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Kubo conductivity in two-dimensional Fibonacci lattices

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Abstract

The electronic transport at zero degrees in quasiperiodic systems is investigated by using the Kubo–Greenwood formula and a novel renormalization method, which allows an evaluation in an exact way of the products of the Green's function in macroscopic Fibonacci chains. The analysis of transport properties in two-dimensional Fibonacci superlattices and in double quasiperiodic lattices is carried out by means of the convolution technique. The spectrally averaged conductance shows a linear dependence with the width of the system and a power-law decay as its length increases along the applied electric field.

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1. Introduction

The transport property is one of the most remarkable characteristics of quasiperiodic systems, since their electronic wave functions are critical, neither extended nor localized [1]. A number of numerical studies for two-dimensional (2D) quasiperiodic systems have been done and anomalous electronic conduction is observed [2], despite that only small approximants have been addressed due to the absence of a general Bloch-type theorem for the quasiperiodic systems. Recently, we have developed a new renormalization method for the Kubo–Greenwood formula in Fibonacci chains [3], and it has been extended to the bond problem. In general, the Fibonacci sequence (F_n) of generation n can be built by defining $F_1 = \mathrm{A}$, $F_2 = \mathrm{BA}$, and the addition rule, $F_n = F_{n-1} \oplus F_{n-2}$, understood as the joining of sequences. For instance, $F_4 = \mathrm{BAABA}$. For the bond problem, the on-site energies are the same ($\varepsilon_i = 0$) and the hopping integrals, t_A and t_B, are organized following the Fibonacci sequence. The 2D quasiperiodic superlattices can be built by stacking periodically Fibonacci chains, which are connected by a hopping integral t. The doubly quasiperiodic lattices are constructed following the sequence of Fibonacci in both directions. On the other hand, the dc electrical conductivity at $T = 0$ can be studied by means of the Kubo–Greenwood formula, which is written as [3]

$$\sigma(E) = \frac{2e^2\hbar}{\pi\Omega m^2} Tr[p\,\mathrm{Im}G^+(E)p\,\mathrm{Im}G^+(E)], \tag{1}$$

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where Ω is the volume of the system, $G^{+}(E)$ is the retarded one-particle Green's function, and $p = \frac{ima}{\hbar}\sum_j \{t_{j,j+1}|j\rangle\langle j+1| - t_{j,j-1}|j\rangle\langle j-1|\}$ is the projection of the momentum operator along the applied electric-field direction.

In this paper, we report an analysis of the 2D electrical conductance, $g^{2D}(E) = \sigma^{2D}(E)L_{\perp}/L_{\parallel}$, where $L_{\perp}$ and $L_{\parallel}$ are respectively the width and the length of the system in reference of the applied electric field, and the 2D conductivity is calculated by using the convolution technique [4]

$$\sigma^{2D}(E) = \int_{-\infty}^{\infty} dE' \sigma_{\parallel}^{1D}(E')\mathrm{DOS}_{\perp}^{1D}(E - E'), \tag{2}$$

being DOS the density of states. In order to analyze global properties of the spectra, an spectral average of the conductance ($\langle g^{2D}\rangle$) can be defined as

$$\langle g^{2D}\rangle = \frac{\int dE\, g^{2D}(E)\mathrm{DOS}^{2D}(E)}{\int dE\, \mathrm{DOS}^{2D}(E)}. \tag{3}$$

In the following section, $\langle g^{2D}\rangle$ as a function of the width and the length of the quasiperiodic systems is investigated.

