Modeling the electrical conductivity of icosahedral quasicrystals

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A model for the electronic structure of icosahedral quasicrystals is proposed on the basis of a number of pertinent experimental results. From this model we obtain a closed analytical expression for the electrical conductivity accurately describing the most remarkable features observed in the $\sigma(T)$ curves of high quality quasicrystals. As a convenient working example we compare the theoretical description provided by our treatment with a series of suitable experimental data for the *i*-AlCuRu, unveiling a relationship among the density-of-states structure, the sample stoichiometry, and the electrical conductivity of different samples at different temperature ranges.

I. INTRODUCTION

The discovery of thermodynamically stable quasicrystalline alloys of high structural quality in the AlCu(Fe,Ru,Os) and AlPd(Mn,Re) systems,[1] and decagonal AlCo(Cu,Ni) system,[2] has allowed for detailed experimental studies of transport properties in quasicrystals (QC's). In this way, unusual behaviors in the temperature dependence of electrical conductivity, Hall and Seebeck coefficients, specific heat and thermal conductivity, have been reported.[3–6] From these experimental results a fundamental question arises, concerning whether the purported anomalies in the quasicrystals transport properties should be mainly attributed (or not) to the characteristic *quasiperiodic order* of their structure. Two different approaches to this question can be found in the literature. On the one hand, attempts are made to explain the transport properties of QC's in terms of concepts originally developed to describe amorphous solids. On the other hand, more specific treatments aimed to exploit the physical implications of the quasiperiodic order notion have been progressively introduced. Both approaches have obtained partial successes in describing different experimental data, thus spurring the interest for a suitable theory of quasicrystalline matter.[7]

Theoretical efforts towards this goal have rendered two main results concerning the electronic structure of QC's. The first one refers to the presence of a pronounced pseudogap at the Fermi level. The second one concerns the existence of spiky features in the density of states (DOS) near the Fermi level. The presence of a pseudogap was theoretically predicted in order to explain the stability of quasicrystalline alloys[8] and its physical existence has received strong experimental support in the last few years, as indicated by measurements of the specific-heat capacity at low temperatures,[9] photoemission[10] and soft x-ray spectroscopies,[11] or magnetic susceptibility and nuclear magnetic resonance probes.[12] On the other hand, the existence of a spiky fine structure of the electronic DOS over an energy scale of about 10 meV has been obtained in self-consistent *ab initio* calculations dealing with several suitable quasicrystalline approximants.[13] The physical origin of such peaks may stem from the structural quasiperiodicity of the substrate via a hierarchical cluster aggregation resonance[14] or through *d*-orbital resonance effects.[15] However, the possible existence of spiky features in the DOS has remained quite elusive to experimental confirmation,[16–18] until two recent works have provided feasible support to both the physical existence of a spiky DOS component and its possible self-similar nature.[19,20]

In the light of this broad collection of experimental results it becomes quite appealing to reconsider one of the most important open questions in the field, namely, that regarding whether the purported anomalies in the transport properties observed in high quality QC's can be satisfactorily accounted for by merely invoking band-structure effects or, alternatively, these anomalies should be traced back to the critical nature of the electronic states. At this stage, it seems quite reasonable that the proper answer may likely require a *proper combination* of both kinds of effects. In fact, on the one hand, certain experimental facts, such as the relative insensitivity of the specific-heat electronic term γ to thermal annealing (as compared to the strong dependence of the electrical conductivity itself), suggests that the purported low values of σ_{4K} cannot be satisfactorily explained by solely invoking the existence of a pseudogap. This conclusion is further stressed by the unrelated variations of σ_{4K} and γ among different and AlPdRe samples,[21] as well as for the relative insensitivity of γ to the chemical composition observed in several AlCuFe samples.[22] On the other hand, it has been suggested that when the energy spacing between the electronic bands in the vicinity of the Fermy level becomes very small, as it occurs in the case of quasicrystalline approximants, the transport may turn out to be anomalous because tunneling occurs between different bands, causing the instability of the wave-packet coherence,[23] hence reinforcing the view that band-structure effects should also play a significant role in the anomalous transport properties of QC's.

