Fermi surfaces and anomalous transport in quasicrystals

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Electronic transport properties of quasicrystals is discussed theoretically. By means of ab-initio Linear Muffin Tin Orbitals (LMTO) calculations, electronic band structure and corresponding Fermi surfaces of several quasicrystalline approximants are obtained. A criterion for distinguishing between metallic and anomalous transport properties in intermetallics is proposed. Unconventional temperature dependence of conductivity of quasicrystals and approximants is addressed in a second part. It is shown that power law exponents can be directly deduced from scaling analysis of the Kubo formula. Finally in relation to our results, we briefly summarize actual knowledge on low temperature transport regimes.

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I. INTRODUCTION

In 1984, the five-fold symmetric quasicrystals (QC) were discovered in AlMn based intermetallic alloys. So far, a lot of theoretical and experimental work have been done in order to describe their crystallographic properties. Concerning physical properties, electronic and magnetic behaviours have unveiled very interesting phenomena and somehow disconcerting physics. In particular, contrary to conventional metallic alloys, the thermal and electrical conductivities of quasicrystalline phases have been found to be unusually low, almost as low as those of insulators. Features like strong hardness, low friction coefficients, resistance against oxidation and corrosion, and optical properties have turned QC into interesting alternatives for several technological applications.

Theoretical works have been concerned with the relation between quasicrystalline order (short, mesoscopic and long-range) and electronic localization and diffusion modes. The electronic structure of real quasicrystals can be deduced from ab-initio LMTO calculations, performed on realistic structural models of their approximants. A pseudo-gap at Fermi level and a dense concentration of low dispersive bands in its close vicinity, constitute the main features of their electronic structure.

In this paper, the topic of Fermi surfaces of quasicrystals is addressed. Such a concept may appear meaningless in quasiperiodic systems for which no reciprocal space can be properly defined, due to the lack of translational symmetry. Notwithstanding, quasicrystals share similar physical properties with certain crystalline alloys called quasicrystalline approximants. Indeed, these alloys do approximate quasicrystalline order on a length scale which actually defines the characteristic size of their unit cell. Such a family of increasing length approximants \((1/1, 2/1, 3/2, 5/3, \ldots)\) enables a natural scaling procedure from which physical properties of real quasicrystals may be deduced.

We will construct the basic idea of electronic states near the Fermi energy with help of the knowledge of the Fermi surface of crystalline approximants.

Anomalous transport in quasicrystals stems from non ballistic quantum diffusion between electronic eigenstates, and has been shown to prevail even at higher temperatures. From scaling analysis of the Kubo formula of electronic conductivity, power law exponents of temperature dependence conductivity will be found qualitatively. A discussion on metal-insulator in quasicrystals will conclude the paper.

II. ELECTRONIC STRUCTURE AND FERMI SURFACES OF QUASICRYSTALLINE APPROXIMANTS

Quasicrystals are highly ordered and anomalously resistive when compared to their amorphous counterparts. Due to a lack of periodicity, an analytic form of the Fermi surface (FS) cannot be written down. On the other hand, it is now well established that some quasicrystalline approximants share similar anomalous properties with pure icosahedral or decagonal phases, so that strict quasiperiodicity may not be an unavoidable requirement to account for such physical properties. It is therefore interesting to investigate the Fermi surfaces of approximant phases, which are well-defined and easier to calculate.

Fermi surface in metallic alloys is indeed, a meaningful concept, enabling the determination of most of the physical properties which depend, in some way, on the behaviour of conduction electrons. It turns out that mag-
nentic field can be used as a powerful probe of the shape of the Fermi surface. For instance, de Haas-van Alphen -dHvA- (magnetization) and Shubnikov (magnetoresis-
tivity) low temperature experiments yield to reliable and quantitative geometrical informations such as radii or cross-sectional areas, whereas magnetoresistance at high fields, reveals whether or not open orbits are allowed in the plane normal to the magnetic field. Nevertheless, the role of open electronic orbits is quite complicated to figure out as they are thought to entail additional quantum interference effects.

