Conductivity of Quasiperiodic Systems: A Numerical Study

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We develop a new real-space method which allows one to evaluate the Kubo-Greenwood formula for dc conductivity of independent electrons in a static potential. We apply it to a numerical study of propagation modes in three dimensional quasiperiodic systems. These modes are strikingly different from those of periodic ones with regard to the effect of disorder. In particular, for Fermi energies in pseudogaps the conductivity can be stable or can even increase when disorder increases. [S0031-9007(97)04045-3]

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Recently, studies on transport in general topologically disordered media have emphasized the importance of understanding how localization of states and anomalous quantum transport are related [1]. For example, in disordered systems, close to a metal-insulator transition (at or close to mobility edges), localization aspects of wave functions can be described by multifractal analysis [2] and related to critical exponents of conductivity [3]. Another example is the problem of localization and transport properties in quasiperiodic systems. This has attracted a growing attention since the discovery of quasicrystals in 1984 [4]. Historically, Kohmoto *et al.* [5] were the first to propose that, at least in 1D systems, *quasiperiodicity induced long range correlations giving rise to an intermediate state of localization,* namely, "critical states" associated to *singular continuous* spectra. Numerical studies of quantum dynamics of wave packets [6] and Landauer resistances [7] manifested peculiar features such as bounded resistance $\rho_N \leq \rho_0 N^{\alpha}$, for energies E in the spectrum of the Hamiltonian, with α encoding the memory of these "quasiperiodic correlations." More recently, correlations between quantum dynamics and localization properties in Fibonacci chains have been rigorously analyzed by means of renormalization group treatments [8] and through new numerical methods (iterated function systems [9]).

Experimentally quasicrystalline phases have unique electronic properties. They are characterized by a low conductivity, which increases when temperature or disorder increases, and a proximity to a metal-insulator transition [10]. Since real systems always contain some defects either static, due to chemical or structural disorder, or dynamic, due to phonons, it is of great interest to know how conductivity is affected by disorder in a quasiperiodic system.

In this context, band structure calculations of periodic approximants have been performed. They predict flat bands which are associated to very low Fermi velocity. These flat bands are associated to states that have a multifractal character [11,12]. Estimates of the conductivity within the Bloch-Boltzmann theory (and the relaxation time approximation) lead also to small conductivities. However, the application of the Bloch-Boltzmann theory to these systems has been criticized [11,13]. Indeed, the propagation of electrons in the perfect quasiperiodic structure is neither ballistic as in the case of periodic systems nor diffusive as in the case of disordered systems. One expects, rather, scaling laws of the form $L(t) = At^{\beta}$ for the extension $L(t)$ of a wave packet, where β depends on the energy and on the Hamiltonian parameters. Thus in a first approximation the diffusivity will be given by $D = L(\tau)^2/3\tau = B\tau^{2\beta-1}$ where τ is the finite lifetime induced by disorder. In the context of a model this has been confirmed by the mathematical work of Bellissard and coworkers [14]. Since states tend to be localized, it has also been proposed that the mechanism of conductivity can be a hopping mechanism. In that case, according to the arguments [11,13], inelastic or even elastic scattering could lead to an increase of the conductivity.

In order to go beyond the Bloch-Boltzmann description and be able to test the various schemes that have been proposed, there is a natural starting point given by the linear response theory. This treatment does not make any assumption on the transport mechanism. In this Letter we present the first study, to our knowledge, of Kubo-Greenwood conductivity for independent electrons in static quasiperiodic potential at $T = 0$ K. Using a new real-space method, it will be shown that the electronic conduction in quasiperiodic systems differs strikingly from the prediction of a Bloch-Boltzmann approach. In particular, if V_{dis} measures the amplitude of the static disordered potential we will show that the conductivity does not vary like $\sigma = \sigma_0/V_{\mathrm{dis}}^2$ (where σ_0 is independent of disorder) in the weak scattering limit. Furthermore, the variation of conductivity with disorder is rather complex, and in particular it depends strongly on the position of the Fermi energy with respect to pseudogaps.