Keeping in mind both possible contributions, the aim of this work is twofold. In the first place, we consider the temperature dependence of the electrical conductivity $\sigma(T)$, showing that its behavior can be satisfactorily described in terms of a closed analytical expression over a wide temperature range (4–650 K). To this end, we will introduce a suitable model for the electronic structure of icosahedral QC's, along with some reasonable assumptions about the physical behavior of charge carriers associated with critical states.

Our proposed model will take into account *both* the existence of a pseudogap near the Fermi level *and* the presence of a *self-similar distribution of spiky features* in the DOS. In the second place, we consider the purported sensitivity of the $\sigma(T)$ curves to the chemical composition, arriving at the conclusion that it should be mainly attributed to a *systematic shift of the Fermi level* position due to the different stoichiometry of the corresponding quasicrystalline samples. To this end, we will compare the theoretical $\sigma(T)$ curves derived from our model with pertinent experimental data for *i*-AlCuRu QC's of different compositions.[24,25] By properly adjusting a number of physical parameters, we obtain a remarkable agreement between experimental and theoretical conductivity curves. In this way, our approach may be considered as a promising first step to gain a better understanding of transport properties in quasicrystalline matter in terms of a *phenomenological* description of the electrical conductivity in QC's.

The paper is organized as follows. In Sec. II we describe our approach to the study of the electrical conductivity and introduce the main features of the electronic structure proposed in our DOS model. In Sec. III we obtain a closed analytical expression for the electrical conductivity. Section IV is devoted to compare the analytical expressions with experimental conductivity curves. Final comments and discussions are contained in Sec. V.

II. THE MODEL

A. Electrical conductivity

Following previous works by Pierce and collaborators,[25,26] we will start by assuming that the electrical conductivity can be described by the general expression[27]

$$\sigma(T)=\frac{e^2}{\Omega_0}\int_{-\infty}^{+\infty}dE\left(-\frac{\partial f}{\partial E}\right)\sigma(E), \tag{1}$$

where e is the electron charge, Ω_0 is the unit-cell volume, E is the energy, f is the Fermi function, and $\sigma(E)$ is the conductivity spectrum defined as the $T\rightarrow 0$ conductivity with the Fermi level at energy E. Expression (1) describes a weighted average of the conductivity spectrum $\sigma(E)$ over the energy range determined by the Fermi distribution at a given temperature. Generally speaking the conductivity spectrum will take into account both band-structure effects and those effects which may be related to the critical nature of the eigenstates. Consequently, we can express $\sigma(E)\equiv N(E)D(E)$, where $N(E)$ is the DOS and $D(E)$ is the electronic diffusivity. Then, by integrating expression (1) by parts, we obtain

$$\sigma(T)=\frac{e^2}{\Omega_0}u(T)\left[D(E)-\int_{-\infty}^{+\infty}dE\left(-\frac{\partial D}{\partial E}\right)\right], \tag{2}$$

where

$$u(T)\equiv\int_{-\infty}^{+\infty}dE\left(-\frac{\partial f}{\partial E}\right)N(E). \tag{3}$$

Expression (2) indicates that the conductivity variation with the temperature will be dependent on the electronic structure, through the factor $u(T)$, but also on the nature of the electron wave functions through the diffusivity dependent factor. Within the Bloch-Boltzmann treatment it is customary to express $D(E)\simeq v^2(E)\tau(E)$, where $v(E)$ denotes the carriers group velocity and $\tau(E)$ is the relaxation time. The application of Bloch-Boltzmann theory to quasiperiodic systems has been criticized[3,28,29] on the basis that scaling properties of critical wave functions may lead to nonballistic transport of the electrons. However, at present, we cannot definitively exclude the Bloch-Boltzmann scheme. In fact, it has been shown that, in some instances, quasiperiodic models are able to support *extended* electronic states.[30,31] Consequently, the role played by the peculiar nature of critical states in the anomalous transport properties observed in QC's requires a closer scrutiny aimed to clarify the relationship between the spatial structure of critical states and their related transport properties.[32]

