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AC Conduction in Quasiperiodic Lattices

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ABSTRACT

The electronic transport in Fibonacci lattices at zero temperature is studied by means of the Kubo-Greenwood formula within the tight-binding scheme, where a renormalization process capable to address the electrical conductivity in macroscopic quasiperiodic systems is used. The effects of the Fermi-energy location on the *ac* conductivity are analyzed in detail for a wide range of the system sizes. Special attention is paid to the transparent states, whose transmission coefficient is unity. The results show a rapid decay of their *ac* conductivity as the frequency increases in comparison with that of periodic systems, and the spectra scale with the inverse of the system size as occur in periodic ones, where analytical results are obtained. Furthermore, a new low-frequency minimum appears when the inhomogeneity of the Fibonacci lattice grows.

INTRODUCTION

The localization and transport of electrons in quasiperiodic systems have been an interesting and controversial issue, since the discovery of quasicrystalline alloys in 1984. Nowadays, there is a consensus that the eigenvalue spectrum produced by a quasiperiodic potential is singular continuous and the associated eigenfunctions are critical [1]. Moreover, the level statistics show an inverse-power-law level-spacing distribution [2], neither Wigner nor Poisson ones. Hence, the electrical conduction of these critically localized states becomes an especially interesting subject. In particular, Fibonacci quasiperiodic superlattices have been built [3] and their properties can be well understood by means of simple models [4]. The hopping conductivity in Fibonacci chains has been addressed by using the Miller-Abrahams equations [5] and the optical conductivity has been analyzed recently within a generalized Drude formula [6]. On the other hand, *transparent states* with unity transmission coefficient have been found [7] in mixing Fibonacci systems (MFS) and their *ac* conductivity has been studied by using the Kubo-Greenwood formula [8]. In general, a good probe of the nature of the electronic eigenvalue spectrum and the localization of wave functions is the *ac* electrical conductivity at zero temperature, since it depends not only on the states at the Fermi level but also on the global structure of the spectrum. In Ref. [8] the electrical conductivity for two different MFS with k=2 and 3, as defined in Ref. [9], has been studied. However, the effects of the Fermi-energy location and the system inhomogeneity on the *ac* conductivity are not widely analyzed in the literature. In this work, we investigate three different MFS within k=3 and report a system-size scale invariance and a new minimum of the Fibonacci *ac* conductivity which deepens when the system becomes more inhomogeneous.

DENSITY OF STATES AND DC CONDUCTIVITY

A mixing Fibonacci system (MFS) is built by alternating two sorts of atoms A and B following the Fibonacci sequence ($F_n=F_{n-1}\oplus F_{n-2}$) and the hopping integral between atoms depends on the nature of them. In this work, the first two generations are chosen as F_1=A and F_2=BA, and then, for example, F_4=BAABA. The energies of the transparent states in these systems should satisfy [9] $E=\alpha(1+\gamma^2)/(1-\gamma^2)$ and $E^2-\alpha^2=4t^2\cos^2(k\pi/N)$, where α ($-\alpha$) are the self-energies of atoms A (B), $\gamma=t_{AA}/t_{AB}$ is the ratio of the hopping parameters, k and N/k are integer numbers. A single *s*-band tight-binding Hamiltonian is considered in order to isolate the quasicrystalline effects.

The *ac* electrical conductivity of a one-dimensional system at zero temperature can be calculated by means of the Kubo-Greenwood formula [10]

$$\sigma(E_F,\omega)=\frac{2e^2\hbar}{L\pi m^2\hbar\omega}\int_{E_F-\hbar\omega}^{E_F}\mathrm{Tr}\left[p\,\mathrm{Im}G^+(E+\hbar\omega)\,p\,\mathrm{Im}G^+(E)\right]dE\,, \tag{1}$$

where L is the system length, p is the linear momentum operator, $G^+(E)$ is the retarded one-particle Green's function, and Tr indicates the trace of the matrix. For a periodic linear chain of N atoms saturated by two semi-infinite periodic chains, the *dc* conductivity within the energy band is [see Eq.(A4) in Appendix]