2. Results

Fig. 1 shows the dc conductivity [$\sigma^{2D}(E)$], normalized by that of a periodic chain [$\sigma_P = 2e^2a(N_{\parallel} - 1)/h$] [3], versus the Fermi energy (E) for a 2D periodic lattice (dot line), Fibonacci superlattices (gray lines), and doubly quasiperiodic lattices (black lines), in which the hopping integrals ($t_A = t$ and $t_B = 0.9t$) are arranged following the Fibonacci sequence and an uniform bond length ($a = 1$) is taken for the sake of simplicity. The imaginary part of the energy in $\sigma_{\parallel}^{1D}(E)$ is $10^{-11}|t|$ and in $\mathrm{DOS}(E)$ is $10^{-2}|t|$, in order to perform easily the integration in Eq. (2). The grey and black solid lines from up to down in Fig. 1 correspond respectively $N_{\parallel} = 90$, 6766, 514 230, and 165 580 142 atoms and a fixed width of 121 394 atoms, showing that $\sigma^{2D}(E)$ of the quasiperiodic systems decrease when their length ($L_{\parallel} = N_{\parallel}a$) grows.

To analyze global behaviors of the spectra in Fig. 1, a spectral average of the conductance ($\langle g^{2D}\rangle$) is performed and it is plotted versus the width ($L_{\perp} = N_{\perp}a$) in Fig. 2 for 2D periodic lattices (circles), Fibonacci superlattices (squares) and doubly quasiperiodic lattices (rhombuses), with the same hopping integrals as in Fig. 1. The total length of these lattices is 165 580 142 atoms, corresponding to the generation $n = 40$, connected to two semi-infinite leads with hopping integrals t. In

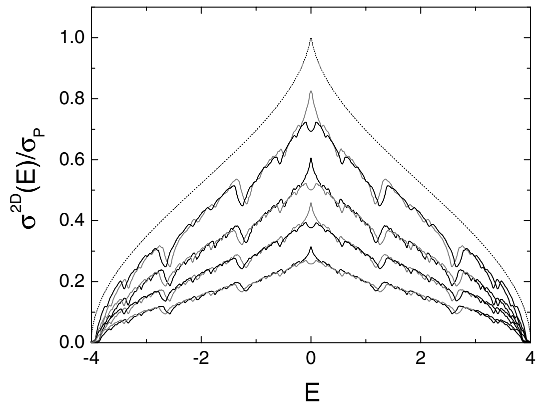

Fig. 1. The dc electric conductivity [$\sigma^{2D}(E)$] as a function of the Fermi energy (E) for a periodic lattice (dot line), Fibonacci superlattices (gray lines) and doubly quasiperiodic lattices (black lines). From up to down the grey and black solid lines represent systems with $N_{\parallel} = 90$, 6766, 514 230, and 165 580 142 atoms, which correspond respectively generations $n = 10$, 19, 28, and 40 of the Fibonacci sequence. These systems have a fixed width of 121 394 atoms.

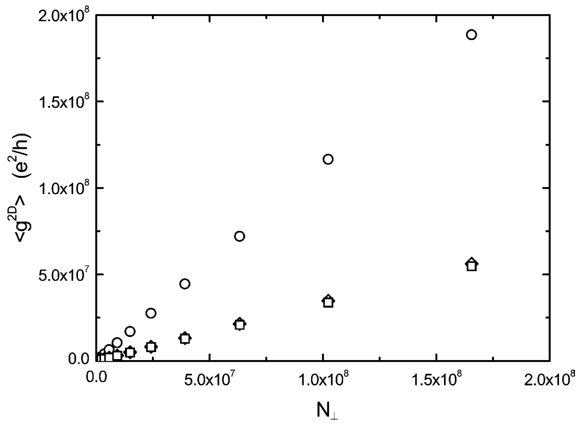

Fig. 2. Spectrally averaged conductance ($\langle g^{2D}\rangle$) versus the number of atoms in the perpendicular direction to the applied electric field ($N_{\perp}$) for 2D periodic lattices (○), Fibonacci superlattices (□) and doubly quasiperiodic lattices (◇). The length of these lattices is 165 580 142 atoms and for the quasiperiodic systems, we have $t_A = t$ and $t_B = 0.9t$.

