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Exact results of the Kubo conductivity in macroscopic Fibonacci systems: a renormalization approach

Vicenta Sánchez, Chumin Wang*

Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Apartado Postal 70-360, 04510 México D.F., Mexico

Abstract

In this work, the Kubo–Greenwood formula is used to investigate the electrical conduction in macroscopic Fibonacci lattices within a single-band tight-binding model. This investigation is carried out by means of a renormalization method, which allows the iterative evaluation of the products of the Green's function in an exact way. The results of d.c. conductivity show an extremely fine band structure and a periodic oscillating pattern in the neighborhood of the transparent state. The a.c. conductivity of these transparent states as a function of the frequency shows a regular oscillating behavior, whose maximums decay following an inverse power law. Furthermore, the d.c. conduction in two-dimensional Fibonacci superlattices reveals a smooth dependence on the Fermi energy location and finally the transition from one- into two-dimensional conductivity is also analyzed.

Keywords: Quasicrystals; Electrical transport; Electronic states

1. Introduction

The electronic conduction in macroscopic quasicrystalline lattices is an interesting but not widely studied subject, since both the quantum transport and macroscopic-scale quasiperiodic system per se are not easy topics. Nowadays, there is a consensus that in these systems the electronic wave functions are critical and the corresponding eigenvalue spectra are singular continuous [1]. The level-spacing analysis shows an inverse-power-law distribution of gaps [2,3] and a semi-Poisson distribution of bands [4], both neither conventional Poisson nor Wigner ones. Hence, the transport properties of these critically localized states are a fascinating and still unclear theme. The hopping conduction in Fibonacci chains has been addressed by means of the Miller–Abrahams equations [5,6]. The optical conductivity has been analyzed within a generalized Drude formula [7] and the temperature dependence has been investigated by summing the relevant ladder diagrams of electron–phonon interactions [8]. Recently, transparent states with unity transmission coefficient have been found in mixing Fibonacci chains [9] and its a.c. conductivity has been studied within the Kubo–Greenwood formalism [10]. In this paper, we report a detailed analysis of the d.c. and a.c. conductivity in macroscopic Fibonacci chains by using a novel renormalization method [11]. Also, the d.c. conduction in two-dimensional Fibonacci superlattices is investigated.

2. Results

A mixing Fibonacci chain (MFC) is constructed by alternating two sorts of atoms, A and B, following the Fibonacci sequence and the hopping integrals between these atoms depend on the nature of them, leading to the existence of two different parameters t_{AA} and $t_{AB}=t_{BA}$ [9]. Let us define the first generation $F_1 = A$, and the second $F_2 = BA$. The next generations are given by $F_n = F_{n-1} \oplus F_{n-2}$, for example, $F_5 = BAABABAA$. It would be worth mentioning that this sequence is chosen in order to obtain the transparent states reported in Refs. [9] and [12], whose energies (E_T) are determined by $E_T = \alpha(1+\gamma^2)/(1-\gamma^2)$ and $E_T^2 - \alpha^2 = 4t^2 \cos^2(K\pi/N)$, where $+\alpha(-\alpha)$ are the on-site energies of atoms A(B), $\gamma = t_{AA}/t_{AB}$ is the ratio of the Fibonacci hopping parameters, t is the hopping integral of the periodic leads, K and N/K are integer numbers [12]. On the other hand, a two-dimensional mixing Fibonacci superlattice (2D-MFS) can be built by

*Corresponding author.
E-mail address: chumin@servidor.unam.mx (C. Wang).

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repeating periodically the MFC, which are connected by a hopping integral $t_\perp$.

In order to isolate the quasicrystalline effects on the transport properties of the system, a simple s-band tight-binding Hamiltonian is considered as given in Ref. [10]. For the sake of simplicity, a uniform bond length, $a=1$, is taken in both directions of a 2D-MFS. The analysis of the electrical conduction is carried out by means of the Kubo–Greenwood formula [13]

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

where Ω is the volume of the system, $f(E)=\{1+\exp[(E-\mu)/k_BT]\}^{-1}$ is the Fermi–Dirac distribution with Fermi energy μ and temperature T, $G^+(E)$ is the retarded one-particle Green's function, and $p=im/\hbar\ \Sigma_j\{t_{j,j+1}|j\rangle\langle j+1|-t_{j,j-1}|j\rangle\langle j-1|\}$ is the projection of the momentum operator along the applied electrical-field direction.

