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To cite this version:

Jean-Pierre Julien, Guy Trambly de Laissardière, Didier Mayou. Ab-initio quantum diffusion in quasicrystals. J.P. Julien, J. Maruani, D. Mayou, S. Wilson, G. Delgado-Barrio. Recent Advances in the Theory of Chemical and Physical Systems, Springer, pp.535-546, 2006, Progress in Theoretical Chemistry and Physics. hal-00012392

HAL Id: hal-00012392

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Submitted on 21 Oct 2005

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ccsd-00012392, version 1 - 21 Oct 2005

AB-INITIO QUANTUM DIFFUSION IN QUASICRYSTALS

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Abstract. We compute the velocity correlation function of electronic states close to the Fermi energy, in approximants of quasicrystals. As we show the long time value of this correlation function is small. This means a small Fermi velocity, in agreement with previous band structure studies. Furthermore the correlation function is negative on a large time interval which means a phenomenon of backscattering. As shown in previous studies the backscattering can explain unusual conduction properties, observed in these alloys, such as for example the increase of conductivity with disorder.

1. Introduction

In 1984, Schechtman, Blech, Gratias, and Cahn [1] presented a new metastable phase of an Al–Mn binary alloy. The diffraction pattern was formed by intense Bragg peaks organized according to the icosahedral symmetry strictly forbidden from conventional crystallography. The underlying order was claimed to be described by the mathematical concept of quasiperiodicity [2, 3]. The confirmation of a new state of matter has been an intense subject of controversy. In particular, Pauling proposed an alternative description of five-fold diffraction patterns based on icosahedral glasses formed

by twins [4]. However, the situation changed after the discovery of stable phases (icosahedral AlCuFe, AlPdMn, AlCuCo...) by Tsai et al. [5], and the existence of quasiperiodic crystals (quasicrystals) is now well accepted. Furthermore, these materials have revealed a lot of unexpected physical properties [6].

Among many fascinating properties, quasicrystals with high structural quality, such as the icosahedral AlCuFe and AlPdMn alloys, have unconventional conduction properties when compared with standard intermetallic alloys. Their conductivities can be as low as 150–200 $(\Omega\,\mathrm{cm})^{-1}$ [7]. Furthermore the conductivity increases with disorder and with temperature, a behaviour just at the opposite of that of standard metal. In a sense the most striking property is the so-called *"inverse Mathiessen rule"* [8] according to which the *increases of conductivity* due to different sources of disorder seems to be *additive*. This is just the opposite that happens with normal metals where the increases of resistivity due to several sources of scattering are *additive*. Finally the Drude peak which is a signature of a normal metal is also absent in the optical conductivity of these quasicrystals.

An important result is also that many approximants of these quasicrystalline phases have similar conduction properties. For example the crystalline α-AlMnSi phase with a unit cell size of about 12 Å and 138 atoms in the unit cell has a conductivity of about 300 $(\Omega\,\mathrm{cm})^{-1}$ at low temperature [7, 9]. The conductivity has the same defect and temperature dependence as that of the AlCuFe and AlPdMn icosahedral phase. There is, to our knowledge, no experimental result on the optical conductivity of this α-AlMnSi phase, but it is very likely that it is similar to that of AlCuFe and AlPdMn icosahedral phase.

The interpretation of these unconventional conduction properties is still a challenge for condensed matter physicists. Several models have been proposed including thermally activated hopping [10] band structure effects due to small density of states and narrow pseudo-gap [11, 12] or anomalous quantum diffusion [13, 14]. Yet all these models are difficult to compare in a quantitative way with experiments.

In this paper we present preliminary results of an *ab-initio* study of quantum diffusion in the crystalline α-AlMnSi phase. The number of atoms in the unit cell (138) is sufficiently small to permit computation with the *ab-initio* Linearized Muffin Tin Orbitals (LMTO) method and provides us a good starting model. Within the Density Functional Theory (DFT) [15,16], this approach has still limitations due to the Local Density Approximation (LDA) for the exchange-correlation potential treatment of electron correlations and due to the approximation in the solution of the Schrödinger equation as explained in next section. However, we believe that this starting point is much better than simplified parametrized tight-binding like s-band models.