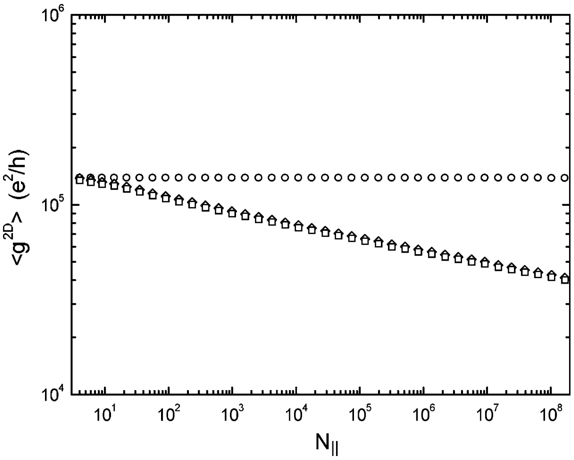

Fig. 3. Spectrally averaged conductance ($\langle g^{2D} \rangle$) as a function of the number of atoms along the applied electric field ($N_{\|}$) for the same systems in Fig. 2, except with a fixed $N_{\perp} = 121\,394$.

Fig. 3, $\langle g^{2D} \rangle$ as a function of the length ($L_{\|} = N_{\|} a$) is shown for the same systems in Fig. 2, except with a fixed $N_{\perp} = 121\,394$, corresponding to the generation $n = 25$.

3. Discussion

It would be worth mentioning that for the periodic case the normalized dc conductivity $[\sigma^{2D}(E)/\sigma_P]$ in Fig. 1 is independent on the system length, contrary to the quasiperiodic case. Indeed, for infinite-width periodic systems the dc conductivity $[\sigma_P^{2D}(E)]$ can be obtained analytically [5] and it is given by

$$\sigma_P^{2D}(E) = \frac{\sigma_P}{\pi} \cos^{-1}\left(\frac{|E| - 2t}{2t}\right) \theta(|4t| - |E|), \qquad (4)$$

where $\theta(x)$ is a step function.

In Fig. 2, observe that $\langle g^{2D} \rangle$ grows linearly with $N_{\perp}$, i.e., $\langle g^{2D} \rangle = e^2(\alpha N_{\perp} + \beta)/h$, where for the periodic lattices $\alpha = 1.13855$ and $\beta = 10.02583$, for the Fibonacci superlattices $\alpha = 0.33047$ and $\beta = -3.94034$, and for the doubly quasiperiodic lattices $\alpha = 0.33923$ and $\beta = -3.06046$. The values of β are essentially zero if they are compared with the scale of the graph (10^8), and the slope (α) is expected to be 2 for the periodic case if the parallel linear chains (or conducting channels) are totally independent. Furthermore, notice that $\langle g^{2D} \rangle$ of doubly quasiperiodic lattices is larger than those of Fibonacci superlattices, possibly originated from the better structural coherence in the doubly quasiperiodic case.

Finally, notice in Fig. 3 that $\langle g^{2D} \rangle$ of periodic systems is constant, while for quasiperiodic systems it decays as a power law $[\langle g^{2D} \rangle = e^2(\mu N_{\|}^{-\nu})/h]$ when the system length increases, as reported for finite Penrose lattices [6]. We found $\nu = 0.06961$ and $\mu = 146\,994.13$ for Fibonacci superlattices, and $\nu = 0.06955$ and $\mu = 150\,750.93$ for doubly quasiperiodic case. It is important to stress that $\langle g^{2D} \rangle$ of Fibonacci superlattices is smaller than those of doubly quasiperiodic lattices, similar to that occurred in Fig. 2.

4. Conclusions

We have studied the electronic transport in macroscopic 2D Fibonacci systems within the Kubo–Greenwood formulation. This study has been carried out by using the renormalization method and the convolution technique. The spectrally averaged conductance shows a power-law decay length dependence, similar to that happened in Penrose lattices. This power-law decay reveals the critical localization nature in quasiperiodic systems, contrary to the constant and exponential decay behaviors in the periodic and randomly disordered systems, respectively [7].

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