For an infinite periodic linear chain with null self-energies and hopping integral t, the conductivity of a segment of N atoms at zero temperature can be calculated analytically and it is given by [14]

$$\sigma_P^{1D}(\mu=0,\omega)=\frac{8e^2t^2}{\pi(N-1)\hbar^3\omega^2}\left\{1-\cos\left[(N-1)\frac{\hbar\omega}{2|t|}\right]\right\}, \quad (2)$$

where the segment length is $\Omega=(N-1)$, since $a=1$. In the limit of $\omega\to 0$, the d.c. conductivity within the energy band is $\sigma_P\equiv\sigma_P^{1D}(\mu,0)=(N-1)e^2/(\pi\hbar)$.

Two-dimensional quasiperiodic superlattices can be built by stacking periodically MFC and its electrical conductivity in the MFC direction can be calculated by taking advantage of the translational symmetry in the periodic-lattice direction, defining a $k_\perp$ vector, which leads to [15]

$$\sigma_\parallel^{2D}(\mu,0)=\frac{1}{2\pi}\int_{-\pi}^{\pi}\sigma_\parallel^{1D}[\mu-2t_\perp\cos(k_\perp),0]\,\mathrm{d}k_\perp=\int_{-\infty}^{\infty}\sigma_\parallel^{1D}(E,0)DOS_\perp^{1D}(\mu-E)\,\mathrm{d}E, \quad (3)$$

where $\sigma_\parallel^{1D}$ is the one-dimensional conductivity along the applied-electrical-field direction and $DOS_\perp^{1D}$ is the density of states of periodic chains, which is given by

$$DOS_\perp^{1D}(E)=\frac{\theta(|2t_\perp|-|E|)}{\pi\sqrt{4t_\perp^2-E^2}},\quad \text{being } \theta(x)=\begin{cases}1, & \text{if } x\geq 0\\ 0, & \text{if } x<0\end{cases}.$$

Note that the results of Eq. (3) can also be obtained within the convolution scheme [16].

In particular, for the periodic-superlattice case, being $t_\perp=t_\parallel=t$ and $\mu\leq|4t|$, analytical results exist and they are

$$\sigma_P^{2D}(\mu,0)=\sigma_P\int_{-2t}^{2t}\frac{\theta(|2t|-|\mu-E|)\,\mathrm{d}E}{\pi\sqrt{(2t)^2-(\mu-E)^2}}=\frac{\sigma_P}{\pi}\cos^{-1}\left(\frac{|\mu|-2t}{2t}\right). \quad (4)$$

For quasiperiodic systems, the Kubo–Greenwood formula is evaluated by using a previously developed renormalization procedure [11], which computes iteratively the products of the Green's function in Eq. (1). Let us consider a MFC with $k=N/K=3$, as defined in Ref. [12], connected to two infinite periodic leads with hopping integrals t and null on-site energies. Fig. 1a shows the zero-temperature one-dimensional d.c. Kubo conductivity as a function of the Fermi energy position, for a MFC with $\alpha=0.225|t|$, $t_{AA}=1.25t$, $t_{AB}=t_{BA}=t$ and $n=35$. The spectrum contains 800 000 items of data and has been calculated in quadruple precision. The imaginary part of the energy in the Green's function is $10^{-10}|t|$ and the transparent state energy ($E_T=-1.025|t|$) is indicated by a dashed line. Observe that the band structure is quite fine in comparison with that obtained in Ref. [10], since now the MFC contains 14 930 352 atoms for $n=35$. An almost constant behavior is found in the neighborhood of the transparent state. An amplification of this zone (Fig. 1a′) shows a periodic oscillating pattern, which can be obtained by a perturbation analysis of the transmittance formula [11]. Note that the spectrum around the transparent state is scaled by the inverse of the system size, in spite of the fact that the whole spectrum does not. Fig. 1(b–d) show the d.c. Kubo conductivity of 2D-MFS with the same parameters as Fig. 1a but $t_\perp=10^{-4}t$, $t_\perp=10^{-2}t$, and $t_\perp=t$, respectively. These spectra are calculated by integrating

