Field-induced confinement in quasi-one-dimensional organic conductors

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We show within a quantum-mechanical calculation that in Bechgaard salts the electron transport along the least conducting c axis is dramatically affected by a magnetic field applied parallel to the intermediate conducting b axis. Above a threshold field, the system undergoes a field-induced dimensional crossover from a three-dimensional (3D) phase to a two-dimensional phase where the electrons are confined in the most conducting (ab) plane. This leads to a significant change in the temperature dependence of the electron scattering rate. The latter exhibits strong deviations from the T^2 Fermi-liquid (FL) rule, which is only obeyed in the low-temperature 3D phase where the interplane hopping is coherent. Despite the departure of the scattering rate from the FL behavior, the transport properties at high temperature are found to be in accordance with FL predictions. Our results, which correctly account for the c-axis transport measurements in Bechgaard salts, provide a possible understanding of the striking behavior of the interlayer conductivity in cuprate based compounds in a parallel magnetic field.

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I. INTRODUCTION

The low dimensional nature of the electronic properties of the highly anisotropic Bechgaard salts denoted $(TMTSF)_2X$ ($X=PF_6$, ClO_4, ReO_4…) is at the origin of a rich variety of physical phenomena.[1,2] The quasi-one-dimensionality of these systems is due to the crystal structure consisting of stacked organic molecules (TMTSF) in the a direction, along which the highest conductivity takes place. These organic chains are coupled along the b direction to form conducting planes, which are weakly coupled along the c axis. The bandwidths along the crystal axes are $t_a:t_b:t_c=3000:200:10$ K. The Fermi surface (FS) is consists of slightly warped parallel sheets at $k_x \sim \pm k_F$ parallel to the k_y and the k_z directions.

These compounds can exhibit a variety of ground states ranging from spin-density wave (SDW) insulator to a metallic state to a superconducting phase by either changing pressure or the anion X.

Applying a magnetic field perpendicular to the most conducting (ab) plane gives rise to a second-order transition from the metallic state to a cascade of field-induced SDW (FISDW) phases, which are one of the substantial phenomena that the growing area of organic quasi-one-dimensional (Q1D) conductors has produced. The overall features of the FISDW phases has been explained successfully in the framework of the quantized nesting model (QNM) based on the idea that—under a magnetic field—nesting properties of the Fermi surface are improved, which furthers the formation of the SDW phases.[3,4]

This field-induced feature has made way for investigating the dimensionality of the electronic system for different orientations of the magnetic field. Studying the transport properties has proved to be a reliable tool for such investigations. In particular, a number of unusual effects are observed (such as the angular dependent magnetoresistance), which, in spite of intensive studies, continues to rise open questions.[5–7] Moreover, attractive results have been obtained for the temperature dependence of the c-axis resistance for the field aligned along the b direction.[8–11] This geometry has been argued to be the best for measuring magnetoresistance effects in Bechgaard salts.[8]

It should be noted that the unit cell (a,b,c) of Bechgaard salts is triclinic, but for sake of simplicity, an orthorhombic (a,b',c^*) cell is used where the b' axis is the projection of the b axis perpendicular to the a direction and c^* is normal to the (ab) plane.

The temperature dependence of the c-axis resistivity ρ_c is found to be marked by a large magnetoresistance and a pronounced minimum, which moves toward higher temperature as the magnetic field increases. However, no magnetoresistance has been measured in the transport properties along the a axis showing a metallic behavior even at high magnetic field.[11,12] This anisotropic behavior between ρ_a and ρ_c rules out any interpretation in terms of charge localization.[10] Actually, it is the signature of a three-dimensional (3D) to two-dimensional (2D) crossover induced by the orbital effect of the field parallel to the b direction $(H\|b)$, which reduces the effective hopping process t_c along the least conducting axis. Such a crossover is expected when the magnetic energy $\omega_c = ev_F Hc/c_0$ is of the order of t_c. Here e is the unit charge, v_F is the Fermi velocity, c is the interplane distance, and c_0 is the speed of light.

In a semiclassical picture, the reduced dimensionality of the system in the presence of a magnetic field along the b direction can be understood as a consequence of the Lorentz force—which causes the electrons on the Fermi surface to move in the k_z direction according to the equation of motion:

$$\frac{dk_z}{dt} = \frac{ev_F H}{\hbar c_0}.$$

In real space, this leads to a periodic open orbit along the a axis with a c-axis velocity component $v_c = 2t_c c/\hbar \sin(k_z c)$

$=2t_c c/\hbar \sin(ev_F Hc/\hbar c_0 t)$. The electron motion is, then, periodically extended along the a direction with a spatial modulation at the magnetic wavelength $\lambda=\hbar c_0/eHc$ but is localized along the c axis with a width of $A_z=4t_c c_0/ev_F H$. The amplitude of the real-space orbit is then decreased as the magnetic field increases, making the conductivity more 2D and reducing the effective dimensionality of the system. Eventually, the carriers become confined in the (ab) plane once $A_z \sim c$, namely, if $\omega_c \sim 4t_c$. As a consequence, the system undergoes a 3D-2D crossover inducing a metal-insulator transition in the temperature dependence of the c-axis resistivity, while the transport properties along the a and the b directions remain metallic.

This *field-induced confinement* should not be confused with the *field-induced localization*, for which the metal-insulator transition is expected to occur in both directions perpendicular to the field.

We have proposed a quantum-mechanical treatment to account for the temperature dependence of the c-axis resistivity in $(TMTSF)_2ClO_4$ under the magnetic field $H\|b$.[11] The model was substantially dependent on the in-plane electron scattering rate $\hbar/\tau$, which was derived within a Fermi-liquid (FL) description with a T^2 temperature-dependence law. However, a major physical question regarding the field-induced confinement could be the following: "Does the FL description stand out when the dimensionality of the system is reduced by the 3D-2D crossover?" Actually, there is a long-standing controversy on the validity of a FL approach for the transport properties in Bechgaard salts.[13]

The aim of this paper is to extend the model discussed in Ref. 11 by going beyond the FL assumption to derive the temperature and the field dependence of the relaxation rate, from which we deduce the quantum-mechanical criterion for the field-induced confinement. Moreover, we determine—besides the c-axis resistivity—the magnetoresistance $\Delta\rho_c/\rho_0$ (where $\Delta\rho_c=\rho_c(H)-\rho_0$ and ρ_0 is the zero-field c-axis resistivity). We also calculate the a-axis resistivity ρ_a and discuss the obtained results in connection with the experimental data of different Bechgaard salts. We shall argue that the present model is actually consistent with the interplane transport behavior of layered conductors in the presence of an in-plane magnetic field.

In the following we will briefly review the experimental studies and the theoretical approaches dealing with interplane transport under a magnetic field parallel to the intermediate conducting b axis. Then, we will present our model in Sec. III and discuss the obtained results in Sec. IV. Section V is devoted to the concluding remarks.

II. FIELD-INDUCED CONFINEMENT: EXPERIMENTS VERSUS THEORY

Forró *et al.*[14] have reported the resistivity and the magnetoresistance measurements along the c axis for a magnetic field parallel to the triclinic b axis in the case of $(TMTSF)_2ClO_4$ at low temperature (below 20 K) and up to 7 T. The authors found that the magnetoresistance obeys the Kohler rule (KR), which states that the relative variation of the resistance is a universal function of H/ρ_0; $\Delta\rho_l\rho_0=mH^2/\rho_0^2$, where ρ_0 is the zero-field resistivity and m is a constant.

