Ferroelectrics, 305: 261–264, 2004

ISSN: 0015-0193 print / 1563-5112 online
DOI: 10.1080/00150190490462991

Taylor & Francis
Taylor & Francis Group

Fractal Quantization of the Electrical Conductance in Quasiperiodic Systems

C. WANG, V. SÁNCHEZ, and F. SALAZAR

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

(Received 9 September 2003; accepted 17 October 2003)

In this work, the Kubo-Greenwood formula is used to investigate the electronic transport in multidimensional macroscopic quasiperiodic lattices within the tight-binding model. This investigation is carried out by means of a novel renormalization method and the convolution technique. The dc electrical conductance of two-dimensional (2D) periodic systems shows uniform steps in units of $2e^2/h$, as observed in 2D electron-gas experiments, and a fractal distribution of these steps is found when the atoms in perpendicular direction to the applied electric field are quasiperiodically ordered. The spectral integral of these conductances presents a strong dependence on the imaginary part of energy in the Green's function, contrary to the case of density of states.

Keywords Quasicrystals; electronic conduction in metals and alloys; renormalization group methods

1. Introduction

Recent advances in the fabrication of two-dimensional (2D) electron gases formed at the high-mobility GaAs-AlGaAs heterostructures have enabled the experimental study of ballistic transport in 2D systems, finding a quantization of the conductance in units of $g_0 = 2e^2/h$ [1, 2]. On the theoretical side, the electrical conductance can be quantified by means of the Kubo-Greenwood formula

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

where Ω is the volume of the system, $G(E)$ is the retarded one-particle Green's function, $f(E) = \{1 + \exp[(E-\mu)/k_B T]\}^{-1}$ is the Fermi-Dirac distribution with Fermi energy μ and temperature T, and p is the projection of the momentum operator along the applied electric-field direction. For one-dimensional systems, the momentum operator can be determined by using the relations $p = (\mathrm{im}/\hbar)[H, x]$ and $x = \sum_j x_j |j\rangle\langle j|$, where x_j is the coordinate of site j. Hence, in the Wannier representation, we have

$$p = \frac{ima}{\hbar}\sum_j (t_{j,j+1}|j\rangle\langle j+1| - t_{j,j-1}|j\rangle\langle j-1|),$$

Address correspondence to C. Wang, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Apartado Postal 70-360, 04510, México D.F., México. E-mail: chumin@servidor.unam.mx

where $t_{j,j+1} = \beta_{j,j+1}(x_{j+1} - x_j)/a$, and $\beta_{j,j+1}$ is the hopping integrals within the tight-binding model. Notice that for the periodic case $t_{j,j+1} = \beta_{j,j+1} = \beta$.

In this paper, we study the electronic transport in two- and three-dimensional (3D) quasiperiodic systems, paying special attention to the imaginary part of energy in the Green's function and its effects on the conductance spectra.

2. Multidimensional Fibonacci Systems

For the bond problem, two kinds of bonds, β_A and β_B, are organized following the Fibonacci sequence and the self-energies of the atoms are assumed to be zero. The first and the second generations of the Fibonacci sequence (F_n) are respectively defined as $F_1 = A$ and $F_2 = BA$, and the generation n is given by $F_n = F_{n-1} \oplus F_{n-2}$. Along the applied electric field all the systems considered in this paper are connected to two semi-infinite periodic leads with vanishing self-energies, hopping integrals $\beta = \beta_A$ and a lattice constant a, in order to resemble the real measurement conditions. A novel renormalization method [3] is used to calculate the electric conductivity in quasiperiodic chains.

