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Electronic transport in multidimensional Fibonacci lattices

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In this article, the Kubo-Greenwood formula is used to investigate the electronic transport behaviour in macroscopic systems by means of an exact renormalization method. The convolution technique is employed in the analysis of two-dimensional Fibonacci lattices. The dc electrical conductance spectra of multidimensional systems exhibit a quantized behaviour when the electric field is applied along a periodically arranged atomic direction, and it becomes a devil's stair if the perpendicular subspace of the system is quasiperiodic. The spectrally averaged conductance shows a power-law decay as the system length grows, neither constant as in periodic systems nor exponential decays occurred in randomly disordered lattices, revealing the critical localization nature of the eigenstates in quasicrystals. Finally, the ac conductance along periodic and quasiperiodic directions is compared with the optical conductivity measured in decagonal quasicrystals.

1. Introduction

The synthesis of thermodynamically stable and structurally near-perfect quasicrystals, such as AlCuRu and AlCuFe systems [1, 2], has provided the possibility to explore the intrinsic properties of quasiperiodic alloys. Among their peculiar characteristics, the transport property is perhaps the most surprising one. Unlike their metallic constituents, the quasicrystals (typically aluminium-rich alloys) are extremely poor conductors of electricity and heat. In fact, they become more resistive when they are more perfect. Moreover, their electrical resistivity (ρ) has a strong temperature dependence, e.g., the ratio $\rho(4.2\,\mathrm{K})/\rho(300\,\mathrm{K})$ is larger than 10, in comparison with 1.2 for amorphous and less than 0.1 for crystalline metals [3]. The optical conductivity is also unusual, showing linear frequency dependence in icosahedral quasicrystals [4] and a strong anisotropy in decagonal ones, in which the optical conductivity decays with the frequency along periodic direction and increases slightly in the low frequency region along the quasiperiodic one [5]. These amazing

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non-Drude responses to the oscillating external electric field are still not fully understood. They are generally believed to be consequences of a peculiar localization nature derived from the long-range quasiperiodic structural order. Nowadays, there is a consensus that the eigenvalue spectrum produced by a quasiperiodic potential is singular continuous and the associated eigenfunctions are critical [6], neither extended nor exponentially localized. In this article, we report an eight orders of magnitude scaling analysis of the dc conductance, revealing a clear power law localization nature of the states, whose exponent shows a linear relationship with the quasiperiodicity strength. Furthermore, we extend this analysis to the finite frequency region and the results show an absence of the Drude peak when the external electrical field is applied along the quasiperiodic direction, as observed in decagonal quasicrystals.

2. The method of renormalization plus convolution

There are several ways to examine the localization and the transport capability of an excitation in solids [7]. In this work, we choose the Kubo formalism to quantify the dc and ac electrical conductivity (σ) of multidimensional Fibonacci systems. Within the linear response approximation, the Kubo-Greenwood formula is given by [8]

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

where Ω is the volume of the system, p is the projection of the momentum operator along the applied electrical field, G^{+} is the retarded one-particle Green's function, and $f(E)=\{1+\exp[(E-\mu)/k_BT]\}^{-1}$ is the Fermi-Dirac distribution with Fermi energy μ and temperature T. In order to isolate the quasicrystalline effects on the conductivity, we consider a simple s-band tight-binding Hamiltonian given by

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

where ε_j is the self-energy at site j and $t_{i,j}$ denotes the hopping integral between nearest-neighbour sites i and j. Using the relation $p=(im/\hbar)[H,x]$, the momentum operator can be written as $p=ima/\hbar\sum_j\{t_{j,j+1}|j\rangle\langle j+1|-t_{j,j-1}|j\rangle\langle j-1|\}$.

Recently, we have developed a novel renormalization method for the Kubo-Greenwood formula in Fibonacci chains [9]. It is very efficient, allowing the study of truly macroscopic systems, as illustrated in figure 1, where the computing time spent through direct calculation of the Green's function (figure 1a) and by using the renormalization method (figure 1b) are comparatively shown. The numerical computations were carried out on a Silicon Graphics O2 workstation with a MIPS R12000 microprocessor.