The central quantities are the velocity correlation function of states of energy E at time t: $C(E,t)$, and the average square spreading of states of energy E at time t along the x direction: $\Delta X^2(E,t)$. The velocity correlation function is defined by:

$$C(E,t) = \Big\langle V_x(t)V_x(0) + V_x(0)V_x(t)\Big\rangle_E = 2\,\mathrm{Re}\Big\langle V_x(t)V_x(0)\Big\rangle_E\,, \tag{1}$$

and the average square spreading:

$$\Delta X^2(E,t) = \Big\langle [X(t) - X(0)]^2\Big\rangle_E \tag{2}$$

where $\langle \mathrm{A}\rangle_E$ is the average of the operator A on states of energy E of Hamiltonian H, explicitly given by the traces fraction:

$$\langle A\rangle_E = \frac{Tr[\delta(E-H)A]}{Tr[\delta(E-H)]} \tag{3}$$

In (1), $\mathrm{Re}\,B$ is the real part of B and $V_x(t)$ is the Heisenberg representation of the velocity operator along x direction at time t. $C(E,t)$ is related to quantum diffusion by:

$$\frac{\mathrm{d}}{\mathrm{dt}}\Big(\Delta X^2(E,t)\Big) = \int_0^t C(E,t')\mathrm{dt}'. \tag{4}$$

Once the bandstructure is computed in a self-consistent way the velocity correlation function can be computed exactly in the basis of Bloch states. Relation (4) shows that an anomalous behaviour of $C(E,t)$ also implies an anomalous behavior of the quantum diffusion which is the basis for the model [13,14] of optical conductivity of quasicrystals. In the long time limit one knows that the propagation is ballistic, this means that $\Delta X^2(E,t)$ is given by $v_{\mathrm{F}}^2 t^2$ at large time. From (4) one deduces that $C(E,t)$ is of the order of $2v_{\mathrm{F}}^2$ at large time. But at intermediate times (see below) the behaviour of $C(E,t)$ is more specific of the crystal and we show that the α-AlMnSi phase is different compared to other good metals such as Al (f.c.c.), cubic $\mathrm{Al_{12}Mn}$ ...

In particular we find that there is on the average a phenomenon of *backscattering* in α-AlMnSi phase. This means that the velocity correlation function is often negative. This negative value has been shown previously [14] a sufficient condition to explain the unusual conduction properties of these alloys.

2. *Ab-initio* electronic structure

2.1. LMTO METHOD

Electronic structure determinations have been performed using the self-consistent LMTO method in the Atomic Sphere Approximation (ASA).