To proceed we introduce a simplifying working hypothesis and assume that the energy dependence of the electronic diffusivity in expression (2) is quite smooth as compared with the energy dependence of the DOS, so that to a first approximation $D(E)\simeq D_0$ and the integral appearing in Eq. (2) vanishes. In fact, a low value for the electronic diffusivity has been obtained in a number of numerical simulations dealing with realistic quasiperiodic systems.[29] In addition, experimental evidence supporting this assumption comes from angle-resolved photoelectron spectra showing *flat narrow* bandlike features indicating quite small group velocities for the charge carriers.[33] By expressing Eq. (3) in terms of the scaled variable $x\equiv(E-\mu)/k_BT$, where μ denotes the Fermi level position, and k_B is the Boltzmann constant, and plugging it into Eq. (2) we get

$$\sigma(T)=A\int_{-\infty}^{+\infty}N(x)\,\mathrm{sech}^2(x/2)\,dx, \tag{4}$$

where $A\equiv e^2D_0/4\Omega_0$ and we have expressed the derivative of the Fermi function in terms of hyperbolical functions. At this point it is worth noticing that with the working hypothesis introduced before we are not neglecting the possible role of critical states in the transport properties of QC's, since such influence is included in the (phenomenological) parameter A. This important question will be further elaborated in Sec. III.

B. DOS model

Low resolution (in general about 0.3–0.5 eV) photoemission spectroscopy has provided substantial evidence on the existence of a broad and smooth pseudogap in several quasicrystalline alloys.[11,16] Photoemission studies of better resolution (in the range 0.15–0.05 eV) are also consistent with this broad feature, without any fine spiky component.[10,33] Investigation of AlCuFe quasicrystalline films by scanning tunneling spectroscopy at low temperatures has given evidence for a narrow, symmetric dip about 60 meV wide located around the Fermi level.[34] A subsequent STM investigation of better resolution on AlCuFe and AlPdRe quasicrystalline ribbons confirmed the presence of a pseudogap about 50 meV wide and did not show evidence for finer structures in the DOS over the energy region extending about 0.5 eV from the Fermi level.[35] The existence of a sharp DOS valley of about 20 meV at the Fermi level in

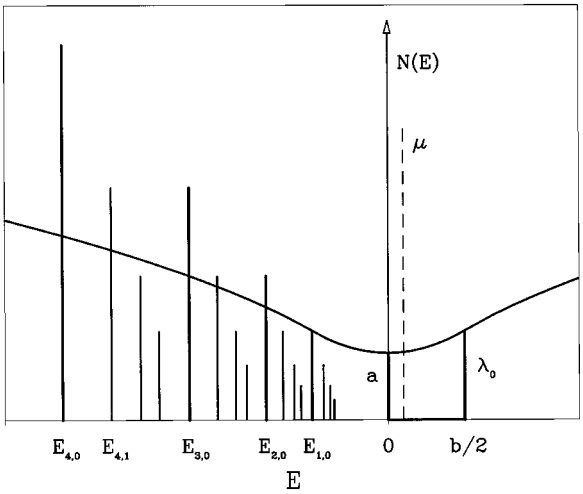

FIG. 1. Diagram showing the different contributions to the QC electronic structure in our proposed DOS model.

both quasicrystalline and approximant phases has been confirmed by nuclear magnetic-resonance studies, which are able to probe the bulk properties of the considered samples.[36] These observations indicate that the dip centered at the pseudogap is not a surface feature and that both its width and depth are sample dependent. On the other hand, the possible dependence of the pseudogap structure with the temperature has been recently investigated by means of tunneling and point contact spectroscopy, and it has been reported that the width of the broad pseudogap remains essentially unmodified as the temperature is increased from 4 to 77 K. On the contrary, the dip feature centered at the Fermi level exhibits a significant modification, progressively deepening and narrowing as the temperature is decreased.[19]