Observe that in the first case, figure 1a, the computing time grows as a third power of the system size, and for the second case, figure 1b, it grows linearly with the number of generation, i.e., grows logarithmically with the system size. For example, for a system with 988 atoms the direct-calculation time is 3 932 891 ms versus 27 ms

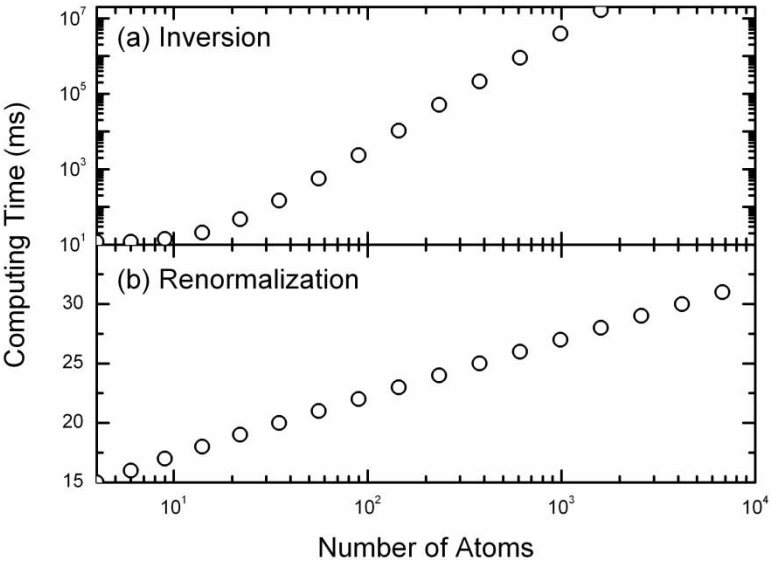

Figure 1. The Kubo-Greenwood formula computing time spent (a) through direct calculation of the Green's function and (b) by using the renormalization method. The numerical computations are performed on a Silicon Graphics O2 workstation with a MIPS R12000 microprocessor.

if the renormalization method is used. It would be worth emphasizing that the results obtained by both methods are exactly the same and the quadruple precision should be used when the system size reaches the macroscopic scale. Therefore, in the rest of this paper we will use the renormalization method to evaluate the Kubo-Greenwood formula.

This renormalization method is difficult to be extended to multidimensional systems, since for each generation only the interior sites of the lattice can be renormalized and all the border sites should be explicitly kept in order to calculate the Green's function of next generations, i.e., for a d-dimensional system, the number of border sites increases as a system of $d-1$ dimensions [10], except $d=1$ where the number of border sites is always two. However, there is an alternative way to address the multidimensional quasiperiodic systems, which is through the convolution technique, when the Hamiltonian of the system is separable, i.e., $H = H_{\|} \otimes I_{\perp} + I_{\|} \otimes H_{\perp}$, with $H_{\|}$ ($I_{\|}$) and $H_{\perp}$ ($I_{\perp}$) being respectively the Hamiltonian (the identity of the corresponding Hilbert space) of the parallel and perpendicular subsystem with respect to the applied electric field [11]. For instance, the decagonal quasicrystals can be visualized as a periodic stacking of quasiperiodic layers and their Hamiltonian can be expressed as a sum of the periodic and quasiperiodic parts within the first-neighbour tight-binding approximation. Combining the renormalization and convolution methods, the electrical conductivity can be expressed as [12]

$$\sigma(\mu, \omega, T) = \frac{1}{\Omega_{\perp}} \int_{-\infty}^{\infty} dy \sigma^{||}(\mu - y, \omega, T) DOS^{\perp}(y) \tag{3}$$

or

$$\sigma(\mu, \omega, T) = \frac{1}{\Omega_\perp} \sum_\beta \sigma^{\|}(\mu - E_\beta, \omega, T), \tag{4}$$

where $\sigma^{\|}$ is the electrical conductivity of the parallel subsystem; $\Omega_\perp$, $DOS^\perp$ and E_β are respectively the volume, the density of states and the eigenvalues of the perpendicular subsystem, i.e., $H_\perp|\beta\rangle = E_\beta|\beta\rangle$.

3. Results

Let us consider a cubic-type lattice, in which the atoms in each direction can be arranged periodically or quasiperiodically [13, 14]. The latter is obtained by alternating two sorts of bonds, t_A and t_B, following the Fibonacci sequence and maintaining the same self-energy $\varepsilon_j = 0$. This bond Fibonacci sequence (F_n) is defined as $F_1 = A$, $F_2 = BA$, and $F_n = F_{n-1} \oplus F_{n-2}$. For example, $F_5 = BAABABAA$. For the sake of simplicity, a uniform bond length (a) is taken. Along the applied electric field all the systems considered in this paper are connected to two semi-infinite periodic leads with null self-energies, hopping integrals $t = t_A$ and a lattice constant a.