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

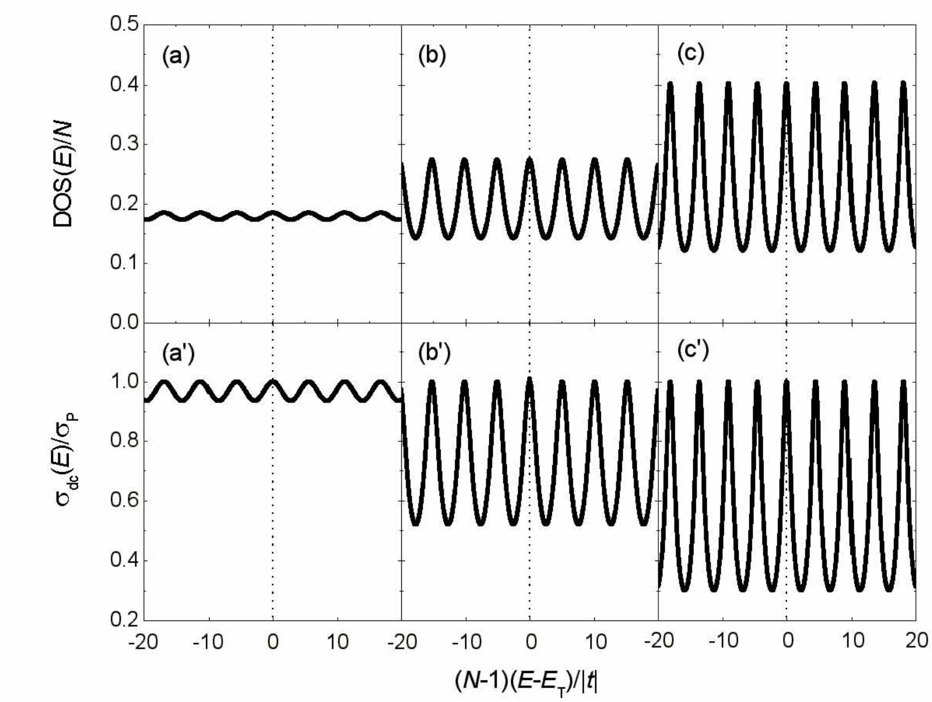

Figure 1. *The density of states (DOS) around the transparent states (E_T), indicated by dashed lines, and the dc Kubo conductivity (σ_{dc}) are shown for three N-atom mixing Fibonacci systems: (a, a') $\alpha=0.225|t|$, $\gamma=1.25$, $E_T=-1.025|t|$, (b, b') $\alpha=0.75|t|$, $\gamma=2.0$, $E_T=-1.25|t|$, and (c, c') $\alpha=1.05|t|$, $\gamma=2.5$, $E_T=-1.45|t|$. All these systems are saturated by two semi-infinite periodic linear chains with hopping integrals t and null self-energies.*

In figure 1, an amplification of the density of states (DOS) around the transparent states and the *dc* Kubo conductivity (σ_{dc}) are comparatively shown for three MFS: (a, a') $\alpha=0.225|t|$, $\gamma=1.25$, $E_T=-1.025|t|$, (b, b') $\alpha=0.75|t|$, $\gamma=2.0$, $E_T=-1.25|t|$, and (c, c') $\alpha=1.05|t|$, $\gamma=2.5$, $E_T=-1.45|t|$, where E_T is the transparent-state energy, indicated by dashed lines in the figure. In the three cases the MFS have $k=3$, *i.e.*, their size, N, is multiple of 3 [9], and they are saturated by two semi-infinite periodic linear chains with hopping integrals t and null self-energies. The DOS is calculated by means of $\mathrm{DOS}(E)=-\mathrm{Im}[\mathrm{Tr}\,G^+(E)]/\pi$, and the imaginary part of the energy in the Green's function is $10^{-10}|t|$. By using a renormalization method [11], we have checked that the curves in Fig. 1 close to the transparent states remain the same for MFS containing 6765, 317811, and 102334155 atoms, *i.e.*, they scale with the inverse of the system size. Likewise, oscillations in both DOS(E) and $\sigma_{dc}(E)$, contrary to the periodic case, are observed. The location of the maxima in these oscillations can be obtained by a perturbation analysis of the transparent-state condition, given in Ref. [9]. It should be mentioned that the normalized *dc* conductivity, σ_{dc}/σ_p, is strictly unity only for the transparent state located at $E=E_T$. Notice also that the amplitude and the frequency of these oscillations increase as the system inhomogeneity is enhanced, *i.e.*, when the parameters α and γ increase.

AC CONDUCTIVITY

In figure 2, we show the *ac* Kubo conductivity [$\sigma(\omega)$] calculated using equation (1) with $E_F=E_T$ for the same three MFS as in figure 1 in comparison with that of the periodic case (open circles), where open pentagons, open squares, and open triangles correspond to the systems of figures 1(a), 1(b), and 1(c), respectively. For the periodic case, the *ac* conductivity at $E_F=0$ is given by Eq. (A3). Notice that when α and γ increase, the minima of $\sigma(\omega)$ move toward lower frequencies, and a new minimum appears and deepens in the low frequency regime. The depth of this low-frequency minimum could be related to the oscillating amplitude observed in DOS(E) and $\sigma_{dc}(E)$ (Fig. 1).