The study was extended by Cooper *et al.*[8] to higher temperatures for the ClO_4 and the PF_6 salts. The authors found that the magnetoresistance in both salts obeys a T^{-3} power law at high temperature ($T>100$ K).

The dependence of the transport properties of $(TMTSF)_2ClO_4$ on the disorder induced by irradiation and alloying was studied by Korin-Hamzić *et al.*[15] for a current flow along the c axis and with a magnetic field parallel to b' axis. The authors reported that the resistance increases as T^2 increases up to 23 K for disordered samples at zero field and that the KR is obeyed for pure and alloyed relaxed samples in the temperature range from 4.2 to 30 K and fields up to 7.8 T. However, significant deviations from KR were observed for irradiated samples. The result was interpreted as a consequence of defect induced decrease in the effective transverse hopping integral t_c. This decrease is expected to be erased by thermal fluctuations around 20 K as observed experimentally.

Danner *et al.*[10] measured the temperature dependence of ρ_c for $H\|b$ in $(TMTSF)_2ClO_4$ and found above 4 T—which has been the lowest reported field value, a minimum of the resistivity that is shifted toward higher temperature as the field increases. The same feature was observed in PF_6 salt by Lee *et al.*[16] above a critical field of 1 T.

Recently Korin-Hamzić *et al.*[9] performed transport measurements in the metallic state of $(TMTSF)_2ReO_4$ above 200 K and analyzed the temperature dependence of the magnetoresistance within FL and non-FL models. The authors argued that the c-axis resistivity for $H\|b'$, which does not agree with Luttinger liquid predictions, cannot be fully understood within the conventional FL description due to the lack of a FL transport theory including anisotropic relaxation times. Moreover, the authors reported a quite interesting results about the temperature dependence of the magnetoresistance, which exhibits at high temperature a T^{-3} behavior as found in ClO_4 and PF_6 salts.

More recently, Joo *et al.*[11] investigated, with accurately aligned magnetic field and in the low-temperature regime, the effect of a magnetic field oriented in the most conducting (ab) plane of ClO_4 compound. The results showed that for $H\|b'$, ρ_c is marked by a field-induced confinement above 1 T while the longitudinal resistivity ρ_a remains metallic. When the field is no more along b', the authors found that the confinement is induced by the field component along the b' axis.

As regards to the theoretical studies, the field-induced dimensional crossover was first pointed out by Lebed[17] when discussing the reentrance of the superconducting phase in organic conductors in high magnetic field parallel to the layers.

Strong *et al.*[18] suggested that the magnetic field leads to a renormalization of the coherent part of the interplane hopping resulting in a coherence-incoherence transition from a 3D FL to decoupled 2D non-Fermi liquids. A magnetic field applied in the b direction dephases the interplane tunneling, which reduces the effective hopping integral t_c. This idea was originally proposed by Anderson to account for the unusual behavior of the interplane resistivity observed in cu-

prate superconductors, which has been ascribed to the non-FL nature of the in-plane electronic ground state. The interplane coherent hopping is expected to be strongly reduced as a consequence of non-FL in-plane electronic features.[19] The model of Strong *et al.* was tested by Danner and Chaikin[20] in the case of $(TMTSF)_2PF_6$, which has been argued to behave as a 2D non-FL above a threshold field as predicted in Ref. 18. However, no quantitative conclusion could be drawn out from the theoretical approach of Strong *et al.* to account for the striking transport features of Bechgaard salts under a magnetic field parallel to the *b* axis.

A field-induced localization scenario was suggested to interpret the large *a*-axis magnetoresistance observed for a field parallel to the *c* axis in $(TMTSF)_2ClO_4$.[12] This effect was ascribed to the opening of a charge gap over the FS. Nevertheless, the absence of any magnetoresistance along the *c* axis rules out this localization model as argued by Danner *et al.*[10]

A semiclassical calculation based on Boltzmann equation was performed to drive an analytical expression for the out-of-plane resistance in transverse magnetic field.[21] The authors found that the obtained expression, which depends on two fitting parameters, is in agreement with experiments up to 7 T. However, a strong discrepancy should be expected between this model and the experimental data at high magnetic field for which the effective coherent hopping along the out-of-plane direction is destroyed. On the other hand, semiclassical models fail to explain the puzzling saturating behavior of the interplane resistance observed at low temperature and high magnetic field.[22,23] We shall discuss this issue in details in Sec. IV.

A quantum-mechanical approach was recently proposed by Lebed[24] to determine the electron wave function in quasi-one layered conductors under a parallel magnetic field. The author showed that, at high magnetic field, all the wave functions are localized on one conducting layer contrary to the weak-field limit where the wave functions can extend over different layers. Lebed suggested to make use of this field-induced 3D-2D crossover to test the existence of a FS in different quasi-2D materials. Nevertheless, the striking behavior of the *c*-axis resistance was not addressed by the theoretical model of Ref. 24.

The outcome of this brief review is that the temperature dependence of the resistivities in quasi-1D conductors under a parallel magnetic field is a though theoretical issue, and quantitative theoretical models are required. Basically, all the proposed models assumed a field independent relaxation time, which is inconsistent with the change from metallic to insulating behavior of the *c*-axis resistance.

Recently, we have performed a quantum calculation of the transverse transport in a parallel magnetic field taking into account the field dependence of both the interplane electron Green's function and the intraplane scattering time. The latter was assumed to obey the T^2 FL rule. The obtained results are consistent with the behavior of the *c*-axis resistance as a function of the temperature observed in the $(TMTSF_2ClO_4)$ salt.[10,11] However, the FL nature of the relaxation time must be taken with a grain of salt in the case of PF_6 compound where no clear conclusion can be drawn about the validity of a FL description. In this paper, we extend discussions about the theoretical results shortly presented in Ref. 11 and address issues dealing with the electronic transport properties in Bechgaard salts in the presence of a parallel magnetic field. We assign the puzzling behavior of these properties to two key ideas, which make the originality of our model: (i) the confinement of the electron Green's function to a single layer and (ii) the temperature and the field dependences of the in-plane scattering rate. The latter shows departure from the T^2 FL law. The obtained results are in good agreement with the experimental data reported in numerous layered conductors.

III. FIELD-INDUCED CONFINEMENT: THEORETIC APPROACH

We consider, for simplicity, an orthorhombic crystal structure instead of the real triclinic one, which should not affect the outcomes of the model. We denote, hereafter, the orthorhombic (a,b',c^*) basis by (a,b,c).

Within a tight-binding model, the dispersion relation of quasi-one-dimensional conductors can be described by

$$\epsilon(\vec{k}) = v_F(|k_x| - k_F) - 2t_b \cos k_y b - 2t_c \cos k_z c, \qquad (1)$$

where *b* and *c* are, respectively, the interchain and interplane distances. We have taken a linear dispersion around the Fermi level along the chains direction *a* corresponding to the highest conductivity and with a Fermi velocity v_F. t_b stands for the hopping integrals to the first-nearest neighbors in the *b* direction, whereas t_c describes the hopping along the least conducting axis *c* perpendicular to the conducting plane (a,b). The strong anisotropy of the hopping parameters leads to an open two-sheet Fermi surface. It is worth to note that, we have neglected in Eq. (1) the second-neighbor hopping integral t_b' along the *b* direction since it is irrelevant for the physics of field-induced confinement.