In figure 2, we show the two-dimensional (2D) ac electrical conductance (g) at zero temperature, defined as $g(\mu, \omega, 0) = \sigma(\mu, \omega, 0)\Omega_\perp/\Omega_{\|}$, for a lattice whose

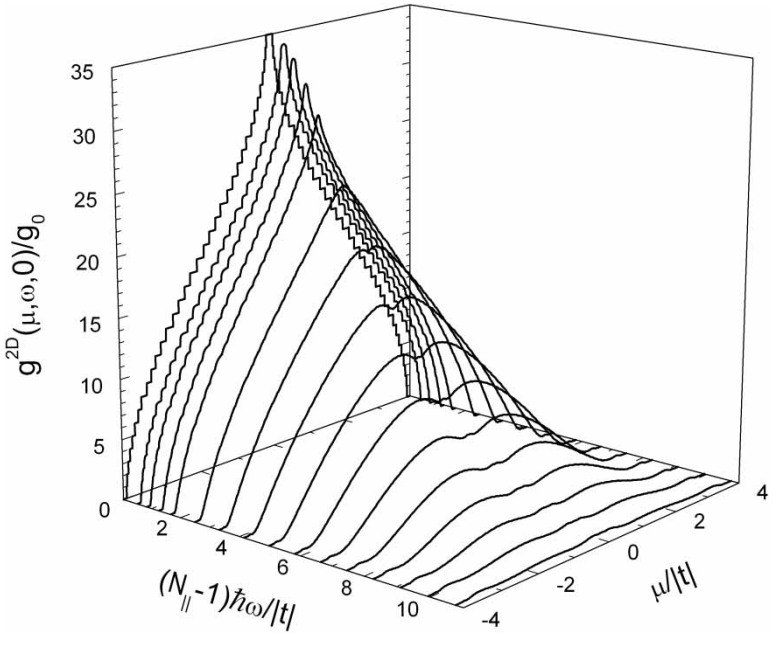

Figure 2. The electrical conductance at zero temperature of a 2D lattice [$g^{2D}(\mu, \omega, 0)$] versus the position of the Fermi energy (μ) and the frequency of the applied electric field (ω). This lattice contains $165\,580\,142 \times 35$ atoms and they are arranged periodically and quasiperiodically, with $\gamma = t_B/t_A = 0.9$, in its longer and shorter sides, respectively. The external electric field is applied along the longer side.

atoms are arranged periodically along the electric field and quasiperiodically in the perpendicular directions with $\gamma = t_B/t_A = 0.9$. The cross section of the lattice contains 35 atoms, and its size along the electric field is of 165 580 142 atoms, corresponding to the generation $n = 40$.

Observe the quantized conductance with a uniform step height $g_0 = 2e^2/h$ at $\omega = 0$, as found experimentally in 2D electron gas devices [15]. However, these steps are not uniformly placed, whose positions are defined by the eigenvalues, E_β, of the perpendicular quasiperiodically-ordered cross section, as shown in equation (4). For frequencies $\omega \neq 0$, these quantum steps are quickly destroyed.

In order to analyze the global localization nature of the states, a spectral average of the conductance, defined as

$$\langle g \rangle = \frac{\int dE\, g(E,0,0)\, DOS(E)}{\int dE\, DOS(E)}, \tag{5}$$

is shown in figure 3 as a function of the number of atoms in the parallel direction ($N_\parallel$), for 2D lattices with different values of the quasiperiodicity strength (γ).

All these lattices contain 165 580 142 atoms in the perpendicular direction to the applied electric field. Notice the well-defined power-law behaviour demonstrated in the log-log plot, i.e. $\langle g \rangle \sim (N_\parallel)^{-\alpha}$. This exponent α depends on γ, as shown in the inset of figure 3, where we can see an almost linear relationship between α and γ.

Finally, let us consider two 2D tapes. Each one contains $165\,580\,142 \times 90$ atoms and orient their longer side on the applied electric field direction.

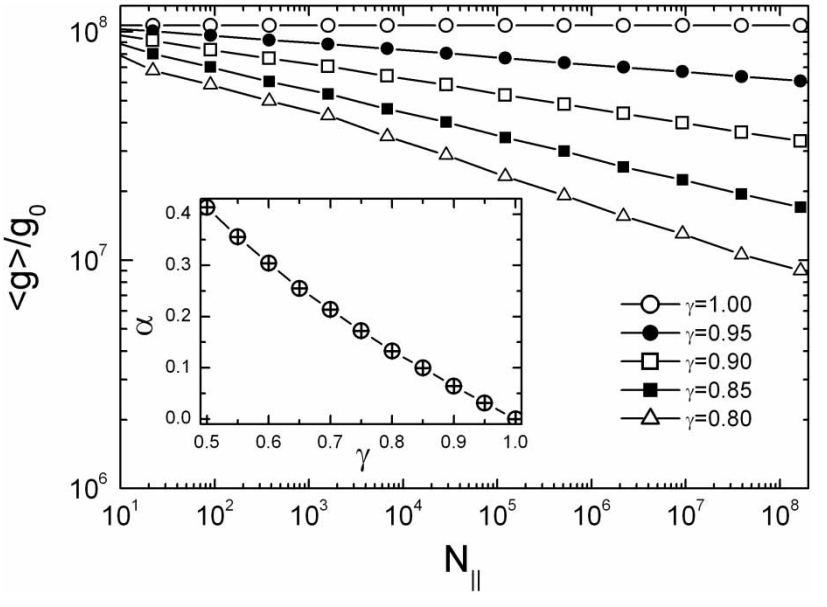

Figure 3. Spectral average of the conductance ($\langle g \rangle$) versus the length ($L_\parallel = N_\parallel a$) for systems with a fixed width of 165 580 142 atoms and different values of the quasiperiodicity strength $\gamma = t_B/t_A$. The data follow a power law as $\langle g \rangle \propto N_\parallel^{-\alpha}$. Inset: the exponent α as a function of γ.