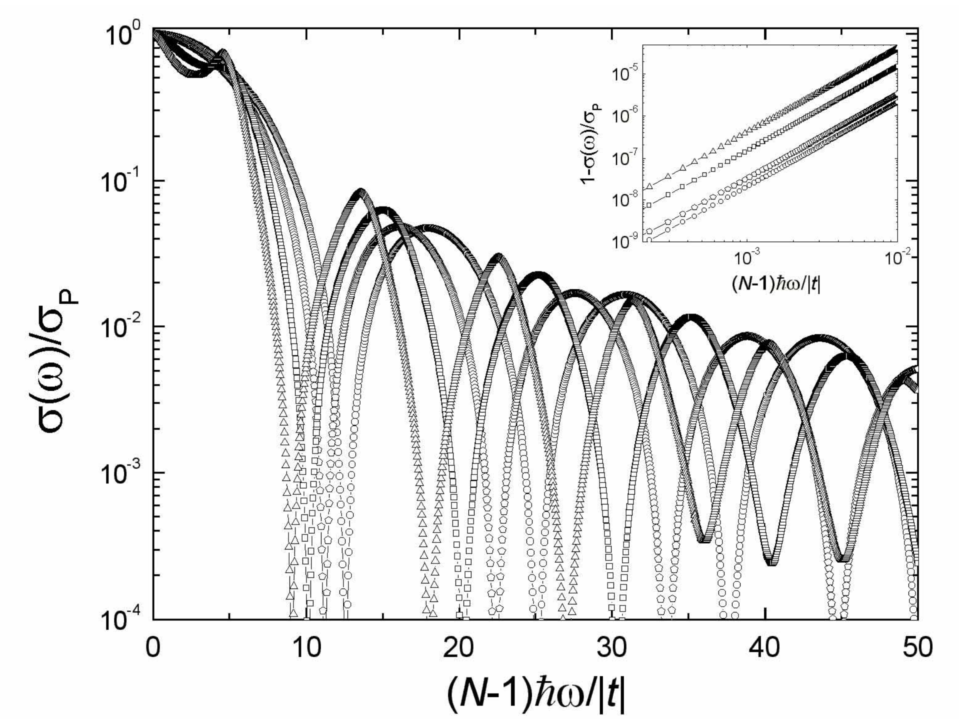

Figure 2. *The ac conductivities [$\sigma(\omega)$] of three MFS indicated by open pentagons, open squares, and open triangles, with the same parameters as in figures 1(a), 1(b) and 1(c), respectively, in comparison with that of a periodic chain (open circles). In the inset a low-frequency log-log plot of $\sigma(\omega)$ is shown.*

In the insert of figure 2, we show a log-log plot of the *ac* conductivity in the low frequency limit, where the numerical calculations were performed in quadruple precision and the imaginary part of the energy in the Green's function is $10^{-14}|t|$, instead of $10^{-10}|t|$ used in the main part of figure 2. For the periodic case, the *ac* conductivity in this limit is given by Eq. (A4). Now, for MFS, in spite of the appearance of the low-frequency minimum, their $\sigma(\omega)$ follows essentially the same relationship of the periodic case, except that the MFS have larger curvatures, *i.e.*, coefficients of 0.03311, 0.14983, and 0.41299 for the systems analyzed in figures 1(a), 1(b), and 1(c), respectively, instead of 1/48 for the periodic case [Eq. (A4)]. It is worth mentioning that the normalized *ac* conductivity of MFS also scales with the inverse of the system size, as found for the periodic case [8].

CONCLUSIONS

The frequency dependence of the transparent-state electrical conductivity in MFS with k=3 has been analyzed in detail. An oscillating behavior around the transparent state has been found for both the density of states and the *dc* conductivity. The amplitude of these oscillations increase when the inhomogeneity of the system is enhanced, *i.e.*, when α and γ grow. Likewise, the *ac* conductivity of MFS present an oscillatory behavior similar to that observed in the periodic chain, except for the appearance of a new minimum in the low-frequency regime, which could be related to the oscillations of the *dc* conductivity around the transparent states. Finally, an universal behavior is observed in $\sigma(\omega)$ of MFS, where the normalized $\sigma(\omega)$ scales with the inverse of the system size in the same way as in the periodic chains.