The LMTO method is well described elsewhere [17, 18] and we would like to remind here only the principal results which are usefull for this paper. In the frame of DFT-LDA band structure calculations, the LMTO method is based on some approximations. The space is divided in atomic spheres where the potential is spherically symmetric and interstitial region where it is flat ("Muffin Tin" potential). In the Atomic Sphere Approximation (ASA), the spheres radii are chosen so that the total volume of the spheres equals that of the solid. One makes a further approximation by supposing that the kinetic energy in the interstitial region is zero (without this non-essential assumption, Laplace equation, as used below, should be replaced by Helmoltz equation). In this intersticial region, the Schrödinger equation reduces to Laplace equation having regular and irregular solutions: $Y_L(\hat{r})r^{\ell}$ and $Y_L(\hat{r})r^{-\ell-1}$ respectively. Here $L = (\ell, m)$ represents the angular momentum index and $Y_L(\hat{r})$ the spherical harmonics in direction $\hat{r} = (\theta, \phi)$. For the sphere centered at site R and in the momentum index ℓ ($\ell = 0, 1, 2 \ldots$), one finds the solution $\varphi_{R\ell\nu}$ of the radial Schrödinger equation for a given so-called linearization energy E_ν, usually taken at the center of gravity of the occupied part of the ℓ-band and the energy derivative of $\varphi_{R\ell\nu}$ noted $\dot{\varphi}_{R\ell\nu}$ (Note that for the velocity correlation function, we need a great accuracy close to the Fermi level. Consequently, after self-consistency, we perform one iteration choosing $E_\nu = E_{\mathrm{F}}$). It can be shown that the corresponding orbitals $\varphi_{R\ell\nu}$ and $\dot{\varphi}_{R\ell\nu}$ are orthogonal to each other and nearly orthogonal to the core levels. It is thus possible to build a basis set of orbitals χ_{RL} centered at sphere of site R in the following way. Outside the sphere, in the interstitial region χ_{RL} is proportional to the irregular solution $Y_L(\hat{r})r^{-\ell-1}$ of Laplace equation and it is augmented (i.e. substituted according to Slater terminology) in its own sphere by a linear combination of $\varphi_{R\ell\nu}$ and $\dot{\varphi}_{R\ell\nu}$ having logarithmic derivative $-\ell - 1$ at the radius s_R of the sphere so that the orbital is continuous and derivable at the sphere boundary. In any other sphere R', the irregular solution of Laplace equation can be expanded in term of regular solutions in that sphere:

$$Y_L(\hat{r}_R)(\frac{r_R}{a})^{-\ell-1} = -\sum_{L'} \frac{1}{2(2\ell'+1)} S^0_{R'L',RL} Y_{L'}(\hat{r}_{R'})(\frac{r_{R'}}{a})^{\ell'} \qquad (5)$$

and the orbital χ_{RL} should be augmented in sphere R' with the same expansion of linear combination of $\varphi_{R'\ell'\nu}$ and $\dot{\varphi}_{R'\ell'\nu}$ having the logarithmic derivative ℓ' at the radius $s_{R'}$ of sphere R'. In (5), a is a scale factor and $S^0_{R'L',RL}$ are the so-called "structure constants" which depend only on the crystallographic structure of the material. In this basis set of the orbitals χ_{RL} both Hamiltonian and Overlap matrices can be expressed in terms of $S^0_{R'L',RL}$, and the potential parameters $\varphi_{R\ell\nu}(s_R)$, $\dot{\varphi}_{R\ell\nu}(s_R)$ and the logarithmic derivative $D_{R\ell\nu}$ and $\dot{D}_{R\ell\nu}$ of these functions at sphere boundary. Since the structure constants $S^0_{R'L',RL}$, decreasing as $r^{-\ell-\ell'-1}$ with distance, are

very long ranged for s and p orbitals, it can be more convenient to change the basis set so that the Hamiltonian can have the Tight-Binding (TB) form or any desired properties (like the orthogonality i.e. overlap matrix equals unit matrix). It can be achieved by adding to the regular solution of the Laplace equation an amount of the irregular solution for a given angular momentum. It is possible to choose this amount $\bar{Q}_\ell$ so that the transformed structure constants S can be screened with a short-range dependence with the distance or so that the orbitals of the transformed basis set are orthogonal (the so-called TB or most localized and orthogonal representations, respectively). With appropriate choice for $\bar{Q}_\ell$, the transformed structure constant matrix obeys to the following equation:

$$S = S^0(1 - \bar{Q}_\ell S^0)^{-1} \tag{6}$$

The Hamiltonian can be written as:

$$H_{RL,R'L'} = C_{RL}\delta_{RL,R'L'} + \Delta_{RL}^{1/2} S_{RL,R'L'} \Delta_{R'L'}^{1/2} \tag{7}$$