By collecting all the relevant information provided by this set of different experimental measurements we propose a DOS structure around the Fermi level which includes *two* main contributions at $T=0$, as it is sketched in Fig. 1. In the first place, we include the contribution due to a relatively broad pseudogap (~ 0.5 eV) which, according to the STM and NMR measurements discussed above, should contain two main features: (i) a contribution due to a narrow (~ 0.06–0.02 eV) and symmetric *parabolic dip* N_d, located close to the Fermi level and, (ii) a contribution due to a *square-root* term N_{sr}, beyond the narrow dip region. Accordingly, the DOS around the Fermi level will be described by the function

$$\begin{cases} N_d(E)=a+\alpha E^2 & |E|\leqslant b/2 \\ N_{sr}(E)=d+c\sqrt{|E|} & |E|>b/2, \end{cases} \tag{5}$$

where a gives the DOS value at the origin of the energy scale [note that, in general, $a\neq N(E_F)$], $\alpha\equiv\frac{1}{2}(d^2N/dE^2)$ measures the curvature of the dip, b is the dip width, and the constants $c=2\alpha b\sqrt{b/2}$ and $d=a-3\alpha b^2/4$ guarantee the derivability and continuity of the DOS at $E=b/2$.

In the second place, we consider an additional contribution due to a *self-similar distribution* of spiky DOS features. The need for such a contribution is well documented on theoretical grounds. In fact, the existence of a dense set of narrow peaks (~ 0.01–0.02 eV) in the DOS appears as a quasiperiodicity related outcome in a number of realistic calculations.[13] In addition, a number of structural models strongly suggest that the DOS should exhibit a self-similar structure originating from long-range correlated cluster packing.[14]

Notwithstanding this, the possible existence of the spiky component of the DOS is still awaiting for a definitive experimental confirmation. Thus, as we have previously mentioned, both high-resolution photoemission and tunneling spectroscopies have failed to detect the theoretically predicted dense distribution of spiky features around the Fermi level. Several reasons have been invoked in order to explain these unsuccessful results. Among them, the existence of some residual disorder present even in samples of high structural quality has been invoked as a plausible agent smearing out the finer details of the DOS.[17] It has also been argued that photoemission and scanning tunnel microscope techniques probe the near surface layers, so that sharp features close to the pseudogap could be removed by subtle structural deviations near the surface from those of the bulk, as reported for annealed QC surfaces.[37]

On the other hand, recent tunneling spectroscopy measurements performed in icosahedral QC's at low temperature (2 K) seem to provide some experimental support for the existence of certain fine structure asymmetrically placed with respect to the Fermi level.[19] In addition, tunneling spectroscopy measurements of decagonal QC's at ultralow temperatures have also revealed very rich fine structures in the DOS around the Fermi level.[20] According to these authors, the complex variation of the tunneling magnetoresistance with a varying applied magnetic field may be related to the self-similar properties of the quasicrystalline structure, exhibiting a hierarchy of spatial scale lengths. It should be mentioned, however, that although these features exhibit certain similarities with the DOS structure predicted by Fujiwara and Yokokawa,[13] a definitive confirmation still requires some additional work.[38]

Consequently, with the aim of shedding some light onto this debated question, we will ascertain the possible influence that a self-similar spiky structure in the electronic structure may play in the resulting transport properties. To this end, and inspired by our previous experience in studying band-structure effects in the dc conductivity of Fibonacci superlattices,[39] we will include a spiky component in the DOS model by means of a *self-similar Dirac comb* given by the expression

$$N_{ss}(E)=\sum_{n=1}^{M}\sum_{j=0}^{M-1}\lambda_{n,j}\delta(E-E_{n,j}), \tag{6}$$

where $\lambda_{n,j}\equiv\eta^{n-j-1}\lambda_0$, with $\lambda_0\equiv N_d(b/2)=a+\alpha b^2/4$, measures the strength of the self-similar peaks, and the series $E_{n,j}\equiv-\eta^{n-2}[1+\eta^{-j}(\eta-1)]b/2$ determines their positions. This self-similar structure includes M main peaks, labeled by the integer n, and $M(M-1)$ subsidiary peaks, labeled by pairs (n, j). The inflation factor $\eta>1$ is related to the QC structure. On the basis of crystallographic data for the i-AlCuFe and i-AlCuRu we will take the value $\eta=\tau_*^3$, τ_* being the golden ratio, as appropriately describing the self-similar structure of the DOS. This assumption has been checked by considering also the values $\eta=\tau_*, \tau_*^2, \tau_*^4$, real-

izing that, in these cases, it is not possible to attain a satisfactory fit between theoretical and experimental curves.