APPENDIX. ANALYTICAL SOLUTION FOR PERIODIC SYSTEMS

In this section we calculate the Kubo conductivity for a periodic chain of N atoms, with lattice constant a, null self-energies and hopping integral t, saturated by two semi-infinite periodic chains with the same parameters. The linear momentum operator for this case is given by

$$p = \frac{imat}{\hbar}\sum_i \left\{ |i\rangle\langle i+1| - |i\rangle\langle i-1| \right\}.$$

We define

$$g_{i,j} \equiv \mathrm{Im}\langle i|G^+(E)|j\rangle \quad \text{and} \quad g'_{i,j} \equiv \mathrm{Im}\langle i|G^+(E+\hbar\omega)|j\rangle,$$

then,

$$\mathrm{Tr}\left[p\,\mathrm{Im}G^+(E+\hbar\omega)\,p\,\mathrm{Im}G^+(E)\right] = -\frac{m^2a^2t^2}{\hbar^2}\left(S_1 - S_2 - S_3 + S_4\right),$$

where

$$S_1 \equiv \sum_{i=1}^{N-1}\sum_{j=1}^{N-1} g_{i+1,j}\,g'_{j+1,i},\ S_2 \equiv \sum_{i=1}^{N-1}\sum_{j=2}^{N} g_{i+1,j}\,g'_{j-1,i},\ S_3 \equiv \sum_{i=2}^{N}\sum_{j=1}^{N-1} g_{i-1,j}\,g'_{j+1,i},\ \text{and}\ S_4 \equiv \sum_{i=2}^{N}\sum_{j=2}^{N} g_{i-1,j}\,g'_{j-1,i}. \quad \text{(A1)}$$

The Green's function for an infinite periodic chain can be written as [12]

$$G_{\ell,m} = \frac{i}{2|t|\sin\theta}e^{i|\ell-m|\theta},$$

where

$$\cos\theta \equiv x \equiv \frac{E-\varepsilon_0}{2t}, \quad \text{and} \quad \sin\theta \equiv -\sqrt{1-x^2}\ .$$

Thus,

$$S_1=\frac{\sum_{i=1}^{N-1}\cos\theta\cos\theta'+\sum_{i=1}^{N-1}\sum_{j<i}\cos(|i-j+1|\theta)\cos(|j-i+1|\theta')+\sum_{i=1}^{N-1}\sum_{j>i}\cos(|i-j+1|\theta)\cos(|j-i+1|\theta')}{4t^2\sin\theta\sin\theta'},\quad \text{(A2)}$$

where $\cos\theta'\equiv x'\equiv\frac{E+\hbar\omega-\varepsilon_0}{2t}$ and $\sin\theta'\equiv-\sqrt{1-(x')^2}$. The first sum in Eq. (A2) gives

$$\sum_{i=1}^{N-1}\cos\theta\cos\theta'=(N-1)\cos\theta\cos\theta'=\tfrac{1}{2}(N-1)(\cos\gamma_1+\cos\gamma_2),$$

where $\gamma_1\equiv\theta+\theta'$ and $\gamma_2\equiv\theta-\theta'$. To evaluate the second sum in Eq. (A2), we define

$$\Sigma(\theta,\theta')\equiv\sum_{i=1}^{N-1}\sum_{j<i}\cos(|i-j+1|\theta)\cos(|j-i+1|\theta')=\sum_{n=1}^{N-2}(N-1-n)\cos[(n+1)\theta]\cos[(n-1)\theta']=\tfrac{1}{2}\left(S^{1,2}+S^{2,1}\right)$$

where

$$S^{a,b}\equiv\sum_{n=1}^{N-2}(N-1-n)\cos(n\gamma_a+\gamma_b)=\mathrm{Re}\left\{\sum_{n=1}^{N-2}\left[(N-1)e^{i(n\gamma_a+\gamma_b)}-ne^{i(n\gamma_a+\gamma_b)}\right]\right\}$$

$$=\mathrm{Re}\left\{(N-1)e^{i\gamma_b}\left[\frac{1-e^{i(N-1)\gamma_a}}{1-e^{i\gamma_a}}-1\right]+e^{i\gamma_b}\,\frac{-(N-1)e^{i(N-1)\gamma_a}+(N-2)e^{iN\gamma_a}+e^{i\gamma_a}}{\left(1-e^{i\gamma_a}\right)^2}\right\}.$$