which is limited to first order in $(E - E_\nu)$ in the TB representation, whereas it is valid up to second order in the orthogonal representation. C_{RL} determines the middle of the band "RL" and Δ_{RL} its width and the strength of hybridization. These parameters are expressed in terms of the 4 potential parameters:$\varphi_{R\ell\nu}(s_R)$, $\dot{\varphi}_{R\ell\nu}(s_R)$, $D_{R\ell\nu}$ and $\dot{D}_{R\ell\nu}$. It should be stressed that hybridization between bands of different angular moments is due to the matrix elements $S_{RL,R'L'}$ which couples RL-states to $R'L'$ ones. Due to the periodicity of the approximant phases, one can apply Bloch theorem. Thus, once the potential parameters are known for each site and each ℓ-component, with an appropriate choice of screening constants, structure constants (6) and Hamiltonian (7) are transformed to k-space. Diagonalization provides energies with their respective eigenstates for each k-point $\overrightarrow{k}$ of the first Brillouin zone. These eigenstates are expressed on the basis of the

$$\chi_{\vec{t}L}(\vec{k}) = \frac{1}{\sqrt{N}} \sum_{\vec{T}} e^{i\vec{k}\cdot\vec{T}} \chi_{(\vec{T}+\vec{t})L} \tag{8}$$

which are the Bloch states obtained from the real space orbital $\chi_{(\vec{T}+\vec{t})L}$, located at site $\vec{t}$ of the unit cell $\vec{T}$: any general atomic site $\vec{R}$ can be decomposed as $\vec{R} = \vec{T} + \vec{t}$. ($N$ is the total number of cells, introduced here for normalization).

2.2. RESULTS: DENSITY OF STATES

For our practical applications, the LMTO basis includes all angular moments up to $\ell = 2$ and the valence states are Al (3s, 3p, 3d), Mn (4s, 4p, 3d).

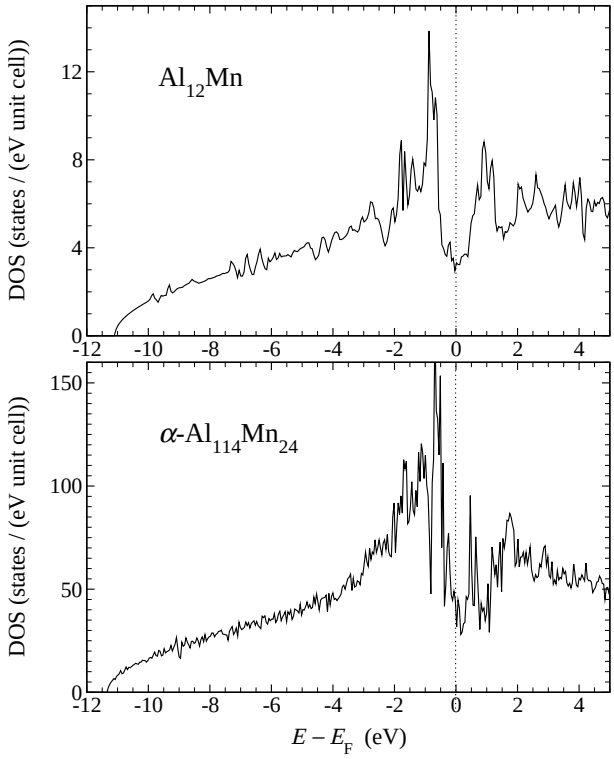

Figure 1. LMTO DOS of cubic $Al_{12}Mn$ (13 atoms / unit cell) and cubic α-$Al_{114}Mn_{24}$ approximant (experimental atomic structure of α-AlMnSi [26] with Si = Al, 138 atoms / unit cell) [22].