Let us consider a magnetic field parallel to the *b* axis $\vec{H}(0,H,0)$ with the gauge $\vec{A}(0,0,-Hx)$. The equation of motion near the right-hand FS sheet is

$$\left\{ i\omega_n + iv_F\frac{d}{dx} - 2t_b \cos k_y b - 2t_c \cos\left(k_z + \frac{eHx}{c}\right)c \right\} \times g_{++}(i\omega_n,k_y,k_z,x,x') = \delta(x-x'), \qquad (2)$$

where $g_{++}(i\omega_n,k_y,k_z,x,x')$ is given by

$$g_{++}(i\omega_n,k_y,k_z,x,x') = e^{-ik_F(x-x')}G_{++}(i\omega_n,k_y,k_z,x,x').$$

Equation (2) is obtained within a mean-field theory by means of Peierls substitution $\vec{p}\rightarrow\vec{p}-\frac{e}{c}\vec{A}$. The Green's function is written in the mixed representation (k_y,k_z,x), which is more convenient for the present problem.[3] Equation (2) can be immediately integrated in the form;

$$G_{++}(i\omega_n,k_y,k_z,x,x') = \frac{\text{sign }\omega_n}{iv_F}\exp i\left\{\frac{i\omega_n(x-x')}{v_F} + k_F(x-x') - \frac{2t_b}{v_F}\cos(k_y b)(x-x') - \frac{4t_c}{\omega_c}\cos\left[k_z + \frac{G_c(x+x')}{2}\right]\sin\left[\frac{G_c(x-x')}{2}\right]\right\}, \tag{3}$$

for $\omega_n(x-x')>0$, where $G_c=eHc/c_0$ is the magnetic wave vector and $\omega_c=v_F G_c$ is the magnetic energy. Taking for Bechgaard salts[7] $v_F=210^5$ m.s^{-1}, $c\sim 14$ Å gives rise to $\omega_c/H=3.3$ K/T.

We substitute the Matsubara frequencies ω_n by $\eta(T,H)-i\omega$—where the scattering rate $\eta(T,H)=\hbar/\tau(T,H)$—and $\tau(T,H)$ is the in-plane quasiparticle lifetime, which is temperature and field dependents. We obtain, by taking the Fourier transform of $G_{++}(i\omega_n,k_y,k_z,x,x')$ with respect to k_z,

$$G_{++}(\omega,k_y,z,E) = \frac{\text{sgn }\omega}{2i\pi c v_F}\exp\left\{\frac{-\eta(T,H)}{E}\right\}\exp i\left\{\frac{\omega}{E} + \frac{E_F}{E} - \frac{2t_b}{E}\cos k_y b\right\}\int_{-\pi}^{\pi}\exp i\left\{\frac{z\theta}{c} - \frac{4t_c}{\omega_c}\cos\theta\sin\left(\frac{\omega_c}{2E}\right)\right\}d\theta. \tag{4}$$

In Eq. (4) we have set $E=v_F/(x-x')$, $\theta=ck_z$, and $X_0=(x+x')/2=0$, since the behavior of the Green's function is not affected by the position of the center of mass X_0.

To derive the z dependence of $G_{++}(\omega,k_y,z,E)$, one should write down the expression of the scattering rate $\eta(T,H)$—which is expected to be substantially dependent on the magnetic field. This is due to the localization of the electron density in a narrower distance along the c axis as the magnetic field increases, which results in an enhanced in-plane scattering rate $\eta=\hbar/\tau$. However, above a threshold field at which the system undergoes a 3D-2D crossover, η tends to saturate since all the electrons are confined in one conducting plane. Lebed[25] has already highlighted the crucial effect of the magnetic field on the temperature dependence of the scattering rate. The latter is found to change with field orientation governing the effective dimensionality of the system.

Moreover, Zheleznyak and Yakovenko[7] have found—based on numerical calculations—that under a magnetic filed the temperature behavior of the Umklapp electron-electron scattering changes from T^2 to T if the temperature is smaller than the magnetic energy. According to Refs. 7 and 25, the in-plane scattering rate is expected to be field dependent.

$\eta(T,H)$ is given by the imaginary part of the self-energy of the electron Green's function:[26]

$$\eta(T,H) = \hbar g^2 v_F T\int_0^{\pi}dq\int_0^{\pi}dQ\int_0^{E_d(T)}\frac{dE}{E^2}\frac{2\pi T}{\sinh^2\left(\frac{2\pi T}{E}\right)} \times\left[\frac{2\pi T}{E(\exp^{4\pi T/E}-1)} + \frac{2\pi T - E}{2E}\right]J_0^2\left(\frac{8t_b}{E}\cos q\right) \times J_0^2\left[\frac{8t_c}{\omega_c}\sin\left(\frac{\omega_c}{E}\right)\cos Q\right], \tag{5}$$

where g is the strength of the electron-electron interaction and $E_d(T)$ is a temperature-dependent cutoff. The latter is a renormalized bandwidth depending on the effective dimensionality of the system. One should expect, as in renormalization group method,[27] different bandwidth cutoffs as the system crosses from a given dimension to the other. In a renormalized mean-field theory, the bandwidth for the 2D phase of Q1D organic conductors is taken as T_{cross} instead of $E_F\sim 3000$ K. $T_{\text{cross}}\sim t_b$ is the temperature at which the system undergoes a dimensional crossover from the 2D phase to the purely one-dimensional (1D) phase.[27]

As argued by many authors,[7,9,25] the switching from a fully 3D to a 2D behavior has dramatic effects on the in-plane scattering rate. Regarding the strong dependence of the dimensionality of the system on the thermal fluctuations, electron-electron scattering processes should then be significantly dependent on the thermal energy scales—which define the different regimes of thermal fluctuations. Crossing from one regime to the other, the temperature behavior of the scattering time is expected to change (reflecting the interplay between dimensionality and thermal fluctuations). Each thermal regime can be identified by an energy scale $E_d(T)$, which marks its extent. Only scattering processes with an energy E [Eq. (5)] less than the cut-off $E_d(T)$ can take place in a given phase. Higher-energy processes will occur in a reduced dimension phase with a higher cutoff.

Referring to the interplane hopping parameter t_c, one could distinguish basically three energy scales for the cut-off $E_d(T)$: (i) $T_{3D}\sim t_c$, below which a coherent interplane hopping takes place leading to a conventional 3D FL. (ii) $T_{3D\text{-}2D}(t_c<T_{3D-2D}<t_b)$, which marks the extent of the transient regime where the system crosses continuously from the 3D to the 2D phase. The interplane hopping, in this regime, becomes more and more incoherent as the temperature increases. (iii) $T_{2D}\sim t_b$ which indicates the crossover temperature from the 1D to the 2D phase. Below T_{2D} but above $T_{3D\text{-}2D}$, the system is effectively 2D and the hopping along the c axis is completely destroyed.

