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Electrical Conductivity and Localization in Quasiperiodic Lattices

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The electrical conductivity of Fibonacci lattices at zero temperature is studied by means of Kubo and Landauer formalisms, in which a tight-binding Hamiltonian of the system is considered. The localization of the eigenstates is quantified by using the participation ratio and the Lyapunov exponent. The results show a close behavior between the dc conductivity and the Lyapunov exponent. In addition, the effects of the boundary conditions on the ac conductivity are also analyzed in detail.

1. Introduction

Since the discovery of quasicrystalline alloys, the electronic localization in these aperiodic materials has been controversial. Nowadays, there is a consensus that the eigenvalue spectrum produced by a quasiperiodic potential is singular continuous and the associated eigenfunctions are critical[1]. Furthermore, the level statistics show an inverse-power-law level-spacing distribution[2], neither Wigner nor Poisson ones. Therefore, the electrical conductivity of these critically localized states becomes an especially interesting subject. In particular, Fibonacci quasiperiodic superlattices have been built[3] and their properties can be well understood by means of simple models[4]. The hopping conductivity in Fibonacci chains has been addressed by using the Miller-Abrahams equations[5] and by the dc Kubo-Greenwood conductivity[6]. Recently, *transparent states* with unity transmission coefficient have been found in mixing Fibonacci systems[7]. However, the ac conductivity of these transparent states is still an unclear issue. In general, the ac electrical conductivity at zero temperature is a good probe of the nature of the electronic eigenvalue spectrum and the localization of wave functions, since it depends not only on the states at the Fermi level but also on the global structure of the spectrum. On the other hand, the effects of the boundary conditions on the conductivity are not widely analyzed in the literature. In this work, a very sensitive influence of the saturator nature on the ac conduction of the system is reported.

2. Wave function localization and dc conductivity

In order to isolate the quasicrystalline effects, a simple *s*-band tight-binding Hamiltonian in a mixing Fibonacci system (MFS) is considered, where the MFS is built by alternating two sorts of atoms A and B following the Fibonacci sequence ($F_n=F_{n-1}\oplus F_{n-2}$) and the hopping integral between atoms depends on the nature of them. In this work, the first two generations are chosen as F_1=A and F_2=BA, and then, for example, F_4=BAABA. On the other hand, the ac electrical conductivity for a one-dimensional system at zero temperature can be calculated by means of the Kubo-Greenwood formula[8]

$$\sigma(E_F,\omega)=\frac{2e^2\hbar}{L\pi m^2}\int_{E_F-\hbar\omega}^{E_F} Tr\left[p\,\mathrm{Im}\,G^{+}(E+\hbar\omega)\,p\,\mathrm{Im}\,G^{+}(E)\right]dE\,,$$

where L is the system length, p is the momentum operator, and $G^{+}(E)$ is the retarded one-particle Green's function. For a perfect linear chain of N atoms saturated by two semi-infinite perfect chains, the dc conductivity within the energy band can be written as[9]

$$\sigma_p=\frac{e^2 a}{\pi\hbar}(N-1)\,.$$

In figures 1(a) the density of states, 1(b) the normalized dc Kubo conductivity, 1(c) the transmittance[1], 1(d) the inverse of the Lyapunov exponent[1], and 1(e) the participation ratio[8] are comparatively shown for a MFS of 2584 atoms with self-energies $\varepsilon_A=\varepsilon_B=0$, hopping integrals $t_{AA}=0.8t$ and $t_{AB}=t_{BA}=t$, and saturated by two semi-infinite perfect chains having hopping integrals t and null self-energies. The transparent state is indicated by a dashed line at E_F=0. Notice that there is an almost identical behavior between the spectra 1(b) and 1(c), since the dc conductivity is proportional to the transmittance through the Landauer formula[1]. Furthermore, a remarkable coincidence between figures 1(b) and 1(d) is also observed, contrary to the case of the figure 1(e), where the participation ratio is shown to be an inadequate quantity to characterize critically localized states.