DHzA shows up as 1/H-periodic oscillations in the magnetization, but is usually observable in crystals of high structural quality, at low temperatures, and in relatively high magnetic fields (above 10 Tesla). From a semiclassical treatment of electron dynamics in a uniform magnetic field, the oscillation frequency can be related to the extremal electronic closed orbit in the related FS. If $\mathcal{S}(E_F)$ is an extremal cross-sectional area of the FS in a normal plane to the magnetic field, then the frequencies $\nu$ of dHvA oscillations is $\nu = h c / 2 \pi e \mathcal{S}(E_F)$ (in Tesla units), whereas effective masses will be given by $m^* = \hbar^2 \partial^2 \mathcal{S}(E_F) / \partial E^2$.

Some attempts have been made to probe Fermi surfaces in pure icosahedral AlPdMn compounds with resistivity of 1250$\mu \Omega \text{cm}$ at room temperature. DHvA signature was found but still needs to be confirmed. It has to be stressed that the measured compounds are anomalously resistive, which is an unfavorable circumstance for the observation of FS by means of DHvA methods.

In the following, first numerical calculations of Fermi surfaces in several crystalline approximants of the icosahedral AlCuFe, AlCuFe-Si and AlMgZn are presented. We believe that experimental investigation of the shape of FS in less resistive quasicrystalline approximants and comparison with theoretical calculations, may facilitate the analysis for pure quasicrystals.

**A. Electronic bandstructure calculations**

Before presenting our results, let us recall the basic features of electronic properties in approximants and quasicrystals. The band structure of quasicrystalline approximants have been calculated by means of LMTO self consistent method. A pseudogap with a width $\sim 0.5$ eV existing at the Fermi energy, attributed to Hume-Rothery distortion, is supposed to be responsible for the stability of the quasicrystals. This pseudo-gap has been found theoretically in models of approximants, and experimentally in approximants or pure icosahedral quasicrystals, so that electronic properties are comparable.

It has also been argued that the pseudogap could be widened and deepened by aggregation of icosahedral clusters or their hierarchical aggregation. Concerning the total electronic density of states (TDOS), self-consistent ab-initio calculations describe TDOS as a dense set of very sharp spikes with a width less or equal to 0.01 eV, sensitively depending upon the scattering length. The spikes may be due to quasi-periodicity, cluster aggregation and d-orbital resonance. Nevertheless, due to finite experimental resolution and averaging information over wide spatial area, these features are difficult to observe experimentally. Very recent low temperature tunneling experiments in AlNiCo decagonal quasicrystals seem to be consistent with such spiky peaks.

Concerning transport properties, it is expected that all the quantities, involving a surface integral over the whole FS, will be affected substantially, if anisotropic effects generate increasing distortion from ideal spherical FS. An illustration has been given in Al$_{62.5}$Cu$_{25.0}$Fe$_{12.5}$ FCI quasi-crystals, by S.E. Burkov et al., who proposed that limited number of Bragg peaks (giving rise to the strongest pseudopotential) might intervene in the Fermi surface-Brillouin zone interaction mechanism. Taking into account the contribution of 42 Bragg planes, an alteration of the shape of spherical Fermi surface was speculated, and a corresponding reduction of electronic conductivity, in the nearly free electron framework, estimated. This heuristic approach reveals how icosahedral symmetry contribute in reducing conductivity from the isotropic case.

**B. Models and Results**

1. $\omega$-AlCuFe

Results from LMTO band structure calculations for several models are presented. The first one is the $\omega$-phase of a crystal AlCuFe (tetragonal symmetry) whose electronic properties are metallic. The electronic structure of this crystal has already been computed, by ab-initio LMTO methods.

On Fig. 1, the total density of states (TDOS) and the Fermi surface in the $K_z = 0$ plane for the $\omega$-phase of AlCuFe are shown ( $K_x, K_y$ are given in $2\pi/\alpha$ units, with $\alpha = 6.336\AA$). The Fermi surface shows the symmetries of AlCuFe alloy and is compatible with band dis-
persion. One notes that this Fermi surface seems to have only closed orbits, and for instance, five shells of closed electronic orbits around the $\Gamma = (0, 0)$ point. To estimate the associated dHvA frequencies, one has to calculate $\int_{\gamma_n} K_y dK_x$ ($\gamma_n$ the countour of the closed orbits). A rough estimation of dHvA frequencies of two quasicircle shaped orbits gives $F \sim 15, 79$ Tesla. The principal frequencies may appear in oscillations of magnetization $M(1/B)$. One notes however there are many "breakdown points" which can couple, because of tunneling, these different closed regions of the FS.