We have considered, for a given temperature, the corresponding energy cutoff $E_d(T)$ to derive the temperature dependence of the scattering rate $\eta(T,H)$ according to Eq. (5).

Taking a unique infinite cutoff—as done in Ref. 26—leads to a field independent scattering rate, which is inconsistent with the field-induced metallic-insulating switching of the ρ_c temperature dependence and with the change in the temperature behavior of the scattering rate with field orientation reported in Ref. 25.

The temperature behavior of $\eta(T,H)$ given by Eq. (5) is depicted in Fig. 1. The numerical values of the different pa-

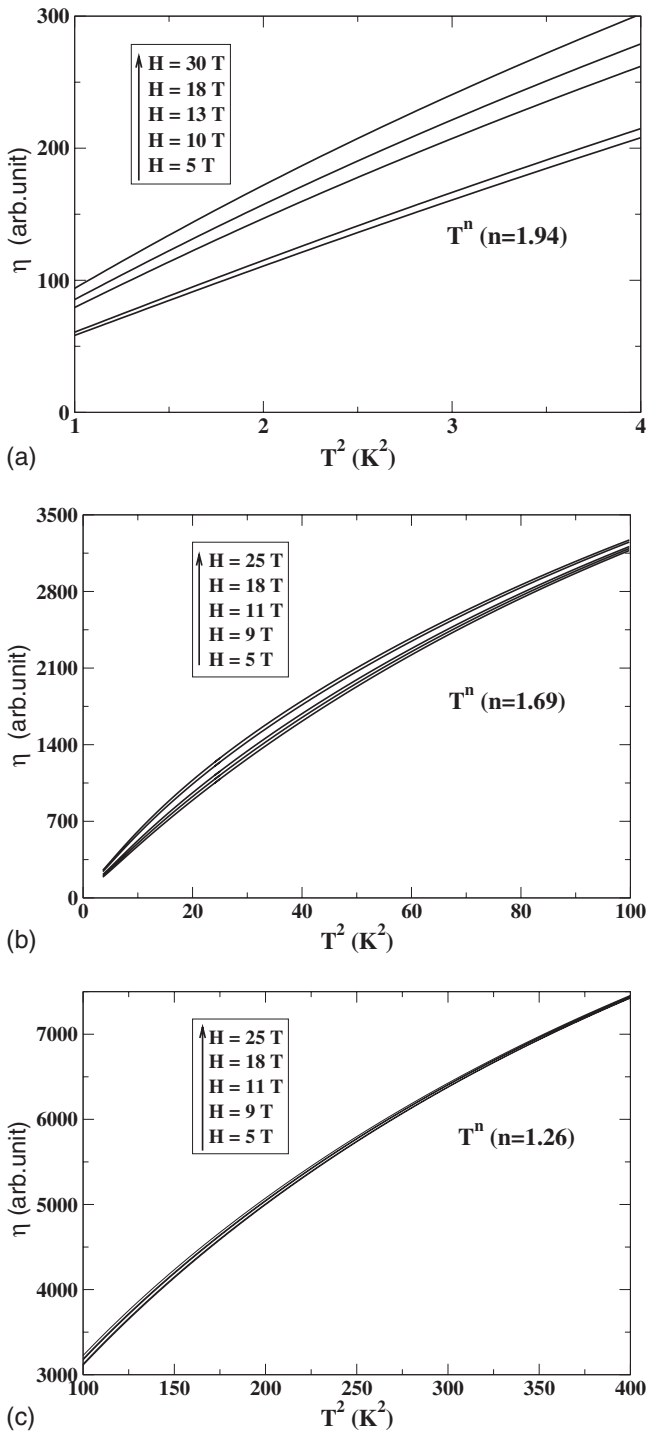

FIG. 1. The calculated scattering rate $\eta(T,H)$ versus T^2 derived from Eq. (5) for different field values (a) in the low-temperature regime ($T<t_c$), (b) in the intermediate regime ($T\sim t_c$), and (c) in the high-temperature regime ($T>t_c$). (a) At low temperature, the T^2 FL law is obeyed, while [(b) and (c)] at high temperature ($T>t_c$), the curves can be fitted by T^n with $n<2$. The calculations are done considering $t_c=10$ K, $t_b=200$ K, and (a) $E_d(T)\sim t_c$, (b) $E_d(T)\sim\frac{t_b}{2}$, and (c) $E_d(T)\sim t_b$. Taking for Bechgaard salts (Ref. 7) $v_F=210^5$ m s^{-1}, $c\sim 14$ Å gives rise to $\omega_c/H=3.3$ K/T.

rameters used in Eq. (5) are given in the caption. It is worth to note that the field-induced confinement scenario depends on t_c value and not on t_b, which is still controversial in Q1D organic conductors. The renormalized bandwidth $E_d(T)$ depends on the effective dimensionality of the system. In the 3D phase, (a) $E_d(T)\sim t_c$ while in the transient regime separating the 3D phase from the purely 2D phase (b) $t_c<E_d(T)<t_b$. In the 2D phase, $E_d(T)\sim t_b$.

Figure 1 shows a clear deviation from the T^2 FL law at high temperature ($T>t_c$). This law is expected to be obeyed when the c-axis hopping is coherent, which is the case of the low-temperature 3D phase where thermal fluctuations are small compared to t_c [Fig. 1(a)].

On the other hand, Fig. 1 shows that the effect of the magnetic field is strongly enhanced as the temperature decreases, namely, when the thermal fluctuations are reduced compared to the magnetic energy ω_c. At high temperature, $\eta(T,H)$ is practically field independent since the system is already in a 2D state resulting from a 3D-2D thermal induced crossover.

A remarkable feature of the scattering rate $\eta(T,H)$ is its dependence on the magnetic field, which is expected to exhibit different behaviors depending on the field magnitude. This is a consequence of the competition between the three energy scales governing the field dependent term in Eq. (5), namely: the interlayer hopping integral t_c, the magnetic energy ω_c, and the energy E, which strongly depends on temperature via the cut-off $E_d(T)$. The behavior of $\eta(T,H)$ as a function of the field should then be marked by three regimes: the first one corresponding to the low-field values ($\omega_c<t_c$) where the electron wave function can overlap several layers leading to a nearly field independent scattering rate. The second regime starts as soon as the magnetic energy overcomes t_c, which is achieved above a threshold field H_1^*. The decoupling of the conducting layers is more and more efficient as the field increases, which results in the confinement of the electrons within a single layer. This gives rise to a substantially enhanced in-plane electron-electron scattering rate with a remarkably large slope compared to that obtained at low field. The third regime is reached at a critical field H_2^*, above which the layers are completely decoupled. The increase in $\eta(T,H)$ is then expected to slowed down with increasing magnetic field. These features are brought out in Fig. 2 where the three regimes can be clearly distinguished. At low magnetic field, where the magnetic energy is smaller than t_c, $\eta(T,H)$ increases slowly with increasing magnetic field reflecting that the system is still in the 3D phase. Above the critical field H_1^*, the slope of $\eta(T,H)$ is strongly enhanced indicating the sharp localization of the electron density in the most conducting plane. H_1^* marks the beginning of the 3D-2D crossover. However, $\eta(T,H)$ tends to saturate beyond the critical field H_2^*, which is the signature of the establishment of the 2D phase where all the electrons are confined in the (ab) plane. The field range from H_1^* to H_2^* is the transient regime where the dimensional crossover takes place. Figure 2 shows that, below a temperature of the order of t_c, H_2^* decreases with increasing temperature—which expresses the competition between the magnetic field and the thermal fluctuations whose effect is to drop the system into the 2D phase. Nevertheless, H_1^* is practically temperature independent