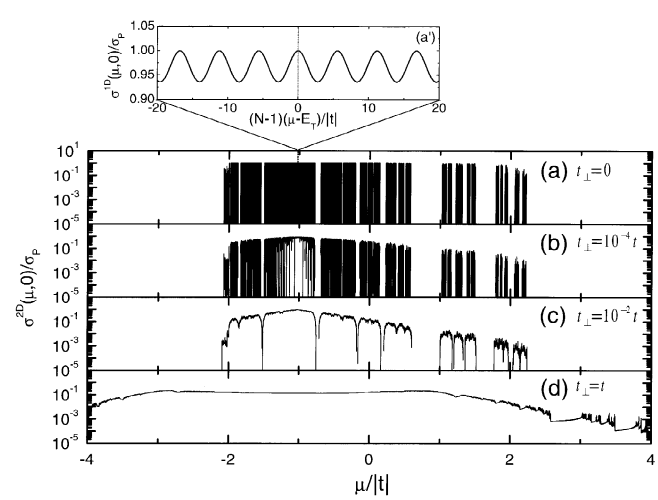

Fig. 1. D.C. conductivity of 2D-MFS (b–d) in comparison with that of a MFC (a). An amplification of the neighborhood around the transparent-state, indicated by dashed lines, is shown in (a′).

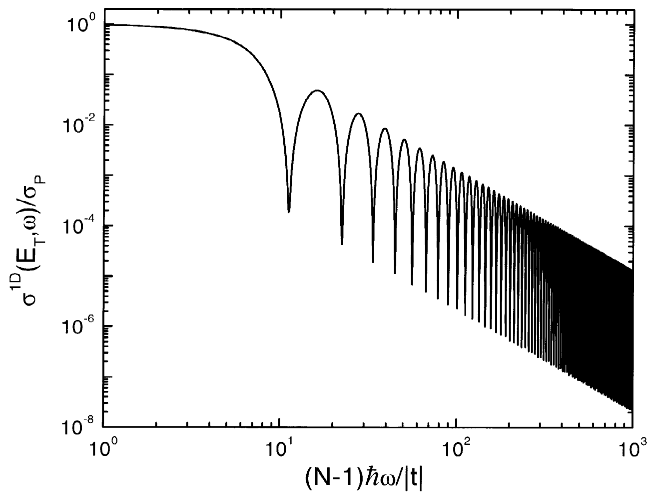

Fig. 2. A.C. conductivity of the same MFC as in Fig. 1a.

Eq. (3). Observe the dimensionality transition and a very smooth behavior revealed in Fig. 1d.

In Fig. 2, the zero-temperature a.c. Kubo conductivity of the same MFC as Fig. 1a is shown for $\mu = E_T$. Note first that the spectrum is also scaled by the inverse of the system size, as found in the periodic case (Eq. (2)). This fact is related to the scaling property observed in Fig. 1a′, since the zero-temperature a.c. conductivity is calculated by integrating a vicinity of $\hbar\omega$ around the Fermi energy (Eq. (1)). Moreover, the maxima of the curve decay following an inverse power law, $\sigma^{1D}_{max}(E_T, \omega)/\sigma_P = C[(N-1)\hbar\omega/|t|]^{-\beta}$, with $\beta = 2$ and $C = 12.68$, instead of $\beta = 2$ and $C = 16$ for the periodic case (Eq. (2)). On the other hand, the minima of the curve should be zero and their finite values observed in Fig. 2 are caused by the finite imaginary part ($10^{-10}|t|$) of the energy used in the calculation of the Green's function.

3. Conclusions

In this paper, we have analyzed the electrical transport in one- and two-dimensional macroscopic Fibonacci systems by means of the Kubo–Greenwood formula. The calculation has been carried out by using a new renormalization method. The results show an inverse-system-size scaling spectrum around the transparent state and an inverse-power-law a.c. behavior. The latter is similar to that of periodic systems, but very different from the a.c. behaviors of other high d.c.-conductivity states in MFC [11]. On the other hand, the smooth d.c. conductivity spectrum obtained from 2D-MFS reveals a high sensitivity of quasiperiodic systems to the periodic stacking and suggests that the Fibonacci superlattices could not be good candidates to observe experimentally the multifractal conduction band structure. Finally, the a.c. conduction in 2D-MFS is currently under study.

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