III. ANALYTICAL EXPRESSIONS

Expressing Eqs. (5) and (6) in terms of x, and substituting them into Eq. (4), we can express the electrical conductivity as a sum of three different contributions,

$$\sigma(T)=\sigma_d(T)+\sigma_{sr}(T)+\sigma_{ss}(T), \tag{7}$$

respectively associated to the corresponding DOS components. In order to perform the pertinent integrations we have made an appropriate expansion of the functions around the Fermi level when required. As a consequence, the domain validity of expressions (8) and (9) below is restricted to the condition $|\mu|<b/2$. In this way we obtain

$$\sigma_d(T)=2A\left[q+\lambda_0 g(T)+\alpha b^2\left(\frac{T}{T_0}\right)\ln f(T)\right], \tag{8}$$

where $q\equiv 2\alpha(b^2/4+\mu^2)$, $g(T)\equiv f(T)\sinh(T_0/T)$, $f(T)\equiv \operatorname{sech}(w_+/2T)\operatorname{sech}(w_-/2T)$, and we have defined $w_\pm\equiv T_0\pm T_\mu$ with $T_0\equiv b/2k_B$ and $T_\mu\equiv\mu/k_B$,

$$\sigma_{sr}(T)=2A\left[2d-dg(T)+\alpha b^2\left(2+\frac{T}{T_0}\right)h(T)\right], \tag{9}$$

where $h(T)\equiv 2\exp(-T_0/T)\cosh(T_\mu/T)$, and finally

$$\sigma_{ss}(T)=A\lambda_0\sum_{n=1}^{M}\sum_{j=0}^{M-1}\eta^{n-j-1}\operatorname{sech}^2\left(\frac{x_{n,j}}{2}\right), \tag{10}$$

where $x_{n,j}\equiv-(|E_{n,j}|+\mu)/k_BT$. The auxiliary functions $g(T)$, $f(T)$, and $h(T)$ verify the following limiting behaviors:

$$\lim_{T\to 0} g(T)=\frac{2}{1+\lim_{T\to 0} e^{-w_-/T}}, \tag{11}$$

$$\lim_{T\to 0} T\ln f(T)=-\frac{w_+}{2}-\lim_{T\to 0} T\ln(e^{w_-/2T}+e^{-w_-/2T}), \tag{12}$$

$$\lim_{T\to 0} h(T)=\lim_{T\to 0} e^{-w_-/T}. \tag{13}$$

Then, since the condition $|\mu|<b/2$ above implies $w_->0$, we obtain the following limiting behaviors for expressions (8)–(10) in the low-temperature regime: $\sigma_{sr}(0)=\sigma_{ss}(0)=0$ and $\sigma_d(0)=4A(a+\alpha\mu^2)$. Consequently, making use of Eq. (7) we get $\sigma(0)=4AN(E_F)$, where $N(E_F)=a+\alpha\mu^2$ measures the value of the DOS at the Fermi level. This relationship allows us to relate the coefficient A to two experimental quantities: $N(E_F)$, which can be determined from specific-heat measurements, and $\sigma(0)$, which can be obtained extrapolating the conductivity curves. Then, expressing A in terms of these physical magnitudes in Eqs. (7)–(10), the electrical conductivity of the system can be rewritten in the closed form

$$\sigma(T)=\sigma(0)[1+\Lambda(T)], \tag{14}$$

where we have introduced the dimensionless function

$$\Lambda(T)=\frac{\alpha b^2}{2N(E_F)}\sum_{1=1}^{3}F_i, \tag{15}$$

with

$$F_1(T)\equiv g(T)+2h(T)-1, \tag{16a}$$

$$F_2(T)\equiv(T/T_0)[\ln f(T)+h(T)], \tag{16b}$$

$$F_3(T)=\frac{\lambda_0}{2\alpha b^2}\sum_{n=1}^{M}\sum_{j=0}^{M-1}\eta^{n-j-1}\operatorname{sech}^2\left(\frac{x_{n,j}}{2}\right). \tag{16c}$$