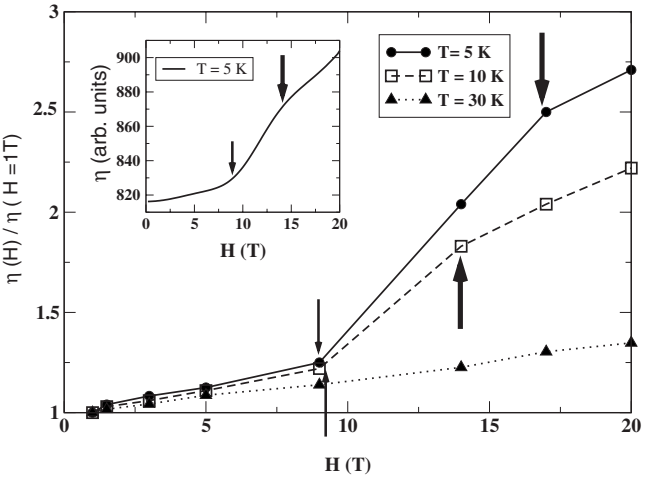

FIG. 2. Field dependence of the scattering rate $\eta(T,H)$ normalized to its value at 1 T derived from Eq. (5) for different temperatures. The symbols are the calculated values at 1, 1.5, 3, 5, 9, 14, 17, and 20 T for which we shall calculate, in the next, the resistivities. The lines joining the symbols are guide for eye. The inset shows the field dependence of the scattering rate at 5 K deduced from Eq. (5). H_1^* (thin line arrows) marks the onset of the 3D-2D crossover, while H_2^* (thick line arrows) is the signature of the collapse of the interplane electron hopping. For the numerical values of the different parameters used in Eq. (5), see Fig. 1.

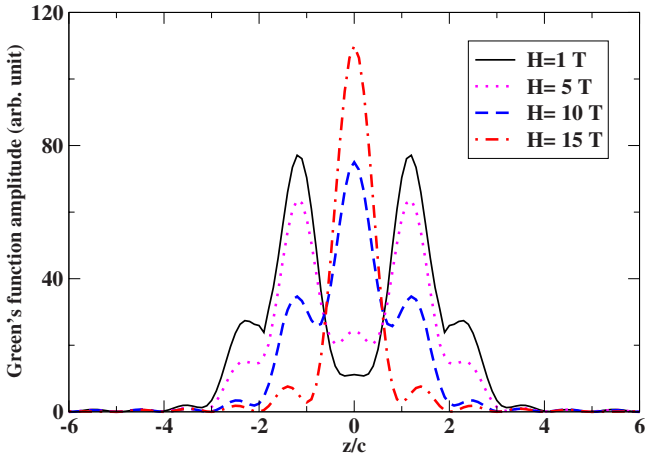

FIG. 3. (Color online) z dependence of the amplitude of the Green's function obtained from Eq. (4) for different values of the magnetic fields. At 15 T, the peak of the Green's function is localized around a single conducting plane, which expresses the collapse of the interplane hopping.

since it is the threshold field at which the magnetic energy bypasses the interplane hopping. As a result, the transient regime (limited by the two critical fields) shrinks as the temperature increases indicating the enhancement of the thermally induced 2D character of the system. Eventually, the field-induced confinement is erased at high temperature ($T \sim 3t_c$) since the system is already in the 2D phase. Figure 2 can be taken as a criterion of the field-induced confinement.

Knowing the temperature and field dependence of the scattering rate, the z dependence of the Green's function can be straightforwardly obtained from Eq. (4). Figure 3 shows the amplitude of the Green's function versus the interplane distance. As the magnetic field increases, the electron Green's function gets more and more confined. At a field of 1 T, the electrons are localized between the $z=-2$ and the $z=2$ planes. By increasing the magnetic field, the amplitude of the Green's function displays a large peak around the $z=0$ plane. This peak is entirely centered at $z=0$ at 15 T leading to a 3D-2D crossover.

To account for the striking transport features of the Bechgaard salts, we have derived (based on the Kubo formula) the interlayer and the a-axis conductivities, respectively, σ_c and σ_a [which are substantially dependent on the scattering rate $\eta(T,H)$] (Refs. 28 and 29):

$$\sigma_i = \frac{e^2\hbar}{\Omega}\int dk_y \int dk_z \int dE v_i^2 \int \frac{d\epsilon}{2\pi}[2\ \mathrm{Im}\ G_R(k_y,k_z,E,\epsilon)]^2 \times [-n_F'(\epsilon)], \quad (6)$$

where $G_R(k_y,k_z,E,\epsilon)$ is the retarded Green's function deduced from Eq. (3) by substituting the Matsubara frequencies ω_n by $\eta(T,H)-i\omega$ (where $\omega=\epsilon$). The setting $E=v_F/(x-x')$, Ω is a normalization factor, $n_F'(\epsilon)$ is the derivative of the Fermi distribution function, and $v_i=\partial\epsilon(\vec{k},\omega_c)/\hbar\partial k_i$ is the electron velocity in the i direction ($i=x,z$).

It is worth to stress that v_z is field dependent since the dispersion component along the c axis is field renormalized. The latter is deduced from the Hamiltonian written in the gauge $\vec{A}=(0,0,-Hx)$—which gives rise, in the equation of motion [Eq. (2)], to the field dependent term[3] $-2t_c\cos(k_zc+\frac{eHxc}{c_0})$ instead of the zero term $-2t_c\cos k_zc$. However, v_x is nothing but the Fermi velocity v_F since the a-axis dispersion is not affected by a magnetic field parallel to the b direction as far as the magnetic energy ω_c is smaller than the intrachain hopping integral $t_a\sim 2000$ K. The conductivity σ_i depends on the magnetic field through the velocity v_i, the Green's function G_R, and the scattering rate η, which is involved in the expression of the G_R [Eq. (3)].

Disregarding the self-energy corrections represented by the scattering rate $\eta(T,H)$ [Eq. (5)], Eq. (6) can be reduced by straightforward calculations to the semiclassical Chambers formula.[21,29,30] The latter gives for the interplane resistivity under a parallel magnetic field ($H\|b$);

$$\rho_c(H,T) = \frac{A}{\tau}(1+\omega_c^2\tau^2). \quad (7)$$

Here τ is the scattering time and A is a constant.

In the next section, we discuss under close scrutiny the signature of the field-induced confinement in the transport properties of quasi-1D organic conductors.