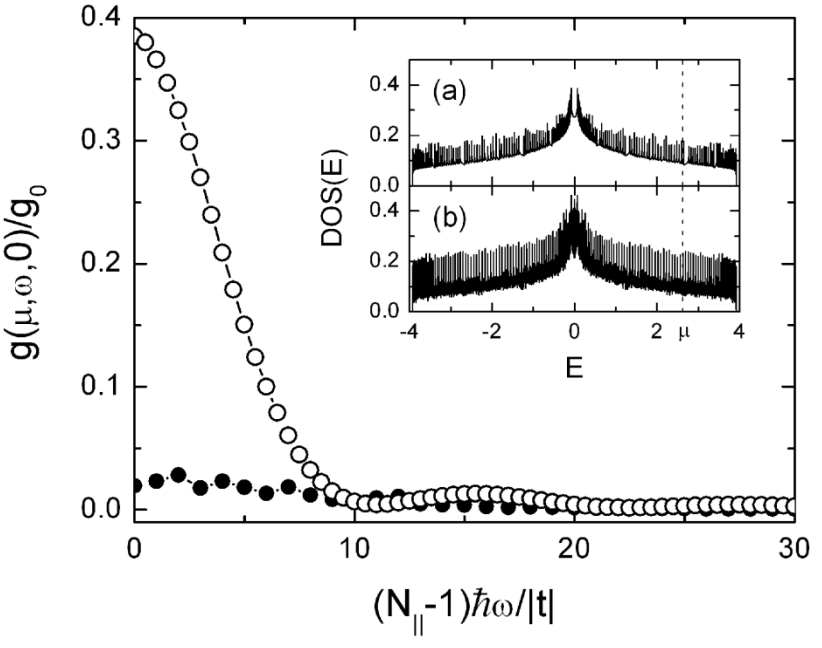

Figure 4. The electrical conductance (g) at zero temperature versus the frequency of the applied electric field (ω) for two 2D tapes of $165\,580\,142 \times 90$ atoms with periodic (open circles) and quasiperiodic (solid circles) order on the longer side, at the same time quasiperiodic and periodic order on the shorter side, respectively. The external electric field is applied along the longer side. Inset: densities of states of these two tapes represented by (a) open circles and (b) solid circles. The Fermi energy (μ) is indicated by a dashed line.

The ac conductance (g) of these tapes evaluated at a pseudo gap as a function of the frequency (ω) is exposed in figure 4, where the first tape (open circles) has respectively its periodic and quasiperiodic atomic orders on the long and short sides and on the contrary, the second tape (solid circles) has the periodic and quasiperiodic atomic orders on the short and long sides, respectively.

Observe that for the first tape the ac conductance falls following a quadratic power law at the very low frequency region, in accordance with the Drude theory [16], while the ac conductance of the second tape remains almost constant, as observed in decagonal quasicrystals [5]. The densities of states (DOS) corresponding to the first and second tapes are respectively displayed in the insets figure 4a and 4b, where the location of the Fermi energy is indicated by a dashed line. The value of the Fermi energy is chosen at a minimum of the DOS verified by magnifications of the spectra.

4. Conclusions

The renormalization method combined with the convolution technique seems to be an interesting approach to multidimensional quasiperiodic systems of macroscopic scale. Using this method we have performed an analysis of dc and ac

conductivities in an *exact* way within the Kubo-Greenwood formalism. The results show a clear quantized conductance when the system is periodic along the applied electric field. The scaling analysis of the dc-conductance spectra reveals a power-law localization nature in the Fibonacci lattices with bond disorder, where the absolute value of the exponent increases almost linearly with the quasiperiodicity strength. The ac conductance evaluated at a pseudo gap shows a quadratic power-law decay with the frequency, in accordance with the Drude theory, when the electric field is applied along the periodic atom-arrangement direction. On the other hand, a weak dependence on the frequency is observed when the electric field is applied along the quasiperiodic direction. These two low-frequency behaviours correspond to $\alpha = 2\beta - 1 > 0$ and $\alpha \approx 0$ cases predicted by the generalized Drude theory [17].

Acknowledgments

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