Since expression (15) satisfies the limiting behavior $\Lambda(T\to 0)=0$, we can interpret expression (14) as indicating that the electrical conductivity curve of a quasicrystalline sample can be separated as the *product* of two different contributions. The first one is given by the $\sigma(0)$ factor and describes the *residual conductivity* of the sample in the limit of vanishing temperatures. This term will be the one responsible for the low conductivity values observed in these materials, as it will be further discussed below. The second contribution is given by the function $1+\Lambda(T)$ and describes the temperature dependence of the electrical conductivity as the temperature is increased. It is worth noting that a splitting of this sort was originally proposed by the LEPES group[6] to describe the remarkable experimental fact that the plots $\sigma(T)-\sigma(4\text{ K})$ for different samples were almost identical. This behavior seems to be a quite general property of most icosahedral QC's of high structural quality (and their approximants) and has been referred to as *inverse Matthiessen rule*.[3,6] However, our expression (14) does not completely coincide with that originally proposed by these authors, namely,

$$\sigma(T)=\sigma(0)+\delta\sigma(T), \tag{17}$$

since, in our description, the $\sigma(0)$ contribution also influences the high-temperature behavior of the conductivity curve, i.e., $\delta\sigma(T)=\sigma(0)\Lambda(T)$. A detailed discussion about this important difference is beyond the scope of the present study and deserves a closer scrutiny.[40]

IV. COMPARISON WITH EXPERIMENTAL RESULTS

To gain a deeper insight into the physical implications of these expressions in Figs. 2 and 3 we compare the theoretical curves derived from expression (14) with experimental data for a set of *i*-AlCuRu samples of different compositions. In Fig. 2 we can appreciate the marked dependence of the electrical conductivity with the sample composition for a series of high quality QC's whose stoichiometry is given by the formula $Al_{65}Cu_{20+x}Ru_{15-x}$, with $x=2,1,0,-1$. The conductivity curves corresponding to the samples with a Ru content in the range 16–14 at. % exhibit low conductivities and are nearly parallel, satisfying the inverse Matthiessen rule. On the contrary, the $\sigma(T)$ curve corresponding to the $Al_{65}Cu_{22}Ru_{13}$ sample exhibits a significantly higher value of the residual conductivity, and also shows a reversed curvature.

As it was indicated above, the variation of the $\sigma(0)$ factor

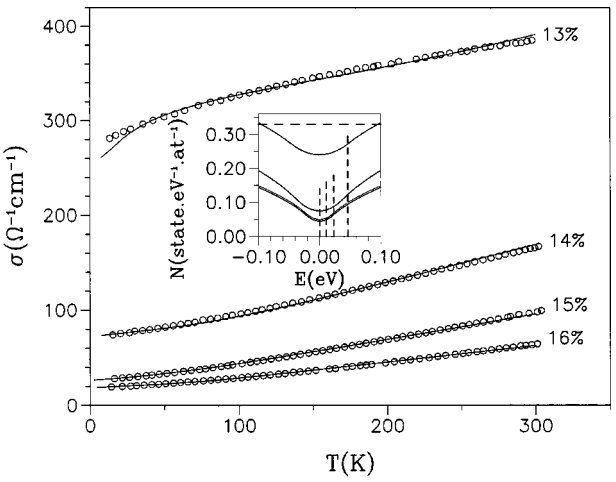

FIG. 2. Comparison between theoretical (solid lines) and experimental (circles) $\sigma(T)$ curves (taken from Ref. 24). From top to bottom, the curves are arranged according to the increasing content of Ru in the samples. The inset shows the DOS structure around the respective Fermi levels (dashed vertical lines) for the different QC's (arranged in the same order), as determined from the fitting parameters listed in Table I.