IV. RESULTS AND DISCUSSION

In Fig. 4(a) we have depicted the temperature dependence of the calculated c-axis resistivity $\rho_c=1/\sigma_c$ [Eq. (6)] for different values of the magnetic fields. Below a threshold field $H^*\sim 1$ T, the system remains metallic over the whole temperature range that goes down to 2 K to avoid the effect of

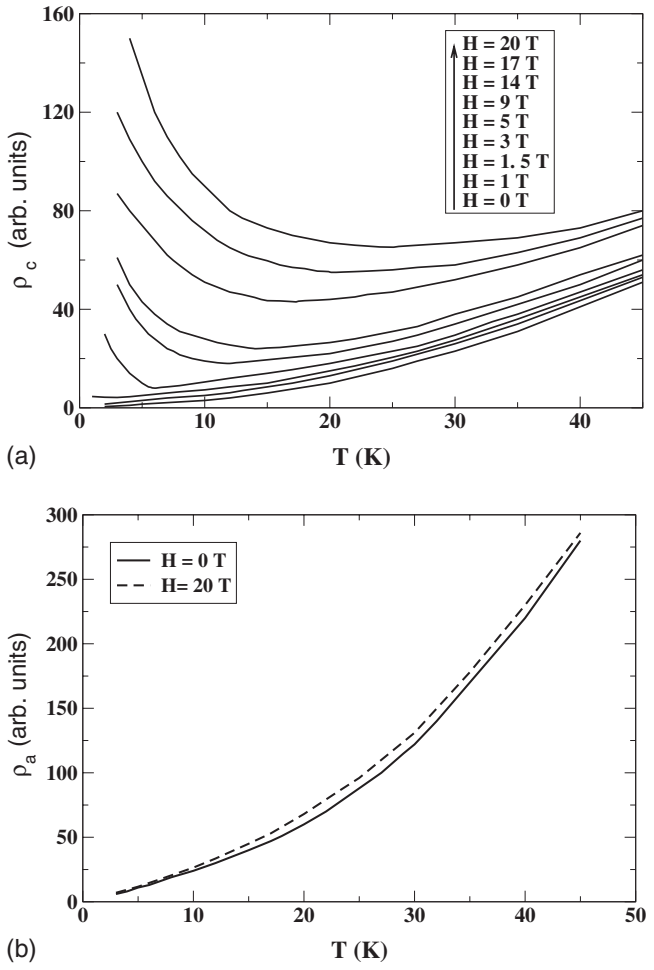

FIG. 4. Temperature dependence of (a) the c-axis and (b) the a-axis resistivities derived from Eq. (6) for different field values. The field is applied parallel to the intermediate conducting axis b. The scattering rate in Eq. (5) is expressed in unit of energy. We have taken for $H=3$ T, $\eta=1$ K, 3, and 12.5 K at, respectively, $T=5$, 10, and 25 K, while for $H=20$ T, we have respectively, $\eta=1.3$, 4, and 12 K at the considered temperatures. The field and temperature dependencies of the chosen values of η obey to the law given in Fig. 1.

superconducting fluctuations (which are expected to be enhanced below this temperature). However, beyond H^*, ρ_c switches from a metallic to an insulating behavior as T is decreased. This crossover occurs at a temperature $T_{\min}$, which increases with increasing magnetic field.

To confirm this field-induced 3D-2D crossover, we have represented the temperature dependence of the calculated a-axis resistivity in Fig. 4(b) (which clearly shows the absence of any confinement even at high magnetic field). The transport along the most conducting axis remains metallic. It is worth to note that, actually, the resistivity ρ_a is slightly increased by increasing magnetic field reflecting the fact that the in-plane scattering rate $\eta(T,H)$ is enhanced by confinement.

To highlight the crucial role of the scattering rate on the interplane transport, we show in Fig. 5 the calculated c-axis resistivity ρ_c derived from Eq. (6) assuming a field independent scattering rate with a T^2 FL temperature dependence. In

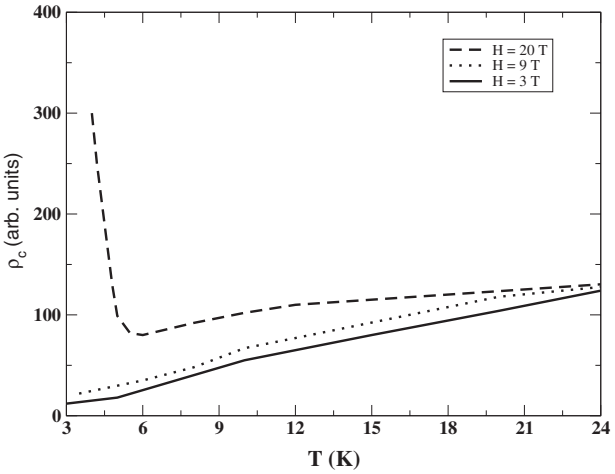

FIG. 5. Temperature dependence of the c-axis resistivity derived from Eq. (6) for different field values assuming a field independent scattering rate η with a T^2 temperature dependence: $\eta=\eta_0 T^2$ with $\eta_0=0.06$ K if expressed in unit of energy.

Fig. 5 no change in the temperature dependence of ρ_c occurs up to 9 T and a very high magnetic field is needed to induce the field-induced confinement. The latter is expected from experimental data to take place above a threshold a of the order of 1 T (Refs. 11 and 16) as shown in Fig. 4(a). It is clear from Fig. 5 that the field dependence of the scattering rate is a keystone in the field-induced confinement scenario.

Figure 6 shows clearly that the T^2 FL law—obeyed by the c-axis resistivity at zero field—is also satisfied at high temperature (above 40 K) even at high field (up to 20 T), which is reminiscent of the experimental data.[9,10] Such result seems to be peculiar since the relaxation rate η does not obey, in the high temperature regime, a T^2 law as it is expected for a FL (Fig. 1). This expresses the fact that the transport FL properties are robust against field-induced confinement when the thermal fluctuations overcome the magnetic energy.

In order to bring out the effect of the magnetic field on the c-axis transport, we plot in Fig. 7 the calculated resistivity ρ_c [Eq. (6)] versus the magnetic field for different temperatures. In the low-temperature regime corresponding to the 3D phase ($T<t_c\sim 10$ K), a clear change in the behavior of ρ_c occurs at a critical field $H_c\sim 5$ T for which the magnetic-field energy is of the order of $2t_c$. The system switches from a H^2 behavior to a H^n ($n\sim 1.7$) indicating a crossover from the 3D to the 2D phase. By increasing temperature, the abrupt change at H_c vanishes and ρ_c shows a rather monotonous increase. However, at high temperature, a field independent behavior can be reached, which is readily understood as the erasing of the magnetic effect in the 2D phase established by thermal fluctuations. This behavior is reminiscent of the magnetic-field dependence of the c-axis resistivity reported in $YBa_2Cu_4O_8$ and $PrBa_2Cu_4O_8$.[31,32] The former is an underdoped cuprate with a metalliclike c-axis response at low temperature and the latter—obtained by Pr substitution of Y and which is also metallic—is thought to be a 3D FL at low temperature, albeit the presence of strong electronic correlations. We suggest that the remarkable features of these compounds, which are still not understood, could be correctly interpreted within the framework of the present model. A