For multidimensional systems, in which one or more directions are quasiperiodic and their Hamiltonians (H) are separable, i.e., $H = H_{||} \otimes I_\perp + I_{||} \otimes H_\perp$, where $H_{||}$ ($I_{||}$) and $H_\perp$ ($I_\perp$) respectively stand for the Hamiltonian (the Hilbert-space identity) of the parallel and perpendicular subsystem with respect to the applied electric field, the convolution theorem [4] is employed. This theorem can be written as

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

or

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

where $\sigma^\parallel$ is the electric conductivity of the parallel subsystem, $\Omega_\perp$, $\mathrm{DOS}^\perp$ and E_β are respectively the volume, the density of states and the eigenvalues of the perpendicular subsystem, i.e., $H_\perp|\beta\rangle = E_\beta|\beta\rangle$. In Figs. 1(a) and 1(b), we respectively show the dc electrical conductances at zero temperature, $g(\mu, 0, 0) = \sigma(\mu, 0, 0)\Omega_\perp / \Omega_{||}$, for 2D ($\Omega_\perp = 46369$ atoms) and 3D ($\Omega_\perp = 90 \times 90$ atoms) periodic lattices, both with $\Omega_{||} = 165580142$ atoms. Figs. 1(c) and 1(d) exhibit the electrical conductances of the same systems as in Figs. 1(a) and 1(b), except that in the perpendicular directions to the applied electric field the atoms are organized following the bond Fibonacci sequence with $\beta_B/\beta_A = 0.8$. Magnifications of Figs. 1(a–d) are respectively illustrated in Figs. 1(a′–d′). Notice that for 2D periodic systems there are perfect quantum steps in units of $g_0 = 2e^2/h$, as observed in 2D electron gas devices [2]. However, in 3D periodic lattices the quantum steps are not uniform, due to the degeneracy and distribution of eigenvalues E_β in last equation. For partially quasiperiodic 2D systems (see Fig. (1c′)), self-similarly distributed quantum steps are observed. In Figs. 1(e) and 1(f), we respectively show the electrical conductances of 2D and 3D fully quasiperiodic systems, i.e., the bond Fibonacci sequence is followed in every direction of the system. Observe that these noisy spectra are one order of magnitude smaller than those of partially quasiperiodic systems. The imaginary part of energy used in all these figures is $10^{-11}|\beta|$.

Another interesting and not widely analysed feature of the dc conduction spectra is its dependence on the imaginary part (η) of the energy in the Kubo-Greenwood formula. In Fig. 2 we show the spectral integral of $g(\mu, 0, 0)$ as a function of η for two fully 2D