The results obtained for this crystal are important since they allow a direct comparison of electronic structure between metallic and anomalous transport compounds. However, one stresses that it may not be sufficient to compare respective bandstructure since electronic transport also requires knowledge of dynamical information that may be only indirectly related to static spectral properties.

2. 1/1 AlCuFe

The bandstructure of 1/1 approximant of i-AlCuFe, based on a hypothetical structural model [24], has been evaluated and is in good agreement with previous calculations. [23] On Fig. 2., the section of the FS in the plane $K_z = 0$ and the TDoS are presented. We estimate four dHvA frequencies, associated to closed orbits, which are respectively 1.44, 4, 7.9, and 13 Tesla ($K_x, K_y$ are given in $2\pi/a$ units with $a = 12.30\,\text{Å}$).

Bandstructure was computed and nearly dispersionless bands were obtained. Fermi velocity was estimated $v_F \sim 0.5 \times 10^7 \text{cm/s}$ (several order of magnitude lower than the corresponding values in amorphous systems), resulting in a mean free path much shorter than the interatomic distance. Accordingly, usual semi-classical treatment of transport may be unreliable. We will discuss later the relation between bandstructure features and anomalous transport.

3. 1/1 AlCuFe-Si

The lowest quasicrystalline approximant 1/1 of AlCuFe-Si (cubic phase with $a = 12.336\,\text{Å}$) is also investigated. The resistivity of this small approximant as a function of temperature has been shown to be anomalous [dσ(T)/dT > 0 (A. Quivy et al. [22])], similar to that of the icosahedral phase of AlCuFe. The model, we used, has been taken from Mizutani et al. [23]. By means of Rietveld method for the powdered X-ray diffraction spectrum, the approximant was found to form a cubic lattice ($a = 12.336\,\text{Å}$) with the space group $Pm3$. Two pseudo-Mackay icosahedral atomic clusters $Cl_1$ (with vacancy in the center) and $Cl_2$ (with Cu atom in the center) were identified, with 139 atoms in the unit cell. Nonetheless, out of this 139 atoms, about 36 position sites were given with occupancy of 50% by Fe and 50% by Cu. To circumvent such uncertainties, we have investigated different models and found that the only proper one, according to the bandstructure results and concentration stoichiometry, is given by considering that $Cl_1$ consists of Cu with 1.0 occupancy in the $M_8$ subcluster, and Fe with 1.0, in the $Mn_1$ subcluster (see reference [24] for details), whereas the situation in $Cl_2$ is reversed.

Results for the 1/1 approximant of $\text{Al}_{55}\text{Cu}_{25.5}\text{Fe}_{12.5}$ – Si$_7$ as described in the structural model proposed by Mizutani [23] are presented on Fig. 3. The TDOS is small at Fermi level (pseudo-gap), and the typical spiky structure is also found. Corresponding electronic bandstructure in the vicinity of the Fermi level exhibits a high density of flat bands. The associated Fermi surface (in $K_z = 0$ plane) is rather different from the one of the tetragonal phase of AlCuFe, in particular by the presence of open orbits. Smallest closed areas (around $\{K_x = 0, K_y = 0\}$) correspond to frequency of about $F \sim 0.7$ Tesla, whereas closed orbits centered around $\{K_x, K_y\} = \{0.5, -0.5\}$ correspond to $F \sim 6.38$ Tesla ($K_x, K_y$ are given in $2\pi/a$ units with $a = 12.336\,\text{Å}$).

