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Sub-diffusive electronic states in octagonal tiling

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Abstract. We study the quantum diffusion of charge carriers in octagonal tilings. Our numerical results show a power law decay of the wave-packet spreading, $L(t) \propto t^{\beta}$, characteristic of critical states in quasicrystals at large time t. For many energies states are sub-diffusive, i.e. $\beta < 0.5$, and thus conductivity increases when the amount of defects (static defects and/or temperature) increases.

Experimental investigations have indicated that the conduction properties of many stable quasicrystals (AlCuFe, AlPdMn, AlPdRe, ...) are unusual and differ strongly from those of simple inter-metallic alloys [1-3]. In particular their conductivity increases with static defects density and when temperature increases. It appears also that the medium range order and the chemical order –over one or a few nanometers– have a decisive influence [4-9]. There is now strong evidence that these non standard properties result from a new type of break-down of the semi-classical Bloch-Boltzmann theory of conduction [10-14]. On the other hand, the specific role of long range quasiperiodic order in electronic properties is still an open question in spite of a large number of studies (Refs. [15-37] and Refs. therein). Many studies support the existence of critical states, which are neither extended nor localised, but are characterised by a power law decay of the wave-function envelope at large distances. In the presence of critical states, the diffusion of charge carrier at sufficiently large time t follows a power law and then the spatial extension L of wave-packets should be, [34-37]

$$L(E,t) \propto t^{\beta(E)} \text{ at large } t, \tag{1}$$

where β, $0 \leq \beta \leq 1$, is an exponent depending on energy E and on the Hamiltonian model. Note that in usual metallic crystals without static defects, $\beta = 1$ and the propagation is ballistic. In strongly disordered systems, $\beta = 0.5$ for a large time range and propagation is diffusive. For a localised state one has $\beta = 0$. When disorder is introduced in the perfect approximant or perfect quasicrystal in the form of static defects (elastic scatterers) and/or inelastic scattering (temperature, magnetic field...), the defects induce scattering and we expect that there is an associated time τ above

which the propagation of the wave-packet is diffusive. The diffusivity D of charge carrier at energy E can be estimated by, $D(E,\tau) \simeq L(E,t=\tau)^2/\tau \propto \tau^{2\beta(E)-1}$, and the conductivity σ at zero frequency is given by the Einstein formula:

$$\sigma(E_F,\tau) = \mathrm{e}^2 n(E_F) D(E_F,\tau) \propto \tau^{2\beta(E_F)-1}, \tag{2}$$

where n is the density of states and E_F the Fermi energy. The case $0.5 < \beta < 1$, called super-diffusive regime, leads to transport properties similar to metal, since the conductivity decreases when disorder increases –i.e. when τ decreases–. Conversely, for $0 < \beta < 0.5$, the regime is sub-diffusive and the conductivity increases when disorder increases like in real quasicrystals. Many authors consider [18-20,29,34-37] that critical states could lead to $\beta < 0.5$ but it has not yet been shown in 2D or 3D quasiperiodic structures (except for some very specific energies).

Model Hamiltonian.– The octagonal, or Ammann-Beenker, tiling [38, 39] is a quasiperiodic tiling analogous to the notorious Penrose tiling. This tiling has been often used to understand the influence of quasiperiodicity on electronic transport [18-25]. A sequence of periodic approximants $X_0, X_1, \ldots, X_k, \ldots$ can be generated [40]. In approximants of order $k \geq 1$, the 6 local configurations around vertexes are the same as in the octagonal quasiperiodic tiling. They have, respectively, coordination number $\eta = 3, 4, 5, 6, 7$ and 8. We consider the simple Hamiltonian,

$$\hat{H} = \sum_i \epsilon_i c_i^* c_i + \sum_{\langle i;j \rangle} \gamma c_i^* c_j + h.c., \tag{3}$$

where i indexes s orbitals located on vertexes, and γ is the strength of the hopping between orbitals. $\langle i,j \rangle$ are the nearest-neighbours at tile edge distance a. To simulate schematically a possible effect of the presence of different chemical elements, the one-site energy ϵ_i is proportional to the coordinance η_i of the site i: $\epsilon_i = \eta_i \gamma$. To obtain realistic time values, we use $\gamma = 1\,\mathrm{eV}$ which is the order of magnitude of the hopping parameter in real inter-metallic compounds. The total density of states (total DOS) of X_7 approximant is shown figure 1(a).

Quantum diffusion.– In the framework of Kubo-Greenwood approach for calculation of the conductivity, we use the polynomial expansion method developed by Mayou, Khanna, Roche and Triozon [41, 42, 31, 27, 28] to compute the mean square spreading of the wave-packet at time t and energy E: $L^2(E,t) = \langle (\hat{X}(t) - \hat{X}(0))^2 \rangle_E$, where $\hat{X}$ is the position operator in the x-direction. The diffusion coefficient $\mathcal{D}(E,t) = L(E,t)^2/t$ is shown in figure 1(b) for X_7 approximant at some energies. The ballistic regime due to the periodicity of the approximant is reached at very large t, when $L(t) > L_k$ where L_k is the approximant cell size; then $L(t) = V_B t$, where V_B is the Boltzmann velocity, *i.e.* the intra-band velocity, $V_B = \langle \partial E_n(k)/\partial k_x \rangle_E/\hbar$, where $E_n(k)$ is the band dispersion relation [12]. For X_7 in time range shown figure 1, this Boltzmann term is negligible and, for all purposes of this discussion, the X_7 approximant is equivalent to the quasiperiodic system. Depending on the t values, three different regimes are observed at each energy:

