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Renormalization–convolution approach to the electronic transport in two-dimensional aperiodic lattices

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Abstract

A novel method combining the renormalization and convolution techniques is developed for the Kubo–Greenwood formula. Using this method, the dc and ac conductance at zero temperature in two-dimensional (2D) quasiperiodic systems are studied. The results show that the ac conductance of quasiperiodic systems could be significantly modified by the presence of periodic leads, which are usually employed as the measurement connections. Furthermore, when the system is periodic along the applied electrical field, a quantized dc conductance spectrum is observed at zero temperature and this quantized spectrum is destroyed when an oscillating electrical field is introduced. However, when the electric field is applied along a quasiperiodic direction of the system, the ac conductance spectrum shows a non-Drude behaviour, in good agreement with experiment results.

Keywords: Electrical transport; Kubo–Greenwood formula; Two-dimensional systems; Renormalization method; Convolution technique

1. Introduction

In the last decades, the thin-film technology had an extremely fast grow and development. Nowadays, it is possible to produce truly two-dimensional (2D) systems, where many quantum phenomena are observed at low temperatures, such as the quantum Hall effect [1]. In addition, the thin-film conductors are pervasive in numerous applications. For example, they are widely used in microelectronics, solar cells, flat panel displays, and sensors. The physical properties of these films are determined by their atomic order and in general, an aperiodic ordering of atoms leads a multiband structure of excitations, such fact could yield new applications. For instance, efficient second- and third-harmonic generations are observed from a quasiperiodic multilayer of nonlinear optical materials [2]. More recently, a quasiperiodic ultrathin film is obtained by the deposition of Cu atoms on the fivefold surface of an icosahedral quasicrystal [3]. On the theoretical side, the electronic transport in 2D aperiodic systems is an interesting but not widely studied subject, since the electronic transport and aperiodic lattices both *per se* are not easy topics. The absence of reciprocal space makes difficult the study of macroscopic systems. In this paper, we investigate the electronic transport in periodic and quasiperiodic 2D lattices within the Kubo formalism. This analysis is carried out by means of a new method that combines the renormalization and convolution techniques developed for the Kubo–Greenwood formula [4]. This method has the advantage of being able to quantify, in an exact way within the Kubo formalism, the electrical conductance of multidimensional periodic or quasiperiodic systems at macroscopic scale.

2. The renormalization + convolution method

There are several ways to examine the localization and the electronic transport in solids [5]. In this study, we

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choose the Kubo formalism to calculate the dc and ac electrical conductivity (σ) of multidimensional Fibonacci systems. The Kubo–Greenwood formula can be written as [6]

$$\sigma_{xx}(\mu,\omega,T)=\frac{2e^2\hbar}{\Omega\pi m^2}\int_{-\infty}^{\infty}\mathrm{d}E\frac{f(E)-f(E+\hbar\omega)}{\hbar\omega}\times Tr[p_x\mathrm{Im}G^+(E+\hbar\omega)p_x\mathrm{Im}G^+(E)] \qquad (1)$$

where Ω is the volume of the system, p_x 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 the Fermi energy μ and temperature T. In order to isolate the quasicrystalline effects on the conductivity, we consider a simple 2D s-band tight-binding Hamiltonian with null self-energies, given by

$$H=\sum_{i,j}\{t_{(i,j),(i+1,j)}|i,j\rangle\langle i+1,j|+t_{(i,j),(i-1,j)}|i,j\rangle\langle i-1,j| + t_{(i,j),(i,j+1)}|i,j\rangle\langle i,j+1|+t_{(i,j),(i,j-1)}|i,j\rangle\langle i,j-1|\}$$

where $t_{(k,l),(m,n)}$ denotes the hopping integral between nearest-neighbour sites indicated by (k,l) and (m,n). Using $p_x=(im/\hbar)[H,x]$, then $p_x=\frac{ima}{\hbar}\sum_{i,j}\{t_{(i,j)(i+1,j)}|i,j\rangle\langle i+1,j|-t_{(i,j)(i-1,j)}|i,j\rangle\langle i-1,j|\}$.