The LMTO density of states (DOS) of an α-AlMn idealized approximant (structural model of Elser-Henley [19]) has been first calculated by T. Fujiwara [12, 20]. This original work shows the presence of a Hume-Rothery pseudo-gap near the Fermi energy, E_F, in agreement with experimental results [7, 11]. E.S. Zijlstra and S.K. Bose [24] gave a detailed *ab initio* electronic structure study of the α-phase. They show the difference between the DOS of the idealized 1/1 approximant and the experimental atomic structure [26]. The pseudogap is present in both cases. But one of the main difference is the spikiness of the DOS which is reduced for the experimental structure with respect to the idealized structure. DOSs of α-$Al_{114}Mn_{24}$ with experimental atomic positions [26] (Si atoms are replaced by Al atoms) is presented Fig. 1. The role of the transition metal (TM) element in the pseudo-gap formation has also been shown from *ab-initio* calculations [21, 22] and experiments. Indeed the formation of the pseudo-gap results from a strong sp–d coupling associated to an ordered sub-lattice of TM atoms. Just as for Hume-Rothery phases a description of

the band energy can be made in terms of pair interactions. We have shown that a medium-range Mn–Mn interaction mediated by the sp(Al)–d(Mn) hybridization plays a determinant role in the occurrence of the pseudo-gap [22, 23]. It is thus essential to take into account the chemical nature of the elements to analyze the electronic properties of approximants. It has been shown [24] that Si atoms are in substitution with some Al atoms. The main effect of Si is to shift E_{F} in the pseudo-gap in agreement with Hume-Rothery mechanism to minimize band energy.

The electronic structures of simpler crystals such as orthorhombic Al_6Mn, cubic $Al_{12}Mn$, present also a pseudo-gap near E_{F} but it is less pronounced than for complex approximants phases [22].

3. Velocity correlation function

3.1. COMPUTATIONAL DETAILS

Starting from the self-consistent LMTO eigenstate Ψ_n with energy E_n, the velocity correlation function is [13]:

$$C(E,t) = 2\left\langle \mathrm{Re}\left\{ \mathrm{e}^{\mathrm{i}\frac{\mathrm{E_n t}}{\hbar}} \langle \Psi_{\mathrm{n}} | \mathrm{V_x}\, \mathrm{e}^{-\mathrm{i}\frac{\mathrm{Ht}}{\hbar}} \mathrm{V_x} | \Psi_{\mathrm{n}} \rangle \right\} \right\rangle_{\mathrm{E_n=E}} \tag{9}$$

By using the closure properties of the eigenstates one obtains easily:

$$C(E,t) = 2\left\langle \sum_p \cos\left((E_n - E_p)\frac{t}{\hbar} \right) \left| \langle \Psi_n | V_x | \Psi_p \rangle \right|^2 \right\rangle_{E_n=E}. \tag{10}$$

where the sum is over all the eigenstates Ψ_p with the same vector $\vec{k}$ than Ψ_n. In (10) the terms $n = p$ are the Boltzmann contribution to the velocity correlation function:

$$C_{\mathrm{B}}(E,t) = 2\left\langle \sum_n \left| \langle \Psi_n | V_x | \Psi_n \rangle \right|^2 \right\rangle_{E_n=E} = 2v_{\mathrm{B}}^2 \tag{11}$$

which does not depend on the time t.

The products $\langle \Psi_n | V_x | \Psi_p \rangle$ are calculated from LMTO eigenstates by using a numerical derivation of the hamiltonian in the reciprocal space: as explained in last section, diagonalization provides the components of eigentstates on the basis set $\chi_{tL}(\overrightarrow{k})$. In this basis the velocity operator, $V_x = \frac{1}{i\hbar}[X, H]$, has the following matrix elements:

$$\langle \chi_{tL}(\overrightarrow{k}) | V_x | \chi_{t'L'}(\overrightarrow{k}) \rangle = \frac{1}{\hbar}\frac{\partial}{\partial k_x} \langle \chi_{tL}(\overrightarrow{k}) | H | \chi_{t'L'}(\overrightarrow{k}) \rangle \tag{12}$$

k_x is the component of k-point $\vec{k}$ in the x direction. Because of Bloch theorem, different k-points are not coupled in the Hamiltonian nor in the