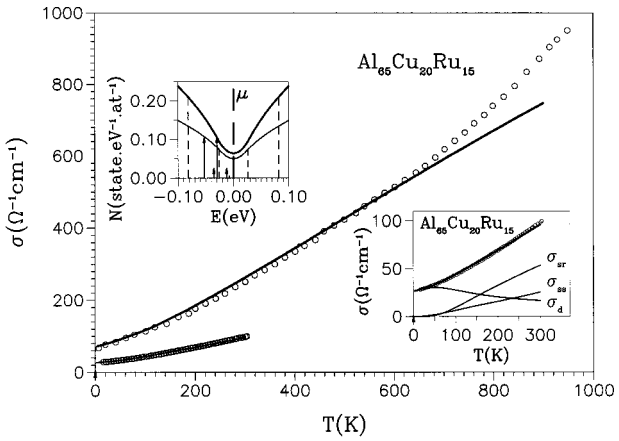

FIG. 3. Comparison between theoretical (solid lines) and experimental (circles) $\sigma(T)$ curves for two different i-$Al_{65}Cu_{20}Ru_{15}$ samples. Data for the curve covering the range 6–950 K are taken from Ref. 25. Data for the curve covering the range 4–300 K are taken from Ref. 24. The upper panel compares the DOS structure around the Fermi level for both samples. The dashed vertical lines indicate the length of the $k_B T_{max}$ interval in the energy scale. The lower panel shows the relative contribution of the different DOS features depending on the temperature range considered.

with the sample stoichiometry accounts for the systematic dependence of the conductivity curves observed in Fig. 2. According to our derivation, the factor $\sigma(0)$ is related to the electronic diffusivity through the relationship $\sigma(0) = e^2 D_0 N(E_F)/\Omega_0$. Therefore our model suggests that the low conductivity values observed in high quality QC's at low temperatures may stem from two different sources. On the one hand, we have the severe depletion of available charge carriers associated with the presence of a pronounced pseudogap around the Fermi level. On the other hand, we must consider the peculiar nature of critical states, most of which may exhibit quite small group velocities. Although our approach does not allow for a precise estimation of the relative importance of both contributions to the final value of the factor $\sigma(0)$, it represents a promising starting point to future detailed studies.

Another interesting result that we can extract from Fig. 2 refers to the change in the sign of the curvature for the $\sigma(T)$ curve corresponding to the $Al_{65}Cu_{22}Ru_{13}$ sample. In fact, since some topological differences exist between the different curves, it is noteworthy to realize that expression (14) provides a *unified description of the electrical conductivity* for the four samples, allowing us to fit the experimental curves quite well *in the entire temperature range considered*, with the only exception of the Ru 13 at. % sample at temperatures lower than 30 K.

In the inset we show the DOS structure around the respective Fermi levels (dashed vertical lines) for the different samples, as determined from the fitting parameters listed in Table I. We have checked that no significant improvement in the fits can be obtained by further increasing the reported M values. This indicates that only the first stages in the fractal growth process determining the self-similar DOS contribution must be considered in order to properly account for the experimental electrical conductivity curves. From the physical viewpoint, this is a quite reasonable result since one expects that the unavoidable presence of phason defects in any real sample significantly contributes to smearing out the finer details of the DOS spiky structure.

From the information graphically summarized in Fig. 2 two main conclusions can be drawn. First, we observe that as the dip minimum rises approaching the metallic value (indicated by the horizontal dashed line in the inset), its width broadens and, consequently, the residual conductivity $\sigma(0)$ progressively increases. Second, a shift in the Fermi level position, depending on the sample composition, is clearly seen. Therefore the variation of the $\sigma(T)$ curves with the sample stoichiometry can be related to a *systematic shift of the Fermi level* around the DOS dip, in such a way that as the Fermi level shifts approaching the DOS symmetry axis and the dip narrows and deepens, the electrical *conductivity*

TABLE I. Parameters used to fit the theoretical curves presented in Figs. 2 and 3. The $\sigma(0)$ values are taken from Refs. 24 and 25.

	a (state/eV at.)	α (state/eV^3 at.)	b (meV)	μ (meV)	$\sigma(0)$ $(\Omega\ \mathrm{cm})^{-1}$	M
$Al_{65}Cu_{19}Ru_{16}$	0.045	36	45	11	18.7	3
$Al_{65}Cu_{20}Ru_{15}$	0.047	40	37	0	26.6	3
$Al_{65}Cu_{20}Ru_{15}$	0.064	45	60	0	70.9	5
$Al_{65}Cu_{21}Ru_{14}$	0.075	24	75	23	72.1	3
$Al_{65}Cu_{22}Ru_{13}$	0.240	15	95	46	258.9	3

TABLE II. Experimental values for several parameters used in our DOS model, as reported for the representative $Al_{65}Cu_{20}Ru_{15}$ QC in literature.