Recently, we have developed a novel renormalization method for the Kubo–Greenwood formula in Fibonacci chains [7], and we address the multidimensional quasiperiodic systems using the convolution technique, when the Hamiltonian of the system is separable, i.e., $H=H_\parallel\otimes I_\perp+I_\parallel\otimes H_\perp$, being $H_\parallel(I_\parallel)$ and $H_\perp(I_\perp)$ respectively the Hamiltonian (the identity of the corresponding Hilbert space) of the parallel and perpendicular subsystem with respect to the applied electric field [8]. 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 nearest-neighbour tight-binding approximation. Therefore, the electrical conductivity can be expressed as [4]

$$\sigma(\mu,\omega,T)=\frac{1}{\Omega_\perp}\int_{-\infty}^{\infty}\mathrm{d}y\sigma^\parallel(\mu-y,\omega,T)DOS^\perp(y) \qquad (2)$$

or

$$\sigma(\mu,\omega,T)=\frac{1}{\Omega_\perp}\sum_\beta\sigma^\parallel(\mu-E_\beta,\omega,T) \qquad (3)$$

where $\sigma^\parallel$ 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 square-type lattice, in which the atoms in each direction can be arranged periodically or quasiperiodically. The latter is obtained by alternating two sorts of bonds, t_A and t_B, following the Fibonacci sequence. 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.

In Fig. 1 we show the electrical conductance (g) at zero temperature, defined by $g(\mu,\omega,0)=\sigma_{xx}(\mu,\omega,0)\Omega_\perp/\Omega_\parallel$, for a 2D lattice of 121394×22 atoms, whose atoms on the long and short sides are respectively arranged periodically and quasiperiodically with $\gamma=t_B/t_A=0.8$. The electrical field is applied along the lengthy direction that is connected to two semi-infinite periodic leads with null self-energies and hopping integrals $t=t_A$. 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 [9]. 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 Eq. (3). For frequencies $\omega\neq0$, these quantum steps are quickly destroyed.

Fig. 2 illustrates a comparison of the ac conductance spectra at $\mu=0$ of the same lattice as in Fig. 1 with (open circles) and without (solid circles) semi-infinite leads. Notice that for the latter case many resonant peaks appear due to the discrete energy spectrum and the resonant frequencies are located at $\hbar\omega=\varepsilon_\alpha-\varepsilon_\beta$, being ε_α and ε_β eigenvalues of the system, since the Kubo–Greenwood formula can be obtained from the Fermi's golden rule within the linear response approximation [10].

Finally, let us consider an isolate finite square lattice, containing 121394×121394 atoms, arranged periodically in one direction and quasiperiodically with $\gamma=0.8$ in the other direction. In Fig. 3(a–c) its optical conductance at high frequencies are shown for different values of μ located

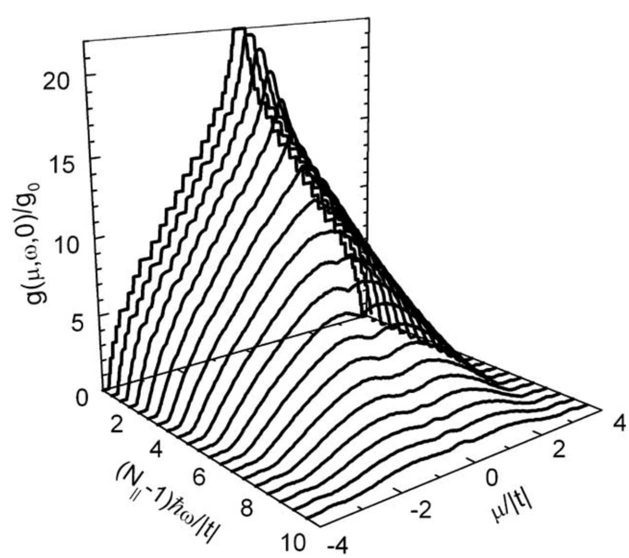

Fig. 1. The electrical conductance at zero temperature of a 2D tape [$g(l,x,0)$] as a function of the Fermi energy (l) and the frequency (x). This tape contains 121394×22 atoms and they are arranged periodically and quasiperiodically, with $c=t_B/t_A=0.8$, in its longer and shorter sides, respectively. The external electric field is applied along the longer side.