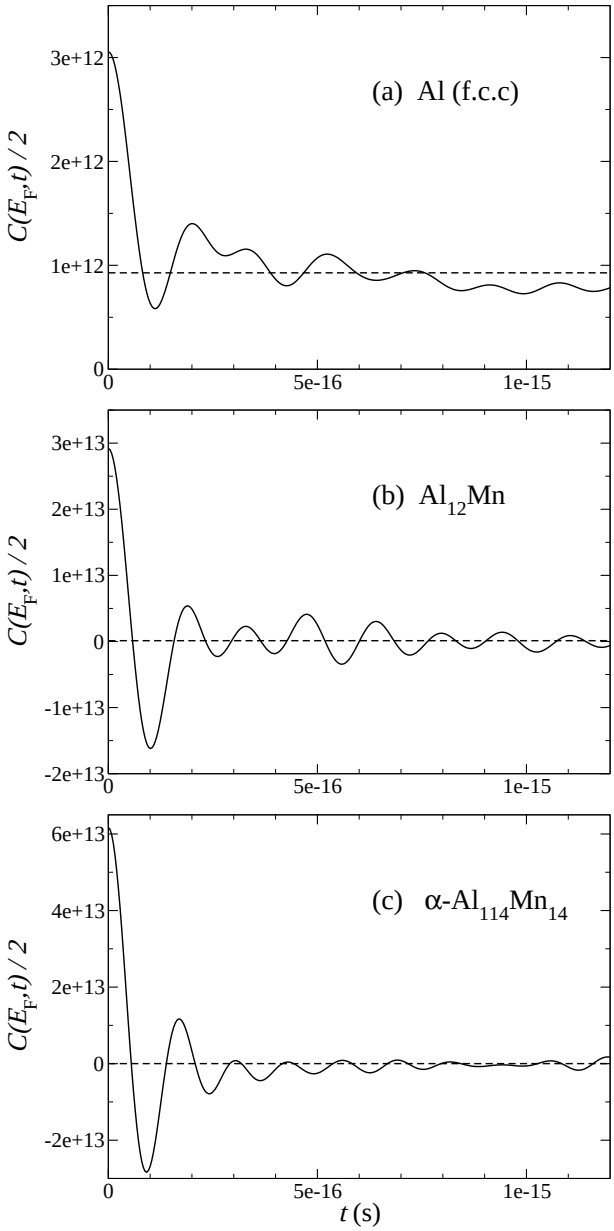

Figure 2. Velocity correlation function $C(E_{\mathrm{F}}, t)$ ($\mathrm{m}^2\,\mathrm{s}^{-2}$) versus time t (s), for (a) Al (f.c.c), (b) cubic $Al_{12}Mn$, and (c) cubic approximant α-$Al_{114}Mn_{24}$. The dashed lines are the Boltzmann velocity correlation function $C_{\mathrm{B}}(E_{\mathrm{F}}, t) = 2v_{\mathrm{F}}^2$. [27]

velocity operator. Having performed the numerical derivation of (12), it is just a matrix multiplication to get expression (10). Formula (12) is an

approximation as one can show that there are additional terms on its right hand side. However these terms are of the order of $(E_n - E_\nu)^2$ and thus vanish for the energies of interest close to E_ν chosen at E_F. Finally equation (10) is integrated according to equation (4), to obtain the average square spreading $\Delta X^2(E,t)$.

3.2. RESULTS: EVIDENCE OF BACKSCATTERING IN AN APPROXIMANT OF QUASICRYSTALS

We compute $C(E,t)$ for crystals (complex approximants and simple crystals). In equations (10)–(11), the average on states of energy E is obtained by taking the eigenstates of each $\vec{k}$ vector with an energy E_n such as:

$$E - \frac{1}{2}\Delta E < E_n < E + \frac{1}{2}\Delta E. \tag{13}$$

ΔE is a kind of energy resolution of the calculation. The calculated $C(E,t)$ is rather sensible to the small number N_k of $\vec{k}$ vectors in the first Brillouin zone. Therefore N_k is increases until $C(E,t)$ does not depend significantly on N_k.