4. 1/1-AlMgZn

Finally, electronic bandstructure and Fermi surfaces of AlMgZn approximants (bcc, $Im\bar{3}$) have been computed by varying atomic compositions in model derived from Rietveld analysis. [23] The band structure of $\text{Al}_{45}\text{Mg}_{40}\text{Zn}_{15}$ near the Fermi level is shown on Fig. 4. Eight bands cross the Fermi energy and each band has large energy dispersion between $\Gamma = \{0, 0\}$ and $H = \{K_x = 0, K_y = -0.5\}$ points (i.e. the (100) direction), which enable to determine whether the orbits of Fermi surfaces are related to hole or electron pockets.

One notes that the $x, y, z$ axes are equivalent due to the $120^\circ$ rotation, but there is no $\pi/2$ rotation symmetry
along x-, y- or z- axes. The large energy dispersion is due to contact of atom clusters along the (100), (010), (001) directions. Furthermore, they are many small electron and hole pockets over the whole region.

On Fig. 5, the corresponding TDoS and FS in the $K_x=K_y$ plane are also given. We precise that $-1 \leq K_x, K_y \leq 1$ are given in units $2\pi/a, a = 14.498\text{Å}$. Six bands provide several closed orbits whereas one band forms an open orbit along the (100) direction. Very small electron and hole pockets, may be rather difficult to observe given the damping effects due to finite electron scattering time. Notwithstanding we estimate the dHvA frequency and the effective mass for the largest orbit surrounding the $\Gamma$ point. From the Fermi surface we estimate $F \sim 11\text{ Tesla}$ and by considering bandstructure along the $\Gamma$--$H$ direction ($H=\{K_x=0, K_y=-1\}$), we find that the corresponding effective mass is of order $m^* \sim 5m_e$ ($m_e$ the free electron mass).

5. Discussion about Fermi surface and relation to anomalous transport

Our studies have shown that many hole and electron pockets emerge in the energy constant contours of the Fermi surfaces. A noticeable feature for the FS of the quasicrystalline approximants seems to be the existence of open orbits which may be manifested through magnetic breakdown at high magnetic field. Methods such as dHvA at low temperature or angle-resolved photoemission spectroscopy, may be suitable to investigate such disconnected Fermi surfaces.

One notes that the band dispersion of the quasicrystalline approximants is so weak that $v_F = 1/\hbar \partial E_n(k)/\partial k$ turns out to be very small. Another noteworthy feature allows to point out a difference between metallic transport and anomalously reported quasicrystalline one. Elastic scattering time $\tau_{\text{el.}}$ is generically related to an impurity concentration in the system, enabling a semiclassical description of the dynamics of wave packet in between scattering events. The exact details of bandstructure being usually neglected. In case of approximants, it turns out that energy spacing between bands, in the vicinity of Fermi energy, becomes very small, so that one has to define a typical time associated to $\hbar/(E_n - E_m)$ (average between two bands $m$ and $n$) as a limit given by Heisenberg uncertainty principle. If there exists a finite number of bands within the energy window defined by a finite $\tau_{\text{el.}}$, then transport may turn out to be anomalous because tunneling occurs between different bands, which cause the instability of the wave packet coherence. Actually, if one considers the crystalline phase $\omega - \text{AlCuFe}$ and the 1/1 approximant of icosahedral AlCuFeSi,AlCuFe-Si,AlMgZn, one finds that, for $\tau_{\text{el.}} \sim 10^{-15}\text{s}$ (typical value found in amorphous of similar resistivities), the energy window is $\Delta E \sim 0.675\text{eV}$ and confines about ten bands for the approximants whereas the crystalline phase presents no bands. One notes that the considered value for the scattering time may be questionable since it is usually deduced from experiment using classical theories (which should be unapplicable in case of anomalous transport). Notwithstanding, the aforementioned difference in the bandstructure does not critically depends on the considered value of $\tau_{\text{el.}}$.

As real experiments do not provide quantitative informations about the bandstructure, a criterion for occurrence of anomalous transport may be defined from detailed analysis of the topology of the Fermi surfaces, by comparison between theoretical results and experiments. For instance, high density of flat bands, in the vicinity of Fermi level may promote the occurrence of open orbits. If such a statement is valid, magnetic breakdown will be observed more frequently for quasicrystalline approximants.