For independent electrons in a given static potential $T = 0$ K, the starting point of the method will be the following form of Kubo-Greenwood (E is the Fermi energy):

$$\sigma_{\mathrm{dc}}(E) = \frac{2\hbar e^2 \pi}{\Omega} \mathrm{Tr}[\hat{V}_x \delta(E - \mathcal{H}) \hat{V}_x \delta(E - \mathcal{H})].$$

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$\hat{V}_x$ is a component of the velocity operator along direction x. $\delta(E - \mathcal{H})$ is the projector on eigenstates H of energy E. Ω is the volume of the system. The factor 2 comes from the spin degeneracy. In this work, the evaluation of the Kubo-Greenwood formula is made through a new real-space method. In a previous work [15] we developed a method for calculating dc and ac conductivity using the formalism of orthogonal polynomials. Here, based on the same formalism, we develop a method which gives access only to dc conductivity. In counterpart this allows an important gain in precision and numerical stability. For convenience, after some simple algebra one can rewrite $\sigma_{\mathrm{dc}}(E)$ as

$$\sigma_{\mathrm{dc}}(E) = \lim_{t\to\infty} F(E,t),$$

$$F(E,t) = \frac{2\hbar e^2\pi}{\Omega}\,\mathrm{Tr}\Big\{\frac{1}{t}[\hat{X}(t) - \hat{X}] \times \delta(E - \mathcal{H})[\hat{X}(t) - \hat{X}]\Big\}.$$

Here $\hat{X}(t) = e^{i\mathcal{H}t/\hbar}\hat{X}e^{-i\mathcal{H}t/\hbar}$ where $\hat{X}$ is the component along direction x of the position operator. At this stage, we define for each orbital $|j\rangle$:

$$|\Phi_j(t)\rangle = \hat{X}e^{-i\mathcal{H}t/\hbar}|j\rangle,$$

$$|\tilde{\Phi}_j(t)\rangle = \frac{|\Phi_j(t)\rangle}{\||\Phi_j(t)\rangle\|}.$$

Here $|\tilde{\Phi}_j(t)\rangle$ is a normalized state. The calculation of conductivity can be reduced to

$$\frac{2\hbar e^2\pi}{\Omega}\sum_j \mathcal{D}_j(t)\langle\tilde{\Phi}_j(t)|\delta(E - \mathcal{H})|\tilde{\Phi}_j(t)\rangle.$$

For each initial state at $|j\rangle = |\Psi(t=0)\rangle$, we can take the origin at j. This means that $\langle j|\hat{X}|j\rangle = 0$. Then $\mathcal{D}_j(t)$ is given by

$$\mathcal{D}_j(t) = \frac{\langle\Psi_j(t)|\hat{X}^2|\Psi_j(t)\rangle}{t}.$$

The conductivity can thus be calculated from $\mathcal{D}_j(t)$ and the spectral quantity related to $|\tilde{\Phi}_j(t)\rangle$. The spectral quantity is calculated by the recursion method [16]. The original part of our method is the evaluation of $|\Psi_j(t)\rangle$. Our method, to solve the Schrödinger equation, avoids the use of Runge-Kutta resolution algorithms, or numerical procedures of diagonalization. It is based on the development of $\delta(E - \mathcal{H})$ already used in [15], which implies also a development of the unitary operator $e^{-i\mathcal{H}t/\hbar}$ on a basis of orthogonal polynomials. Hereafter, we will take Chebyshev polynomials of the first kind associated to the weight $\rho(E) = 1/[\pi\sqrt{4b_\infty^2 - (E - a_\infty)^2}]$ and defined via the recursive relations

$$Q_0(E) = 1, \qquad Q_1(E) = \frac{E - a_\infty}{2b_\infty},$$

$$Q_{n+1}(E) = \left(\frac{E - a_\infty}{b_\infty}\right)Q_n(E) - Q_{n-1}(E),$$

where a_∞ and b_∞ are chosen as band parameters in accordance with the ones of the true density of states (via a first recursion process). Then the vector under study reads

$$e^{-(i\mathcal{H}t/\hbar)}|j\rangle = \sum_n h_n\Big(\int dE\rho(E)Q_n(E)e^{-(iEt/\hbar)}\Big)Q_n(\mathcal{H})|j\rangle$$

$$= \sum_n h_n i^n J_n\left(\frac{-2b_\infty t}{\hbar}\right)e^{(-ia_\infty t/\hbar)}Q_n(\mathcal{H})|j\rangle.$$

$h_0 = 1$ and for other n $h_n = \frac{1}{2}$. As usual with orthogonal polynomials the $Q_n(\mathcal{H})|j\rangle$ are evaluated via the recurrence property [16]. Amplitudes of $e^{-(i\mathcal{H}t/\hbar)}|j\rangle$ on this basis have a rather simple form connected to Bessel functions. The consequent interest is to get nice asymptotic behaviors for these coefficients which converge very quickly as $n \to \infty$, given that $\lim_{n\to\infty} J_n(z) \sim (1/\sqrt{2\pi n})(ez/2n)^n$. It is this development that makes the calculation quick and precise.