$C(E_\mathrm{F},t)$ for Al (f.c.c), cubic $Al_{12}Mn$ [25], and the cubic approximant α-$Al_{114}Mn_{24}$ (with the experimental atomic structure [26]) are shown in figure 2. E_F is the Fermi energy calculated by the self-consistent L.M.T.O. procedure. The energy resolution is $\Delta E = 1.36\,\mathrm{eV}$. The number of $\vec{k}$ points in the first Brillouin zone is $N_k = 80^3$, 40^3 and 10^3 for Al, $Al_{12}Mn$, and α-$Al_{114}Mn_{24}$, respectively.

For large t,

$$\lim_{t\to+\infty} C(E_\mathrm{F},t) \simeq C_\mathrm{B}(E_\mathrm{F},t) = 2v_\mathrm{F}^2\,, \tag{14}$$

where v_F is the Boltzmann velocity (intra-band velocity) at the Fermi energy: $v_\mathrm{F} = 9.6\,10^7$, $3.4\,10^7$, and $6.2\,10^6\,\mathrm{cm\,s^{-1}}$, for Al, $Al_{12}Mn$ and α-$Al_{114}Mn_{24}$, respectively. This last result is very similar to the original work of T. Fujiwara et al. [12] for the α-$Al_{114}Mn_{24}$ (with the atomic structure model of Elser-Henley). The strong reduction of v_F in the approximant phase with respect to simple crystal phases shows the importance of a quasiperiodic medium-range order (up to distances equal to 12–20 Å). This leads to a very small Boltzmann conductivity for the approximant [12].

When t is finite (figure 2), $C(E_\mathrm{F},t)$ and $C_\mathrm{B}(E_\mathrm{F},t)$ differ, and there is a new difference between approximant and simple crystal. In the case of Al (f.c.c.) phase, $C(E_\mathrm{F},t)$ is always positive, and the Boltzmann value is reached rapidly when t increases. But for some t values the velocity correlation function $C(E_\mathrm{F},t)$ is negative for $Al_{12}Mn$ and α-$Al_{114}Mn_{24}$. That means that at these times the phenomenon of *backscattering* occurs.

Roughly speaking, the transports properties depends on the values of $C(E_\mathrm{F},t)$ over all times t from 0 to the scattering time τ [13, 14] (see for

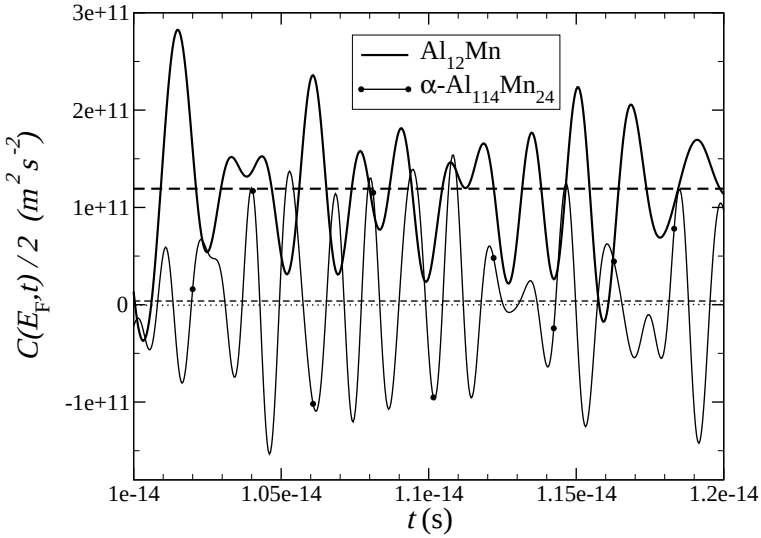

Figure 3. Velocity correlation function $C(E_{\mathrm{F}}, t)$ ($\mathrm{m}^2\,\mathrm{s}^{-2}$) versus large time t (see figure 2). The dashed lines are the corresponding Boltzmann velocity correlation function $C_{\mathrm{B}}(E_{\mathrm{F}}, t) = 2v_{\mathrm{F}}^2$.