III. ANOMALOUS TRANSPORT PROPERTIES

A. Anomalous diffusion and temperature dependence of the conductivity

Unusual electronic transport in quasicrystals is supposed to originate from anomalous quantum diffusion and specific local atomic order. To circumvent the complexity of the structural issues, when considering electronic localization, one may address separately the effects of quasiperiodic potential on electron dynamics, and bandstructure effects, generic of approximants. In principle, scaling analysis based on crystalline approximants should allow a connection between both approaches.

In ordinary metals, neglecting weak localization effects, one usually distinguishes two different regimes for temperature dependent transport (even if the frontier, given by Debye temperature, is by no means universal, but rather alloy-dependent). To calculate $\sigma(T)$, one must treat properly the electron-phonon interaction within the usual linear response scheme. The Kubo formula is a suitable starting point, and can be written as:
\[
\sigma(T) = \frac{e^2 n_0}{m} \int_{-\infty}^{+\infty} \left( \frac{\partial f(E)}{\partial E} \right) \Gamma(k_F, E \pm i\eta) \frac{dE}{2\pi m \Sigma(k_F, E)}
\]

with \(n_0\) the electronic density, \(f(E) = (1 + e^{\beta(E-\mu)})^{-1}\) the Fermi-Dirac function and \(\Gamma(k_F, E \pm i\eta)\) a so-called vertex function which accounts for all the collision process of the propagating electrons with the phonons. \(\Sigma(k_F, E)\) is related to the transition rate of one electron in one eigenstate, due to the coupling with the thermal perturbation.

The evaluation of the Kubo formula is done by summing the relevant ladder diagrams for electron-phonon interactions, and reducing the vertex function to an integral equation, that is solved numerically. \(\tau_\text{tr}\) In the case of weakly disordered metals, the vertex function reduces to 1, whereas inelastic relaxation time \(\frac{1}{\tau_\text{tr}(E)} = -2(3m\Sigma(k_F, E))^{-1}\) is given by Fermi’s golden rule. It is shown that in the temperature regime such that \(\hbar\omega_D \gg k_B T\) (with \(\omega_D \sim c_S/\sqrt{\gamma}, c_S\) the sound velocity and \(\gamma\) the lattice constant), phonons with energies \(\hbar\omega \sim k_B T\) will play a dominant role. Transport time will be given accordingly by \(26\):

\[
\frac{1}{\tau_\text{tr}} \sim \frac{T}{\hbar} \left( \frac{T}{\hbar\omega_D} \right)^4 \sim T^5
\]

and from Drude formula \(\frac{e^2 n_0}{m \tau_\text{tr}}\), Bloch-Gruneisen law will follow \(20\):

\[
\sigma_{\text{DC}}(T) \sim \frac{n_0 e^2 \tau_\text{tr}}{m} \sim T^{-5}
\]

Electronic transport properties in quasicrystals or approximants turn out to be non-metallic, opposite Mathiessen rule being one of the most spectacular manifestation. \(27\) Experiments reveal that the general form of conductivity is generically \(\sigma_{\text{DC}}(T) \sim \sigma_4 + DT\) with \(\Delta \sigma(T) \sim T^\alpha \quad \alpha \in [1,1.5].\) \(20\) Theoretically, recent studies of anomalous electronic transport in presence of inelastic collisions, by Schulz-Baldes and Bellissard \(24\), have strengthened the heuristic arguments for the suggested anomalous Drude law \((\sigma \sim T^{2\beta-1})\) \(8\), where \(\tau\) is supposed to be the relevant inelastic scattering rate at a given temperature. The anomalous Drude law has been shown to account for all the specific electronic properties of quasicrystals.