- At very small time, typically when $L(t) < a$, the mean spreading grows linearly with t, $L(t) = V_0 t$ (ballistic behaviour), where $V_0 > V_B$ [10, 12].
- For times, corresponding to $L(t) \gtrsim$ a few a, the propagation seems to become diffusive as the diffusion coefficient is almost constant, $\mathcal{D}(t) \simeq \mathcal{D}_{dif}$. Therefore L_1,

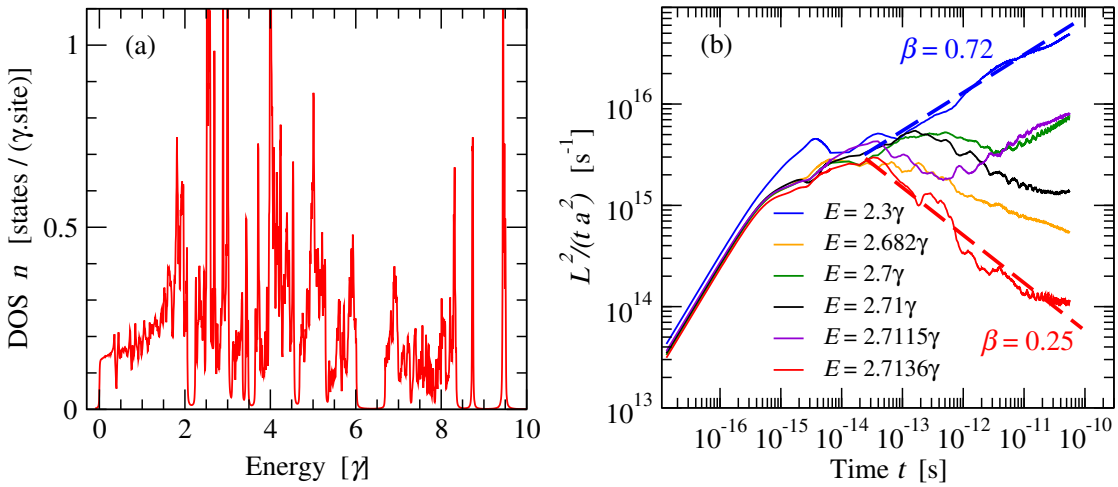

Figure 1. Density of states and quantum transport in perfect X_7 octagonal approximants (number of sites per cell $N = 275807$, unit cell $478a \times 478a$, with a the tile edge length): (a) Total DOS n (the recursion method induces a convolution of $n(E)$ by a Lorentzian of width 5 meV), (b) diffusive coefficient $\mathcal{D}(t) = L(t)^2/t$ for various E.

defined by $L_1 = \mathcal{D}_{dif}/V_0 \simeq$ a few a, is a kind of effective elastic scattering length but it is not due to static scattering events because we consider perfect tilings. The corresponding effective elastic scattering time is $t_1 = L_1/V_0$. Roughly speaking, it seems that when $L(t) \gtrsim L_1$, *i.e.* $t \gtrsim t_1$, the wave-packet feels a random tiling.

- An other distance L_2 (respectively an other time t_2, $L(t_2) = L_2$) appears. For $L(t) > L_2 \simeq$ a few $10a$, a new regime appears and $\mathcal{D}(t)$ follows a power law. It is thus characteristic of the medium and long range quasiperiodic order. Figure 1(b) shows that the β value can switch from a sub-diffusive regime ($\beta < 0.5$) to a super-diffusive regime ($\beta > 0.5$) over a small variation of energy. The t_2 values, $t_2 \simeq 10^{-13}$–10^{-14} s, have the order of magnitude of the scattering time above which measurements show unusual transport properties in quasicrystals [1].

Both distances $L_1 \simeq$ a few a, $L_2 \simeq$ a few $10a$, and the exponent β at time $t > t_2$, depend a lot on the energy value E. $L_1 < L_2$, but at some energy it even seems that $L_1 \simeq L_2$. Further analysis are necessary to understand the energy dependence.

To summarise, we have presented quantum diffusion in a large approximant of the octagonal tiling. The charge carrier propagation is determined by the wave-packet spreading in the quasiperiodic lattice. From numerical calculation, two length scales seem to characterise this quasiperiodic spreading. L_1, typically $L_1 =$ a few a, above which the propagation is almost diffusive in spite of the absence of static defects. L_2, typically $L_2 =$ a few $10a$, above which specific quasiperiodic symmetries lead to a power law dependence of the root mean square spreading, $L(t) \propto t^{\beta}$. For some energies states are super-diffusive or diffusive, *i.e.* $\beta \geq 0.5$, whereas for other energies, a sub-diffusive regime, *i.e.* $\beta < 0.5$, sets in as expected for critical states characteristic of quasiperiodicity. This sub-diffusive regime is the generalisation to quasicrystal of the

non-Boltzmann propagation found in realistic approximants of i-AlMnSi and i-AlCuFe [10, 11], in the complex inter-metallic alloys λ-AlMn [12], and in small approximants of octagonal and Penrose tilings [13, 14].

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