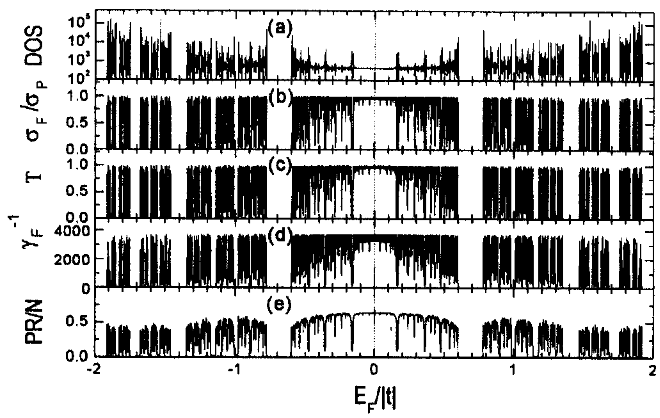
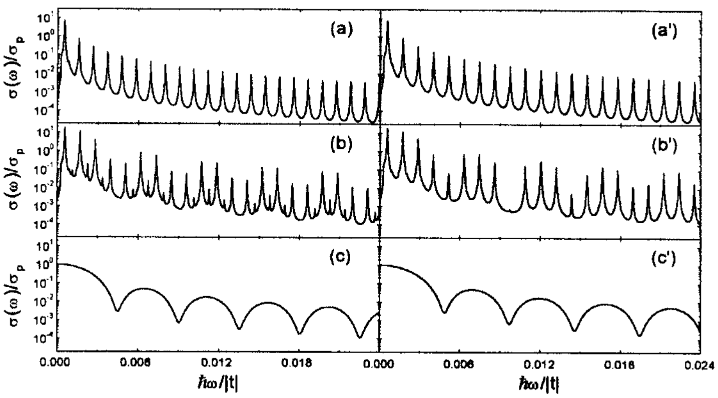


Figure 1: (a) Density of states (DOS), (b) Kubo conductivity (σ_F), (c) transmittance (T), (d) inverse of the Lyapunov exponent (γ_F^{-1}), and (e) participation ratio (PR) for a MFS of 2584 atoms, as explained in the text, with $\mathrm{Im}(E_F)=10^{-10}|t|$.

3. Boundary-condition effects on the ac conductivity

In figure 2, we show the ac Kubo conductivity with $E_F=0$ for three MFS with the same self-energies and hopping integrals as in figure 1, but different boundary conditions, *i.e.*, (a) 10946 atoms without saturators, (b) 2584 atoms with two 4181-atom perfect saturators, and (c) 2584 atoms saturated by two semi-infinite perfect linear chains. The corresponding results calculated for perfect systems are comparatively shown in figures 2(a′), 2(b′), and 2(c′). First, observe that the resonance peaks in figures 2(a′) and 2(b′) are located at the same frequencies, since they have the same eigenvalue spectrum. However, their strengths are very different, since the Kubo formula is evaluated for different system lengths. Similar behavior is found for the quasiperiodic case, except the resonance peaks are not located exactly at the same frequencies and new peaks appear in figure 2(b), because in these figures the Fibonacci segments are different and the selection rule is not expected to obey for the quasiperiodic case. On the other hand, the minima of the figures 2(b) and 2(c) seem to be located at the same values of frequency, and a continuous behavior is observed in figure 2(c) due to the semi-infinite saturators. Finally, notice that in figures 2(a) and 2(b) the ac conductivity exceeds σ_p for several frequencies, since σ_p is calculated using semi-infinite saturators.



Figures 2(a-c): The ac conductivity of three MFS with different boundary conditions, as explained in the text, is compared with the corresponding perfect cases shown in figures 2(a′-c′). The self-energies and hopping integrals of the MFS are the same as in figure 1 but with $\text{Im}(E_F)=10^{-5}|t|$.

4. Conclusions

In this work, we have analyzed the electrical conductivity and the localization behavior of the transparent state in a MFS. Very close spectra obtained from the inverse of the Lyapunov exponent, the Kubo and the Landauer formula are observed, except for the participation ratio, since it quantifies only the fraction of contributing sites to the wave function and does not indicate the coherence of them. It is important to stress that in spite of having presented only a special case of transparent states, the behavior reported in this paper has been verified for other MFS[9]. On the other hand, ac conductivity shows a general diminution as the frequency of the applied electrical field increases. However, it is highly sensitive to the boundary conditions: (1) for the case without saturators the ac conductivity decreases monotonically; (2) with finite saturators an oscillatory decreasing behavior is found; and (3) when semi-infinite saturators are introduced the ac conductivity becomes a smooth oscillating function of the frequency. These results have been confirmed analytically for the perfect case[9]. Finally, the diminution of the transparent-state ac conductivity is faster than that of a perfect linear chain; this fact seems to be related to the isolation of the transparent states in the spectrum of the MFS and the ac conductivity involves states within an interval of $\hbar\omega$ around the Fermi energy.

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