In the following, temperature dependent power law is shown to be consistent with a scaling analysis of the Kubo formula, in the low temperature regime. From the knowledge of exact eigenstates \(|\alpha\rangle\), in the vicinity of Fermi energy, the Kubo formula is evaluated from \(\sigma_{\text{DC}} = \int_{-\infty}^{+\infty} dE (\partial f(E)/\partial E) \sum_\alpha \delta(E-E_\alpha) \tilde{D}_\alpha(E)\)

\[
\tilde{D}_\alpha(E) = -\frac{1}{\pi} \lim_{\gamma \to 0^+} \Im m \langle \alpha| \hat{v}_x \frac{1}{E - \hat{H} + i\gamma} |\alpha\rangle
\]

is the contribution to diffusivity of a given eigenstate \(|\alpha\rangle\). The cut-off \(\gamma\) stands for the relevant relaxation time that will dominate the transport process. Scaling analysis of the Kubo formula has been performed for realistic models of approximants of the decagonal AlCuCo quasicrystals, including sp-d orbitals of all the atomic species. This leads to a self-consistent treatment of sp-d hybridization effects, which are known to produce important alteration of a naive nearly free electronic transport model. Anomalous power law dependence of diffusivity in \(\gamma\) was found \(14, 15\)

\[
\langle \mathcal{D} \rangle \sim \gamma^\nu \sim \left( \frac{1}{\tau_\text{tr}} \right)^\nu, \quad \nu \simeq 0.25
\]

where \(\gamma\) has to be replaced by a suitable scattering rate dominating transport mechanism. We stress that this result gives the first “quantitative exponent” characterizing the transport coefficients in the vicinity of the Fermi level for a realistic model. From Kubo’s formula, the temperature dependent part of the conductivity is related, in a first approximation, to the transport time. In the low temperature limit, using the Debye model, one expects Bloch-Gruneisen law to be applicable. Then from \(\tau_\text{tr} \sim T^\mu\) with \(\mu = -5\), we conclude that :

\[
\Delta \sigma(T) \sim T^{\eta}, \quad \text{with } \eta \simeq 1.25
\]

This is in good agreement with the values obtained experimentally for several quasicrystalline and approximant phases at temperature \(\geq 400 mK\). \(30, 31, 32, 33\) For instance, in icosahedral Al\(_{70}\)Pd\(_{20}\)Re\(_{10}\) bulk samples, Al\(_{70}\)Pd\(_{18}\)Re\(_{12}\), Al\(_{70}\)Pd\(_{22}\)Re\(_8\) ribbon samples \((R = \rho_{20K}/\rho_{300K} \approx 2 - 10)\), and Al\(_{65}\)Cu\(_{20}\)Ru\(_{15}\) ingots, the transport exponents are respectively \(\eta = 1.3\) and \(\eta = 1.4, 1.45,\) \(34\) and \(\eta \approx 1.3\) \(34\), for temperature range \([400mK, 300K]\). One recalls that in quasicrystals, the typical Debye temperature, which limits the “low temperature regime” estimated from specific heat measurements are typically \(\approx 400 \approx 500K\). \(37\)

One also notes that Kubo formula \(\sigma \sim T^{2\beta-1}\) with \(\beta = 0.375\) in the d-AlCuCo approximants, is also consistent with opposite Mathiessen rule. If scattering time increases (improving structural order or decreasing temperature), conductivity decreases.
In summary, scaling analysis of the Kubo formula, combined to temperature dependence of transport time, has been shown to be consistent with the power-laws found in experiments. The main asset of scaling analysis with 3D realistic models of periodic approximants is that complicated effects due to local atomic order (sp-d hybridization, local cluster geometries) have been integrated self-consistently into the ab-initio calculations. This point is critical, given that metal-insulator transition can be induced by a tiny variation of atomic stoichiometry, while the material preserves long range order. For instance, a metal insulator transition has been studied in the Al70.5Pd21Re8.5−x−Mnx quasicrystalline compounds. The signature of such a transition occurs as concentration of manganese is increased from x = 0 to x = 5, whereas long range quasiperiodic order remains unchanged. Finally, from studies of electronic properties in approximants, one may relate non-metallic transport character to specific features of Fermi surface combined to scaling analysis of the transport coefficients.

B. Discussion on low-temperature transport and metal-insulator transition

From experiments, one can basically distinguish two low-temperature transport regimes for quasicrystals. The anomalous power law temperature dependence of the conductivity appears as a criterion for distinguishing both regimes.