For each j the calculation is performed on a cube, centered on the site j, which length is 100 sites (the cube contains about 10^6 sites). Also, for practical calculations, the sum is performed over ~100 sites of origin. We find that this is sufficient for our purpose. We have performed numerous tests (more details can be found elsewhere [17]) to ensure that the convergence is achieved. We estimate that the conductivity is calculated with an energy resolution of a few percent of the bandwidth, which is enough for our purpose. As for the calculation of conductivity, the total computing time is of the order of 100 h on a HP735 for each conductivity curve $\sigma_{\mathrm{dc}}(E)$ (see below).

We performed calculations of quantum diffusion and Kubo-Greenwood conductivity at $T = 0$ K. We consider an s-band tight-binding model on a simple cubic lattice with nearest-neighbor hopping which has already been studied by several authors [18,19]. The hopping integral is the energy unit ($t = 1$) and the on-site energies are given by $\varepsilon_j = \varepsilon_{x_j} + \varepsilon_{y_j} + \varepsilon_{z_j} + \varepsilon_{\mathrm{dis}}$ with $\varepsilon_{\mathrm{dis}} = \text{random number} \in [-(V_{\mathrm{dis}}/2), +(V_{\mathrm{dis}}/2)]$ and $\varepsilon_{j_\alpha} = \pm V_{\mathrm{qp}}$ constraints to quasiperiodic correlations (Fibonacci sequence). This model allows a direct comparison between a quasiperiodic system and a periodic one since for $V_{\mathrm{qp}} = 0$ one recovers the classical Anderson model with diagonal disorder. We note also that for $V_{\mathrm{dis}} = 0$ the Hamiltonian is separable. An eigenstate $\Psi(x,y,z)$ can be written as the product of eigenstates of the chains along each direction $\Psi(x,y,z) = \Psi_1(x) \times \Psi_2(y) \times \Psi_3(z)$, the energy being

the sum of the three energies $E = E_1 + E_2 + E_3$. This means also that for a state that is initially localized on a site j one has $\Psi_j(x, y, z, t) = \Psi_1(x, t) \times \Psi_2(y, t) \times \Psi_3(z, t)$ with $\Psi_1(x, t = 0) = \delta(x - x_j)$ and similarly for y and z. Obviously, the Hamiltonian is no more separable when V_{dis} is nonzero.

We study the quantum diffusion through $D_j(t)$. For $V_{\text{dis}} = 0$ the above relation shows that $D_j(t)$ is the same as for a one dimensional model [8]. In this study we focus on the effect of disorder. Our results (see Fig. 1), clearly show that conduction modes undergo a transition from nonballistic to diffusive regime [i.e., $D_j(t)$ is independent of t at large t]. When the disorder increases, the transition to the diffusive regime occurs at shorter times, and the asymptotic value of $D_j(t)$ tends to decrease. We note also that the fluctuations of $D_j(t)$ are less important when the disorder increases.

We studied also the conductivity $\sigma_{\text{dc}}(E)$ and its variation with the strength of disorder. In a metal one expects a law of the form $\sigma = \sigma_0/V_{\text{dis}}^2$ (σ_0 is independent of disorder). Indeed, this is what we find for $V_{\text{qp}} = 0$. For sufficiently small values of disorder, our numerical results are in good agreement with the prediction of the Bloch-Boltzmann approximation [17]. However, the enhancement of disorder in a quasiperiodic system leads to a different law. For instance, in Fig. 2 the conductivity decreases when the disorder increases but does not follow the law $\sigma = \sigma_0/V_{\text{dis}}^2$ (note that the density of states is nearly independent of disorder in this parameter range). Instead, we get approximately for each energy E a law of the form $\sigma = \sigma_0/V_{\text{dis}}^{\alpha}$. Our results do not strictly follow a power law, probably because such laws apply only to the limit of infinitely small disorder, and also due to the finite accuracy of our method. Depending on the energy E we find $\alpha = 0.4-0.8$ in our calculation.