	$Al_{65}Cu_{20}Ru_{15}$	Measurement	Ref.
$N(E_F)$ (state/eV at.)	0.0467	specific heat	5
	0.0637	specific heat	22
b (meV)	20–50	NMR	36,42
α (state/eV^3 at.)	23–32	NMR	43

of the QC progressively *worsens*. In this sense it is interesting to note that the most symmetric structure ($\mu=0$) is obtained for the $Al_{65}Cu_{20}Ru_{15}$ sample, which according to metallurgical studies,[41] seems to be the most stable of the series.

V. CONCLUDING REMARKS

In order to estimate the applicability domain of our model, we compare in Fig. 3 theoretical and experimental conductivity curves covering different temperature ranges. We see that it is possible to obtain a good fit from below 4 K up to about 650 K. This threshold value is expected from NMR measurements suggesting that a significant change of the DOS structure might take place above the Debye temperature ($\sim$500 K),[43] hence implying that an appropriate dependence of the DOS structure with the temperature should be considered. On the other hand, the fitting parameters listed in Table I are in complete agreement with experimental figures reported in the literature (given in Table II). This fact provides further evidence on the reliability of the model. In this sense, suitable measurements aimed to check the Fermi level position shift predicted by the model should be pertinent.

We can also estimate the relative importance of the three different contributions of the DOS to the overall evolution of the conductivity curve. To this end, we present in the lower panel of Fig. 3 the contribution due to each σ_ν to the overall temperature dependence of the QC electrical conductivity, as determined from expressions (7)–(10). As it can be readily seen, below 50 K the $\sigma(T)$ curve is entirely dominated by the narrow dip component contribution, although the self-similar spiky component plays a minor but significant role in determining the *positive curvature* of the conductivity curve in this temperature interval. On the other hand, above room temperature the contribution due to the σ_{ss} component starts to play also a significant quantitative role, compensating the progressive decrease in the contribution due to the σ_d component. Nonetheless, it should be stressed that, in order to keep the lowest possible number of free parameters during the fitting process, the position of the Fermi level is located far away from the spiky component of the DOS (see Fig. 1). Consequently, one expects that the influence of such a component on the electrical conductivity will be of some importance only in the regime of high temperatures, as it is indeed the case. If the existence of a self-similar spiky component of the DOS were ultimately confirmed, then the model introduced in this work may be readily implemented to account for more realistic parameters defining the main features of this component. Therefore we believe that, on the basis of actual model parameters alone, it is not possible to arrive to any definitive conclusion on the role played by the spiky component in the electrical conductivity of the considered samples.

To conclude, some words are appropriate with regard to the physical relevance of our approach as well as its applicability. In the present treatment the evaluation of the transport properties is mainly based on the energy spectrum function $\sigma(E)$. In our opinion, this approach to the problem offers some appealing advantages. First, such a procedure circumvents many of the approximations usually required in other approaches to the study of transport properties in QC's. Second, we can make use of some current knowledge about the energy spectrum, which has been recently obtained in the course of numerical studies of realistic quasiperiodic systems.[29] Third, this treatment is quite general, thus providing a promising starting point for a more rigorous study of transport properties in QC's within a unified scheme. In this sense, future studies aimed to include relevant effects such as the electron-phonon interaction or quantum interaction effects will be appealing.

In summary, we propose a DOS model which accurately describes the most characteristic features observed in the $\sigma(T)$ curves of high quality QC's over a wide temperature range. In this way, we obtain a closed expression for the electrical conductivity, which exhibits some relevant similarities with the empirically proposed inverse Matthiessen rule. In addition, by properly choosing the physical parameters appearing in the model, we unveil a relationship between the Fermi level position, the DOS structure, and the sample stoichiometry.

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