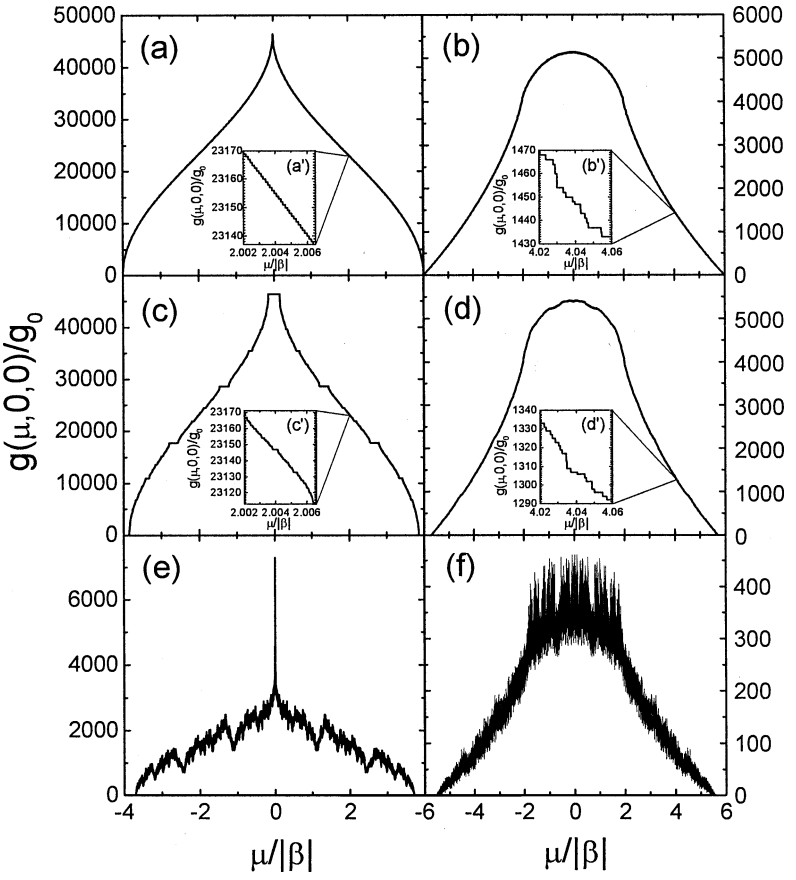

FIGURE 1 Electric conductances (g) for (a) 2D and (b) 3D periodic lattices, (c) 2D and (d) 3D quasiperiodic superlattices, in which the bond Fibonacci sequence is found in the perpendicular directions to the applied electric field, and (e) 2D and (f) 3D fully quasiperiodic systems. The magnifications of Figs. (a–d) are respectively illustrated in Figs. (a′–d′).

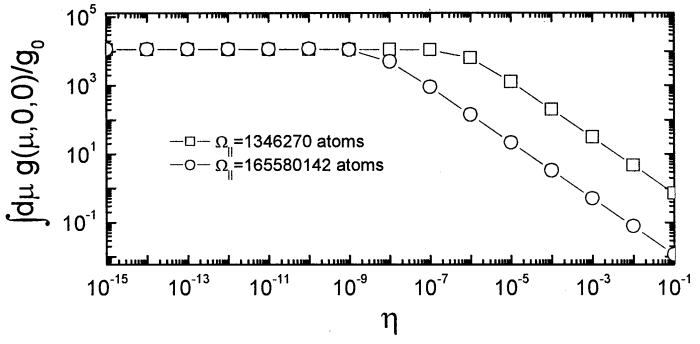

FIGURE 2 The spectral integral of g(μ, 0, 0) as a function of the imaginary part of energy (η) for two fully 2D Fibonacci systems, $\Omega_{||} = 1346270$ atoms (open square) and $\Omega_{||} = 165580142$ atoms (open circles), with the rest of parameters as in Fig. 1(e).

Fibonacci systems, $\Omega_{||} = 1346270$ atoms (open square) and $\Omega_{||} = 165580142$ atoms (open circles), with the rest of parameters as in Fig. 1(e). Observe the existence of a critical value (η_c), i.e., the integrals remain the same value for $\eta < \eta_c$ and diminish following a power law ($\eta^{-\alpha}$) when $\eta > \eta_c$, where $\alpha = 0.82$ for bond Fibonacci systems with $\beta_B/\beta_A = 0.8$. It is interesting to compare with the DOS, whose spectral integral is always a constant, independent of η. Furthermore, we observe that $\eta_c \propto \Omega_{||}^{-1}$ and an imaginary part (η) smaller than η_c is used in Fig. 1. Therefore, quadruple precision calculations are required.

3. Conclusions

In summary, we have studied the electronic transport in macroscopic multidimensional Fibonacci systems, observing an almost uniform distribution of the steps in the conductance spectrum of 2D periodic lattices and a fractal distribution of these steps when the arrangement of atoms in the perpendicular direction to the applied electric field becomes quasiperiodic. The analysis of the imaginary part of energy reveals the existence of η_c for each given $\Omega_{||}$ and suggests the use of $\eta < \eta_c$ for electric conductance calculations. Fig. 2 contrasts to the constant behaviour of the DOS spectral integral, since the Kubo-Greenwood formula involves the products of the Green's function instead of single ones in the DOS calculation.

Acknowledgment

This work has been partially supported by CONACyT-41492-F and DGAPA-IN101701. Computations have been performed at the Bakliz of DGSCA, UNAM.

References

1. B. J. van Wees, H. van Houten, C. W. J. Beenakker, J. G. Williamson, L. P. Kouwenhoven, D. van der Marel, and C. T. Foxon, *Phys. Rev. Lett*. **60**, 848 (1988).
2. R. de Picciotto, H. L. Stormer, L. N. Pfeiffer, K. W. Baldwin, and K. W. West, *Nature* **411**, 51 (2001).
3. V. Sánchez, L. A. Pérez, R. Oviedo-Roa, and C. Wang, *Phys. Rev*. B **64**, 174205 (2001).
4. W. A. Schwalm and M. K. Schwalm, *Phys. Rev*. B **37**, 9524 (1988).