In Fig. 3, we show the conductivity for a quasiperiodic modulation $V_{\text{qp}} = 1.1$. A striking result is that there are particular zones, identified by pseudogaps, which seem quite insensitive to a tremendous increase of disorder (a factor of 16 for V_{dis}^2). The conductivity varies monotonically for intermediate values of disorder not shown here. The inset in Fig. 3 shows the average density of states. The density of states increases slightly with disorder in the pseudogaps. This increase compensates for the decrease of diffusivity leading to a nearly constant conductivity. In regions of high density of states, which correspond also to higher conductivity, both density and diffusivity decrease.

In Fig. 4 we show $\sigma_{\text{dc}}(E)$ for $V_{\text{qp}} = 2.5$ and different values of V_{dis} (again the conductivity varies monotonically for intermediate values of disorder not shown here). The variation of conductivity with energy is rather complex. We note, however, that the conductivity increases with V_{dis} for some energies that correspond to pseudogaps. In contrast to the previous cases there is an important change of the density of states. It increases where the conductivity increases. It means that the electronic structure is deeply modified by the disorder. Thus we prove that the localization induced by a quasiperiodic potential can be destroyed by a disordered potential.

A direct comparison with experimental results on quasicrystals is difficult, since our model does not

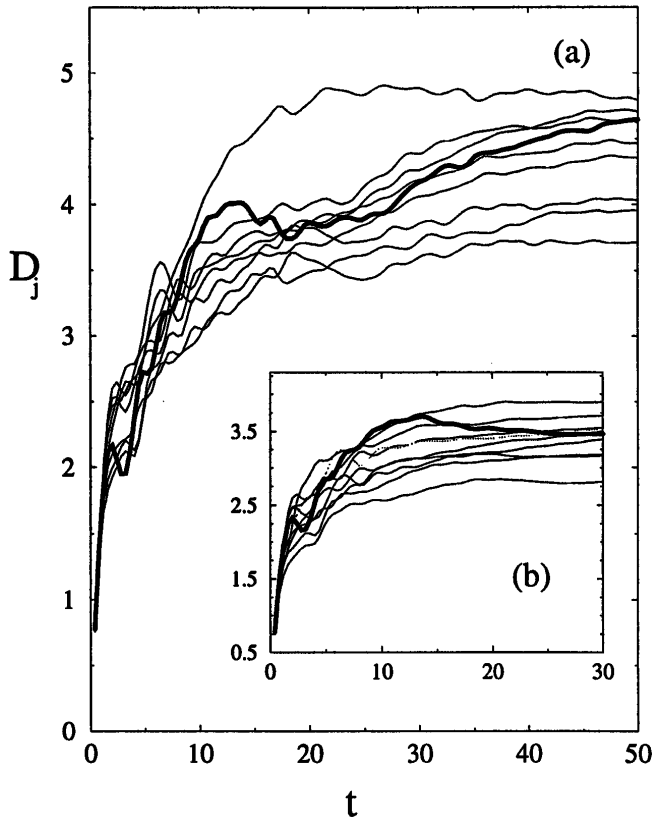

FIG. 1. $\mathcal{D}_j(t)$ represented for several initial sites j and $V_{\text{qp}} = 0.9$. Time is in units of $2\hbar/W$ where W is the bandwidth. Lengths are in units of the nearest-neighbor distance. (a) $V_{\text{dis}} = 2$; (b) $V_{\text{dis}} = 2\sqrt{2}$. The thick line is an aid to visualize one of the curves.