Indeed, in some quasicrystals, low temperature transport is dominated by quantum interferences effects (QIE), as described for weakly disordered systems, and leads to a finite conductivity at zero temperature, and to typical temperature and field dependence of resistivity. Detailed studies have been carried out in particular in pure quasicrystalline phases of AlCuFe, AlPdMn, AlCuCo, AlNiCo. From data analysis and theories of QIE, an estimation of mean free path about 20 ∼ 30 Å was extracted. However, the origin of coherence of wavefunctions in quasicrystals may be different from that given by the conventional theory of QIE, which relies on quantum interference between propagating and backscattered waves. Coherence in quasicrystals may be rather due to the “quasiperiodic mesoscopic order” as recently shown by scaling analysis of electronic participation ratio in realistic structural models.

Another transport regime at low temperatures corresponds to stronger electronic localization induced by quasicrystalline order, and yields to better insulating quasicrystals at zero temperature. Besides, for largest values of $R = \rho_{4k}\phi_{900k} \sim 120$, the associated power law $\Delta \sigma(T) \sim T^0$ seems to prevail down to very low temperature $T \downarrow 4K$. This behaviour is reminiscent of scale invariance, as usually found in systems close to metal-insulator transition. No weak localization effects are revealed from experiments.

Furthermore, at $4K \leq T \leq 16K$, the conductivities of some samples oficosahedral AlPdRe have been successfully described by means of McMillan scaling theory, which treats localization and electron-electron correlation on equal footing. Experiments by Lin et al. have been interpreted through $\sigma(T) = (\sigma_{4k} + \sqrt{T/\Delta})^{\eta}$ where $\Delta$, the Coulomb gap (the relevant energy scale in the insulating phase, $\Delta \propto (\sigma_{4k})$, is determined by conductivity and electron tunneling measurements. This suggests that, unlike disordered amorphous, the metal insulator transition in quasicrystals may be induced by the atomic order on local or mesoscopic scale. The exact physical origin of such a metal-insulator transition is still a challenging unresolved problem.

One may depict the transition from one low-temperature transport regime to another in the following way. Quasicrystalline phases that are dominated by QIE at low temperatures, may suffer screening by tiny impurities and/or disruptions of the relevant mesoscopic atomic order, responsible for stronger geometrical localization (defined by “resonances” as described in [13]). An experimental evidence is provided by the deviations observed in AlPdMn and AlCuRu at about 80K, where typical power law for conductivity can be recovered.

IV. CONCLUSION

Experiments reveal that quasicrystals present remarkable electronic transport properties, hitherto unexpected. In particular, a metal-insulator transition is approached, by improving quasicrystalline order. Within the one electron scheme, several theoretical approaches suggest an intermediate type of algebraic localization between purely extended states and exponentially localized states. Different schemes were proposed to explain original transport properties, amongst which, non-ballistic quantum diffusion for long relaxation times or hopping mechanisms induced by interband transitions at shorter ones. In this paper, we have shown how scaling analysis of the Kubo formula may lead to power-law temperature dependence of electronic conductivity in the low temperature regime.
Features of the Fermi surfaces of several quasicrystalline approximants were presented based on ab-initio calculations. They may hopefully support further experimental investigations of real FS in quasicrystalline materials, and improve our understanding about non-metallic transport in approximants and quasicrystals.

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VI. FIGURES CAPTIONS

Fig. 1. Total density of states and Fermi surface in the Brillouin zone ($K_z = 0$ plane) of the $\omega$-AlCuFe crystalline phase.

Fig. 2. Total density of states and Fermi surface of the 1/1-AlCuFe quasicrystalline phase.

Fig. 3. Total density of states and Fermi surface of 1/1-AlCuFeSi.

Fig. 4. Electronic bandstructure of 1/1-AlMgZn quasicrystalline approximant.

Fig. 5. TDoS and Fermi surface section of 1/1-AlMgZn in the plane $K_x = K_y$. 

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DOS (states/Ry. cell)

Al45Mg40Zn15 (increase #k-pts)

ENERGY (Ry.)

EF