instance equation (4)). A realistic value of τ has been estimated to about 10^{-14} s [8]. For the simple crystals $Al_{12}Mn$, $C(E_{\mathrm{F}}, t)$ is meanly positive when $t > 2\,10^{-15}$ s. But for the complex approximant α-$Al_{114}Mn_{24}$, a lot of t values correspond to $C(E_{\mathrm{F}}, t) < 0$, even when t is close to τ or larger (figure 3). Therefore, in the case of $Al_{12}Mn$, the backscattering (negative range of $C(E_{\mathrm{F}}, t)$) should have a negligible effect on the transport properties, whereas this effect must be determinant for the approximant.

The phenomenon of backscattering leads to unusual quantum diffusion. It is illustrated on the plot of the average spreading of states ΔX^2 (equation (2)) versus time t (figure 4). It shows that ΔX^2 results in two term: a Boltzmann term and a non-Boltzmann term. The Boltzmann term has the usual t^2 behavior: $\Delta X_{\mathrm{B}}^2 = v_{\mathrm{B}}^2 t^2$. The new non-Boltzmann contribution, which comes from the non-diagonal matrix element in (10), has an atypical constant asymptotic behavior. In a normal crystal this last term is negligible with respect to the Boltzmann term. On the contrary, in approximant both terms have the same order of magnitude for realistic times, typically t less than fews 10^{-14} s.

4. Conclusion

We present *ab-initio* calculations of the velocity correlation function of the electronic states close to the Fermi energy, in a complex approximant and simple crystals. These calculations are the first numerical proof of the exis-

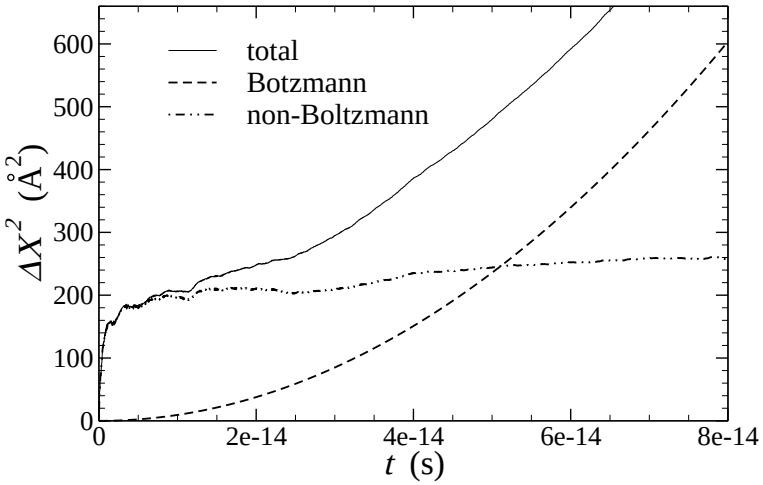

Figure 4. Average spreading of states $\Delta X^2(E,t)$ for energy $E = E_{\rm F}$(LMTO), in α-AlMnSi. $\Delta X^2(E,t)$ can be decomposed in a Boltzmann term and a non-Boltzmann term.

tence of the phenomenon of backscattering in an approximant of quasicrystals. This shows that a Boltzmann approach is not enough to understand the unusual transport properties of quasicrystals. It will be shown elsewhere [28] that these results on the quantum diffusion explain fairly well the experimental conduction properties of the α-AlMnSi phase and of the related QC phases.

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