Likewise, the third term is

$$\sum_{i=1}^{N-1}\sum_{j>i}\cos(|i-j+1|\theta)\cos(|j-i+1|\theta')=\sum_{n=1}^{N-2}(N-1-n)\cos[(n-1)\theta]\cos[(n+1)\theta']=\Sigma(\theta',\theta),$$

and the sum of these last two terms in Eq. (A2) can be written as

$$\Sigma(\theta,\theta')+\Sigma(\theta',\theta)$$
$$=\cos\gamma_2\,\frac{-2(N-1)\cos^2\gamma_1+(4N-6)\cos\gamma_1+(-2N+4)+\cos N\gamma_1+\cos(N-2)\gamma_1-2\cos(N-1)\gamma_1}{4(1-\cos\gamma_1)^2}$$
$$+\cos\gamma_1\,\frac{-2(N-1)\cos^2\gamma_2+(4N-6)\cos\gamma_2+(-2N+4)+\cos N\gamma_2+\cos(N-2)\gamma_2-2\cos(N-1)\gamma_2}{4(1-\cos\gamma_2)^2}.$$

Therefore,

$$S_1=\frac{1}{4t^2\sin\theta\sin\theta'}\left\{\frac{\cos\gamma_2[1-\cos(N-1)\gamma_1]}{2(1-\cos\gamma_1)}+\frac{\cos\gamma_1[1-\cos(N-1)\gamma_2]}{2(1-\cos\gamma_2)}\right\}.$$

Analogously,

$$S_2=\frac{1}{4t^2\sin\theta\sin\theta'}\sum_{i=1}^{N-1}\sum_{j=1}^{N-1}\cos(|i-j|\theta)\cos(|j-i|\theta')=\frac{1}{4t^2\sin\theta\sin\theta'}\left[(N-1)+\sum_{n=1}^{N-2}(N-1-n)(\cos n\gamma_1+\cos n\gamma_2)\right]$$
$$=\frac{1}{4t^2\sin\theta\sin\theta'}\left[\frac{1-\cos(N-1)\gamma_1}{2(1-\cos\gamma_1)}+\frac{1-\cos(N-1)\gamma_2}{2(1-\cos\gamma_2)}\right].$$

Moreover, taking advantage of the dumb indexes in the definition of S_3 [Eq. (A1)], we found S_3 is almost the same as S_2, except that θ and θ' are exchanged. However, S_2 is an even function of γ_2, consequently, $S_3= S_2$. Analogously, $S_4= S_1$. Therefore,

$$\begin{aligned}
&\mathrm{Tr}\left[p\,\mathrm{Im}G^{+}(E+\hbar\omega)p\,\mathrm{Im}G^{+}(E)\right]\\
&=-\frac{m^2a^2}{4\hbar^2\sin\theta\sin\theta'}\frac{-(1-\cos\gamma_2)^2\left[1-\cos(N-1)\gamma_1\right]-(1-\cos\gamma_1)^2\left[1-\cos(N-1)\gamma_2\right]}{(1-\cos\gamma_1)(1-\cos\gamma_2)}\\
&=\frac{4m^2a^2t^2}{\hbar^4\omega^2}\left\{\begin{array}{l}\frac{1}{2}\left[1-\cos(N-1)\theta\cos(N-1)\theta'\right]\left[\frac{(1-\cos\theta\cos\theta')^2}{\sin\theta\sin\theta'}+\sin\theta\sin\theta'\right]\\ -\sin(N-1)\theta\sin(N-1)\theta'(1-\cos\theta\cos\theta')\end{array}\right\}.
\end{aligned}$$

For the case of null Fermi energy (E_F=0) and low frequencies of the applied electrical field, we have $|E|/2|t|<\hbar\omega/2|t|<<1$. Hence, performing a Taylor expansion in the last equation we obtain

$$\mathrm{Tr}\left[p\,\mathrm{Im}G^{+}(E+\hbar\omega)p\,\mathrm{Im}G^{+}(E)\right]\approx\frac{4m^2a^2t^2}{\hbar^4\omega^2}\left\{1-\cos\left[(N-1)\frac{\hbar\omega}{2|t|}\right]\right\};$$

consequently,

$$\sigma(\omega)=\frac{2e^2\hbar}{L\pi m^2\hbar\omega}\int_{-\hbar\omega}^{0}dE\,\mathrm{Tr}\left[p\,\mathrm{Im}G^{+}(E+\hbar\omega)p\,\mathrm{Im}G^{+}(E)\right]=\frac{8\,t^2e^2a}{(N-1)\pi\,\hbar^3\omega^2}\left\{1-\cos\left[(N-1)\frac{\hbar\omega}{2|t|}\right]\right\}, \quad \text{(A3)}$$

where the system length is $L=(N-1)a$. Finally, in the low-frequency limit, we have

$$\sigma(\omega)\approx\frac{e^2a(N-1)}{\pi\,\hbar}\left\{1-\frac{1}{48}\left[\frac{(N-1)\hbar\omega}{t}\right]^2\right\}. \quad \text{(A4)}$$

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