. 1(d). Notice its remarkable coincidence with Figs. 1(b) and 1(c), which is somewhat expected.[18] However, the participation ratio for this system shown in Fig. 1(e) differs clearly from the spectra Fig. 1(b), Fig. 1(c), and Fig. 1(d), which indicates that the PR is not a good quantity to characterize critical states.

Finally, the same analysis as in Fig. 1 is applied to another MFS, in which $\epsilon_A=0.225|t|$, $\epsilon_B=-0.225|t|$, $t_{AA}=1.25t$, and $t_{AB}=t_{BA}=t$. In this case, the transparent state is located at $\mu=-1.025|t|$ for generations $n=4l+3$, being l a positive integer.[12] The results of this analysis are shown in Fig. 2 for a MFS of generation $n=15$ with 987 atoms. First, notice that the spectra lose the symmetry around $\mu=0$, since the lattice is not bipartite. On the other hand, the general behavior observed in Fig. 1 is also present in Fig. 2. In particular, the density of states around the transparent state, indicated by the dashed line in the figures, resembles that of a periodic linear chain.

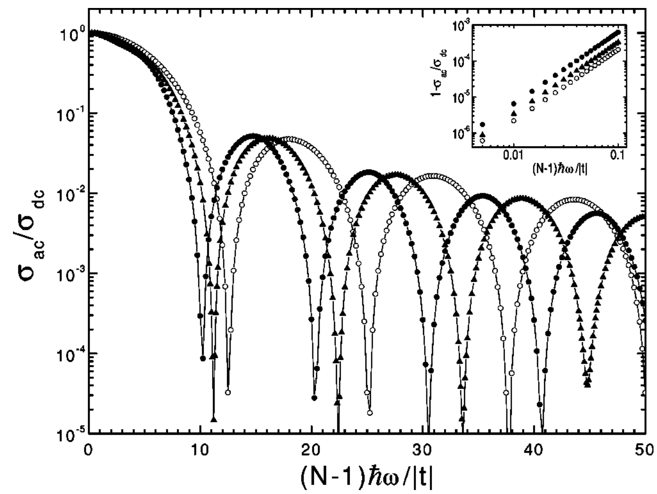

FIG. 3. Transparent-state ac conductivity of a periodic chain (open circles) and of two mixing Fibonacci systems (solid circles and solid triangles) with the same parameters as in Figs. 1 and 2, respectively. In the inset a low-frequency-regime log-log plot of the ac conductivity is shown.

IV. ac CONDUCTIVITY

It is interesting to study the behavior of the transparent states under perturbations such as the application of oscillating external fields, since the ac conductivity is very sensitive to the distribution nature of eigenvalues and the localization of wave functions close to the Fermi energy. In Fig. 3 the ac conductivity of the same two MFS as in Figs. 1 and 2 for μ at the transparent-state energies is shown, in comparison with the *universal* ac-conductivity spectrum of the periodic case obtained from Eq. (5), since it remains the same for any value of N. Notice first that, in general, the conductivity diminishes as the frequency increases, as reported by Albers and Gubernatis for periodic and disordered systems.[19] Furthermore, several minima of the ac conductivity are observed. For the periodic case, they are located at $(N-1)\hbar\omega=4n\pi|t|$, being n an integer number. These frequencies can be obtained from the analytical solution [Eq. (5)], by considering $|E|/2|t|<\hbar\omega/2|t|\ll 1$ for $\mu=0$ and retaining only their linear terms in the Taylor expansion, i.e.,

$$\begin{aligned}\frac{1}{2}\nu(N-1)\left(\frac{\nu^2(1)}{s(1)}+s(1)\right)-s(N-1)\nu(1) &\cong 1-\cos(N-1)\phi\cos(N-1)\phi' \\ &\quad -\sin(N-1)\phi\sin(N-1)\phi' \\ &=0,\end{aligned} \tag{10}$$

where $\phi = E/2|t|$ and $\phi' = (E+\hbar\omega)/2|t|$. On the other hand, in logarithmic scale, it is observed that the diminution of the quasiperiodic case is faster than that of periodic one, a behavior directly related to the nontransparency of the states around the transparent ones. Furthermore, an almost constant separation of the minima is found for the MFS, similar to the periodic case. This fact could be due to the nearly constant density of states close to the transparent states shown in Figs. 1(a) and 2(a).

In particular, for the low-frequency regime the ac conductivity of a periodic linear chain can be obtained analytically from Eq. (5) after performing a Taylor expansion,

$$\sigma_p(\omega) = \sigma_p\left\{1 - \frac{1}{48}\left[\frac{(N-1)\hbar\omega}{|t|}\right]^2\right\}. \tag{11}$$

For the quasiperiodic case, the exponent in Eq. (11) remains unchanged, as shown in the inset of Fig. 3. Nevertheless, the MFS have larger curvatures, i.e., coefficients of 0.06025 and 0.03311 for the systems analyzed in Figs. 1 and 2, respectively, instead of $\frac{1}{48}$ for the periodic case. It would be worth mentioning that for the low-frequency regime a smaller imaginary part ($10^{-10}|t|$) of the energy in the Green's function and quadruple precision calculation are needed. On the other hand, for the high-frequency regime the ac conductivity of both periodic and quasiperiodic systems diminishes rapidly as the frequency increases.

V. CONCLUSIONS

In summary, we have studied the ac conduction of transparent states in the MFS. In spite of having the same dc conductivity as the ordered lattice, the transparent states of MFS do not have the same behavior under an oscillatory electrical field, i.e., their ac conduction decreases much faster than those of the crystalline case. On the other hand, the analysis of the dc electrical transport shows that the participation ratio does not accurately quantify the transport capacity of the critically localized states, since it indicates only the fraction of contributing sites to the wavefunction, and does not specify their spatial distribution.

For the ac case, the rapid diminution of the transparent-state ac conductivity is a general feature in the MFS, since they are isolated in the spectrum,[11] i.e., they are always surrounded by non-transparent states, and the ac conductivity involves states within an interval of $\hbar\omega$ around the Fermi energy. On the other hand, oscillatory length-dependent conductivities have been found by Sokoloff for both periodic and quasiperiodic chains.[20] This fact can be obtained from Fig. 3 by fixing a frequency and changing the system length. Moreover, the almost null ac-conductivity observed at certain frequencies in Fig. 3 is expected to be a strict one-dimensional behavior, since for three-dimensional systems an integration over the first Brillouin zone of the k-space perpendicular to the applied electrical field is required. Therefore, a smooth variation is obtained.[21] In addition, if fluctuations such as the Peierls distortion are considered, the dc conductivity of one-dimensional metals should vanish at $T=0K$. It would be worth mentioning that if free boundary conditions, i.e., without the semi-infinite saturators, are chosen, the ac conductivity becomes a spectrum of peaks,[22] where resonances[23] and wave function-symmetry selection rules are present. Finally, an important extension to this work is the temperature-dependence analysis of the transparent-state ac conductivity including phonon participation, which is currently in progress.

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