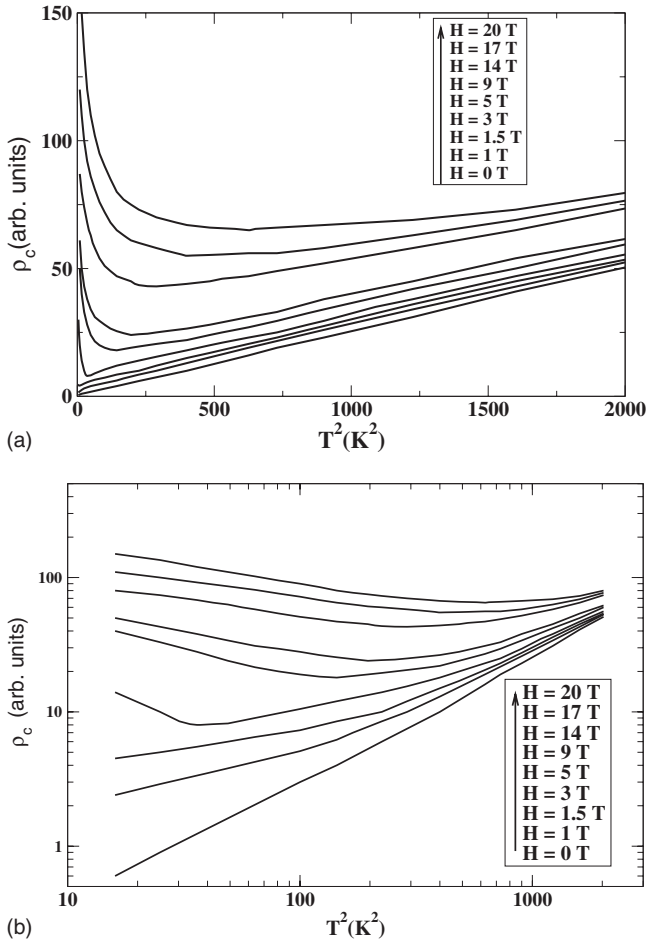

FIG. 6. c-axis resistivity [Eq. (6)] vs T^2 for different values of the magnetic field in (a) a linear and (b) a logarithmic scales.

detailed theoretical analysis and a quantitative comparison with the experimental results of Refs. 31 and 32 will be discussed elsewhere.

A substantially noteworthy experimental result concerns the saturation, at low temperature, of the interlayer resistance R_c under high magnetic field aligned along the b axis.[22,23] A more striking feature is that this behavior is found to be independent of the field orientation in the (ab) plane. These puzzling results cannot be understood within the existing theories. In particular, the semiclassical Boltzmann theory [Eq. (7)] predicts a nonsaturating behavior.[22] In Fig. 8 we report the field dependence of our calculated c-axis resistivity ρ_c at low temperature (solid line) compared to the experimental results of Ref. 10 obtained in the case of $(TMTSF)_2ClO_4$ salt. The calculated ρ_c is in quantitative agreement with the experimental data contrary to the semiclassical result. In particular, the latter does not exhibit any saturating behavior. We found that ρ_c shows an initial rapid rise followed by a nearly field independent behavior. This is reminiscent of the magnetoresistance measurements in the $(TMTSF)_2PF_6$.[22] This saturation can be viewed as a consequence of the field dependence of the in-plane relaxation rate. In the considered field regime, the magnetic energy ω_c is not sufficiently large to induce a decoupling of the 2D layers. Therefore, at low temperature, the electron wave function can overlap many layers and the in-plane relaxation rate remains nearly field independent as far as $\omega_c < t_c$ (Fig. 2). This leads to a saturating c-axis resistance, which can be taken as $\rho_c \sim \eta(T,H)$.[17] The low-temperature condition is necessary to obtain the saturation behavior since the interlayer tunneling, and so the 3D character, are enhanced by decreasing temperature. We then suggest that the saturating resistance of Q1D organic conductors at low temperature is closely related to the nearly field independent behavior of the in-plane relaxation rate (inset of Fig. 8). Let us now turn to the role of the in-plane field orientation in the saturation of the interlayer resistance—which is found to be insensitive to the rotation of the field in the (ab) plane—except the position along the most conducting axis.[23]

Once again, we assign this striking behavior to the field dependence of the electron-electron scattering rate η, which is basically sensitive to the in-plane field component along the b axis. The latter, whatever the field orientation, cannot

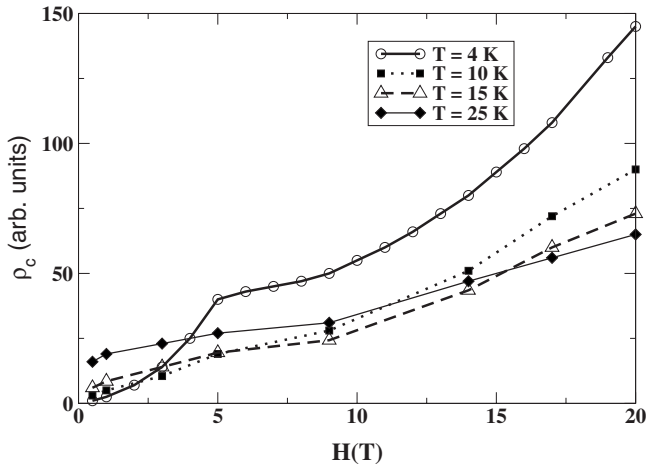

FIG. 7. Field dependence of the calculated c-axis resistivity [Eq. (6)] for different temperature values. The lines are guide for the eye.

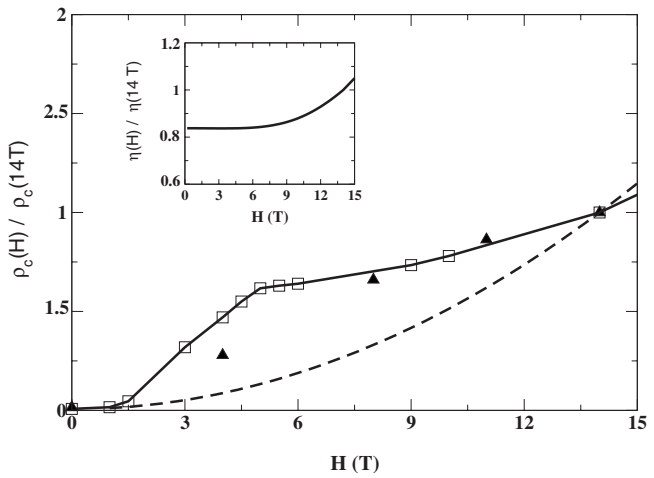

FIG. 8. The calculated c-axis resistivity [Eq. (6)] vs the magnetic field at 2 K (squares) compared to the experimental data (solid triangles) of Ref. 10 and to the results derived within the semiclassical Boltzmann transport theory (dashed line) [Eq. (7)]. The solid line is guide for the eye. The inset shows the field dependence of the scattering rate at 2 K.