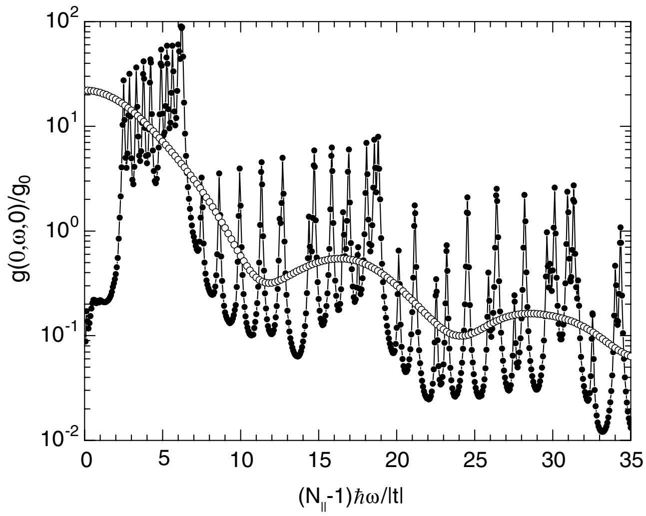

Fig. 2. The ac conductance (g) versus the frequency (ω) of the applied electric field for the same system of Fig. 1, with (open circles) and without (solid circles) semi-infinite periodic leads.

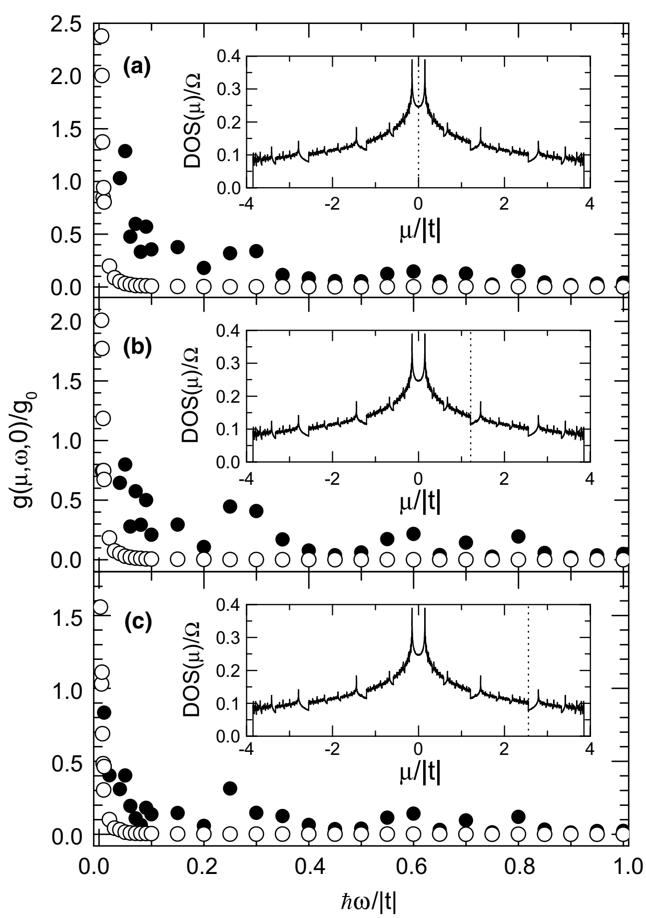

Fig. 3. The frequency dependence of the optical conductance at zero temperature (g) for the Fermi energy (μ) located at (a) $\mu = 0$, (b) $\mu = 1.215|t|$, and (c) $\mu = 2.559|t|$, which are indicated by dashed lines in the spectra of the density of states (DOS). These conductance spectra are obtained from a square lattice of 121394×121394 atoms arranged periodically and quasiperiodically in each direction, when the electric field direction is applied along the first (open circles) and the second (solid circles) direction.

at local minimums (dashed lines in their corresponding insets), when the electrical field is applied along periodic (open circles) and quasiperiodic (solid circles) directions. Observe that for the former case $g(\mu,\omega,0) \propto \omega^{-2}$, as predicted by the Drude theory [11], while for the latter case an oscillating behaviour is observed, both in qualitative agreement with the experimental results obtained from a decagonal quasicrystal [12].

4. Conclusions

The renormalization plus convolution method could be an interesting approach to the multidimensional aperiodic systems. Using this method we have performed an analysis of dc and ac 2D electrical conductance in an *exact* way within the Kubo–Greenwood formalism. The results show a clear quantized dc conductance when the system is periodic along the applied electric field. The boundary conditions of a system seem to be crucial for its ac conductance, which depends significantly on the nature of the measurement contacts. The optical conductance without contacts 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 atomic arrangement direction. On the other hand, an oscillating dependence on the frequency is observed when the electric field is applied along the quasiperiodic direction, as found in a one-dimensional ac conductivity analysis [13].

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