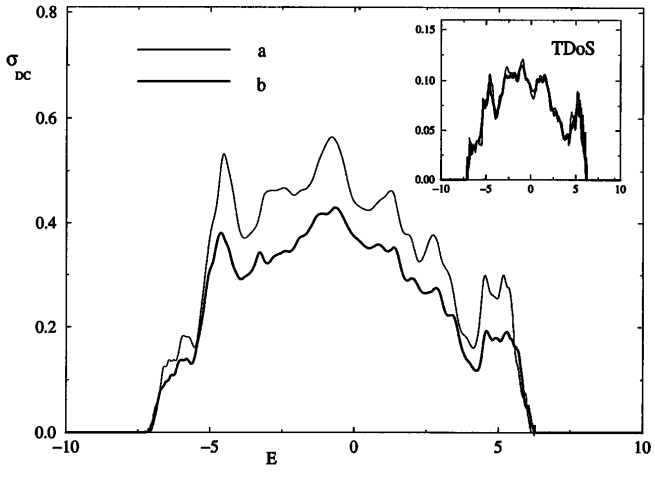

FIG. 2. Conductivity $\sigma_{\text{dc}}(E)$ for $V_{\text{qp}} = 0.7$ [average value over sites "j" of $\lim_{t\to\infty} D_j(t)N_j(E)$ where $N_j(E)$ is the spectral weight on the state $|\tilde{\Phi}_j(t)\rangle$]. The energy unit is the hopping integral t. Inset: Average density of states. (a) $V_{\text{dis}} = 2$; (b) $V_{\text{dis}} = 2\sqrt{2}$.

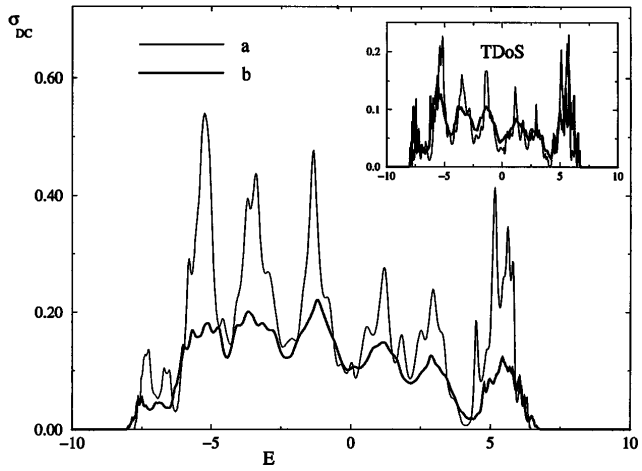

FIG. 3. Conductivity $\sigma_{dc}(E)$ for $V_{qp} = 1.1$ as a function of the Fermi energy E for different values of the disorder parameter. Inset: Average density of states. (a) $V_{dis} = 1/\sqrt{2}$; (b) $V_{dis} = 2\sqrt{2}$.

provide a realistic description of the electronic structure and of the local atomic order. However, quite remarkably, when the Fermi energy lies in a pseudogap, which is the case experimentally, the behavior of the conductivity is reminiscent of the experimental observation that the conductivity increases with disorder or with temperature [10].

In conclusion, the contribution of this paper is twofold. First, our method opens new ways of investigating transport properties. Second, we demonstrate the complexity of electronic transport in quasiperiodic systems, in the context of anomalous localization. For sufficiently small disorder the variation of conductivity follows qualitatively scaling laws. At strong disorder the conductivity can be stable or can even increase upon enhancement of disorder, especially for Fermi energies in a pseudogap.

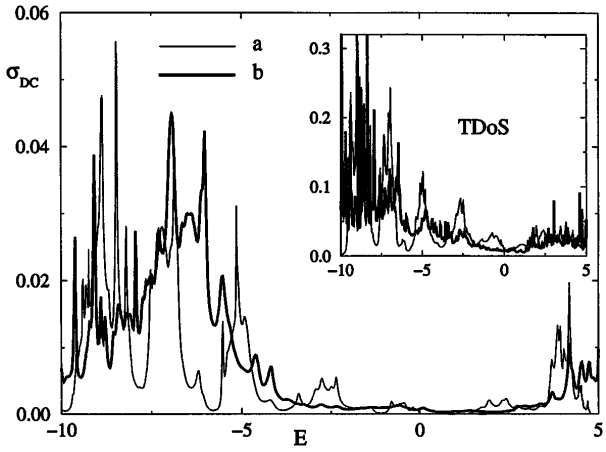

FIG. 4. Conductivity $\sigma_{dc}(E)$ for $V_{qp} = 2.5$ as a function of the Fermi energy E for different values of the disorder parameter. Inset: Average density of states. (a) $V_{dis} = 2$; (b) $V_{dis} = 4\sqrt{2}$.

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