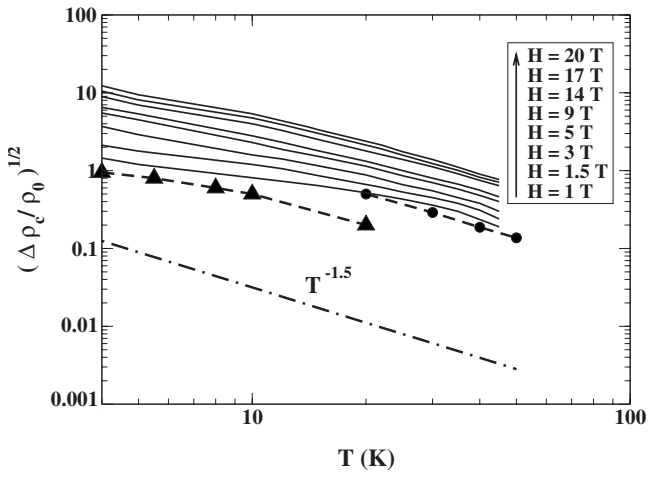

FIG. 9. Temperature dependence of the calculated magnetoresistance $(\Delta\rho_c/\rho_0)^{1/2}$ [Eq. (6)] at different field values. The filled triangles and circles are data from, respectively, Refs. 8 and 9. The dashed lines are guide for eye while the dotted-dashed line is the experimental behavior expected at high temperature

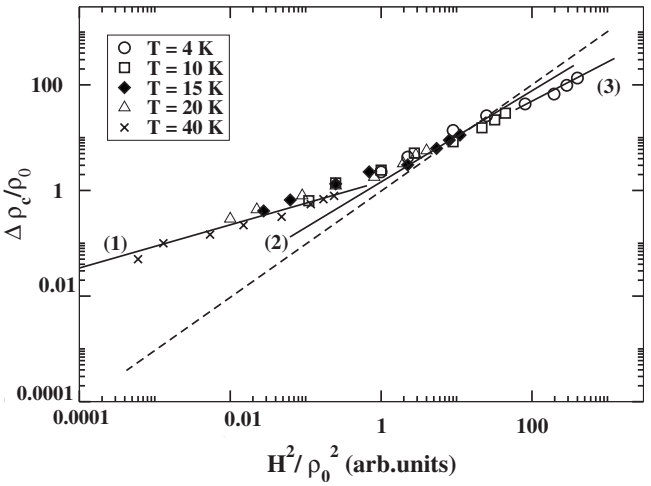

FIG. 10. Kohler's plot of the out-of-plane magnetoresistance derived from the numerical results plotted in Fig. 4(a). Each symbol corresponds to the magnetoresistance at a given field and at a given constant temperature calculated from the value of the resistivity shown in Fig. 4(a). The dashed line has a slope one while the lines (1), (2), and (3) have, respectively, the slopes 0.45, 0.9, and 0.75. ρ_0 is the resistivity at zero field for the considered temperature.

decouple the 2D layers as far as the threshold field H_1^* is not reached. In this field regime, corresponding to the experimental conditions of Ref. 23, the calculated scattering rate and the interlayer resistance are expected to be unaffected by the rotation of the field in the layer (Fig. 8) in accordance with recent experimental results.[23]

It is worth to stress that our results (shown in Fig. 8) may be interpreted in terms of the semiclassical description by taking a field dependent relaxation time $\tau=1/\eta$ of the Chambers formula [Eq. (7)].

As shown in the inset of Fig. 8, the relaxation rate η is constant for $H>6$ T—which leads, according to Eq. (7), to an increasing resistance as the magnetic field increases.

For $H>6$ T, η is enhanced since the magnetic energy ω_c bypasses the interlayer hopping integral t_c. As a result, the increase in ω_c with increasing field is slowed down due to the decrease of τ giving rise to a saturating resistance [Eq. (7)]. Nevertheless, for higher-field values ($H>12$ T)—for which the system is effectively 2D system—the increase in τ can no more compensate the enhancement of ω_c. As a consequence, the saturating regime disappears and the increase in ρ_c resumes again. However, this interpretation raises the question of whether the Chambers formula [Eq. (7)]—derived with a constant relaxation time—holds on if the latter is field dependent? This point should be taken with a grain of salt.

More insight into the field-induced confinement can be learned from the temperature and the field dependence of the magnetoresistance $\Delta\rho_c/\rho_0$. Figure 9 shows a change in the power-law behavior of the temperature dependence of the calculated magnetoresistance, which is smeared out as the magnetic field increases (solid lines in Fig. 9). At high temperature ($T>t_c$) and beyond a threshold field of 5 T, at which the system is effectively 2D, the magnetoresistance exhibits a $T^{-2.6}$ behavior in accordance with the experimental data of Cooper *et al.*[8] (triangles). This behavior turns out to be a universal T^{-3} power law at high temperature as found by Hamzić *et al.*[9] for different Bechgaard salts (filled circles).

The field dependence of the magnetoresistance is displayed in the form of Kohler's plot in Fig. 10. The dashed line corresponds to the expected theoretical curve with a slope one since (according to KR) $\delta\rho/\rho_0=mH^2/\rho_0^2$ [Eq. (7)]. It is worth to note that the data points in Fig. 10 cannot form a unique straight line since they correspond to different temperature and field regimes, which rules out the possibility to describe them with the same law. However, one may gather these data in three straight lines—indicated by (1), (2), and (3) in the figure with, respectively, the slopes 0.45, 0.9, and 0.75. Three regimes can then be distinguished. In the first one, corresponding to the data of line (1) associated to the high temperatures ($T>t_c$) and low field ($\omega_c<t_c$), strong deviations from the KR are observed [slope of line (1) is clearly different from 1]. In this regime, the system is effectively 2D due to thermal fluctuations. The latter destroys the interlayer hopping leading to a departure from KR, which is expected to hold on according to Hamzić *et al.*[15] if the hopping is still coherent. The deviation from KR is ascribed to the reduction in the effective value of t_c.[15] In the second regime, which concerns the low temperatures ($T<t_c$) and low fields ($\omega_c<t_c$), the KR is recovered [slope of line (2) $\sim$1]. In this case, the system is effectively 3D since the c-axis hopping is not destroyed by thermal fluctuations and field-induced confinement. By increasing the magnetic field, the data—corresponding to the low-temperature regime [line (3)]—show small deviations from KR as soon as the field bypasses the value at which the field-induced confinement takes place at the considered temperature. This regime corresponds to the transient phase ($H_1^*<H<H_2^*$) where the dimensional crossover takes place with a reduced interplane hopping integral.

These results sound in agreement with the magnetoresistance measurements of Refs. 14 and 15 in the limit of low field.

The outcome of this discussion is that KR is satisfied if the system is effectively 3D where the *c*-axis hopping is not destroyed by either field-induced confinement or thermal fluctuations.

V. CONCLUSION

In summary, we suggest that the striking behavior of the *c*-axis electronic transport results from the field-induced dimensional crossover, which we have described within a quantum calculation. We showed that the magnetic field applied along the intermediate conducting axis brings the system to an effective 2D phase by localizing the electron Green's function within a single conducting plane. Such dimensional switching has dramatic effects on the in-plane relaxation rate. The latter, which we have derived as a function of temperature and magnetic field, exhibits departure from the T^2 FL law. However, the *c*-axis resistivity still obeys a FL behavior at high temperature—which means that the FL is robust in quasi-1D conductors even if the relaxation rate does not match the FL law. This is an original issue, which has not been addressed so far. We expect that our model, which provides a coherent interpretation of the experimental results in Bechgaard slats, may be a reliable framework to account for the peculiar features reported in some cuprate based compounds in high magnetic fields.

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