Interlayer magnetoresistance in multilayer Dirac electron systems: motion and merging of Dirac cones

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Abstract
We theoretically study the effect of the motion and the merging of Dirac cones on the interlayer magnetoresistance in multilayer graphene-like systems. This merging, which can be induced by a uniaxial strain, gives rise in a monolayer Dirac electron system to a topological transition from a semi-metallic phase to an insulating phase whereby Dirac points disappear. Based on a universal Hamiltonian, proposed to describe the motion and the merging of Dirac points in two-dimensional Dirac electron crystals, we calculate the interlayer conductivity of a stack of deformed graphene-like layers using the Kubo formula in the quantum limit where only the contribution of the \( n = 0 \) Landau level is relevant. A crossover from a negative to a positive interlayer magnetoresistance is found to take place as the merging is approached. This sign change of the magnetoresistance can also result from a coupling between the Dirac valleys, which is enhanced as the magnetic field amplitude increases. Our results describe the behavior of the magnetotransport in the organic conductor \( \alpha-(\text{BEDT})_2\text{I}_3 \) and in a stack of deformed graphene-like systems. The latter can be simulated by optical lattices or microwave experiments in which the merging of Dirac cones can be observed.

(Some figures may appear in colour only in the online journal)

1. Introduction

Since the discovery of graphene [1, 2], systems showing a massless Dirac electron-like dispersion relation continue to attract considerable interest. The signature of such electrons has been recently revealed in the organic conductor [3] \( \alpha-(\text{BEDT})_2\text{I}_3 \) where BEDT denotes bis(ethylenedithio)-tertrathiafulvalene. This compound consists of a stack of conducting BEDT layers separated by insulating iodine planes. The weak coupling between the conducting layers gives rise to the 2D character for the electronic properties of this material. Theoretical studies [3, 4] and band energy calculations [5, 6] have given evidence for the presence of two tilted Dirac cones which move under pressure. It has been argued that the interlayer magnetoresistance is a powerful tool to probe the properties of the Dirac cones [7]. Tajima et al [8] have observed a large negative interlayer magnetoresistance in \( \alpha-(\text{BEDT})_2\text{I}_3 \) for a transverse magnetic field. This effect was ascribed to the carriers of the zero-mode Landau level \( (n = 0) \). The authors have also reported a change to a positive magnetoresistance which was assigned to Zeeman splitting of the \( n = 0 \) Landau level.

A theoretical interpretation of these experimental results has been proposed by Osada [9, 10] by calculating, within a quantum approach, the interlayer magnetoresistance in a system of stacked Dirac electron layers. Osada showed that in the quantum limit the negative magnetoresistance is due to the degeneracy of the zero-mode Landau level which dominates the interlayer transport. At high field, spin splitting becomes relevant and gives rise to the crossover from negative to positive magnetoresistance due to the reduction of carrier density. Osada has also given an explanation of the angle dependence of the interlayer resistivity observed by Tajima et al [8], which cannot be understood within a semi-classical description.

Based on transport measurements, Monteverde et al [11] recently argued that the conduction in \( \alpha-(\text{BEDT})_2\text{I}_3 \) could not only be ascribed to Dirac electrons. Both massive and Dirac...
carriers contribute to the conduction properties. Moreover, no merging of Dirac cones was observed up to 3 GPa [11].

According to theoretical calculations [12], the merging in α-(BEDT)2I3 is expected to occur around 0.5 GPa. More recently, Piéchon et al [13] discussed, based on an analytical approach, the stability of Dirac points and the merging conditions in α-(BEDT)2I3.

The motion and the merging of Dirac points has been observed in a tunable honeycomb optical lattice of ultracold Fermi gas [14]. Lim et al [15] provided a theoretical description of the experiment of Dirac point manipulation in optical lattices.

The topological phase transition from a zero gap band state, with two Dirac points, to a gapped phase was also observed in a microwave experiment simulating a strained graphene [16]. Montambaux et al [17] have proposed a universal Hamiltonian to describe the motion and the merging of Dirac cones in 2D systems. The proposed Hamiltonian offers the possibility to follow continuously the topological transition from the semi-metallic phase, with two Dirac points, to the insulating phase where the Dirac points merge and a gap opens in the energy spectrum.

It is worth emphasizing that the merging in a monolayer graphene could not practically be observed since a very large strain is required [17]. It is thus interesting to investigate the possible signature of this merging in other Dirac electron systems, in particular in multilayer graphene-like systems such as the organic conductor α-(BEDT)2I3.

In this paper, we propose to study the merging of Dirac cones in a stack of undoped Dirac electron layers weakly coupled by a vertical tunneling. We look for evidence of the merging in the behavior of the interlayer magnetoresistance. In the present work, we consider that each layer is described by the universal Hamiltonian proposed by Montambaux et al [17] and we introduce the interlayer coupling perturbatively. For simplicity, we do not consider the tilt of Dirac cones which has been addressed in [7, 19]. Moreover, we neglect the Zeeman effect which has already been found to induce a sign change in the magnetoresistance [8, 9]. We also do not take into account the broadening of the Landau level which may result in a mixing of the Landau levels [9]. We derive, based on the Kubo formula, the interlayer magnetoresistance in the quantum limit where only the zero mode (n = 0) is considered. In the next section, we focus on the behavior of the field and angle dependence of the interlayer magnetoresistance far from the merging of Dirac cones. In section 3, we derive the magnetoresistance at the merging and discuss its experimental fingerprints.

2. Interlayer magnetoresistance: motion of Dirac cones

2.1. Independent Dirac valleys

We consider a stacking structure of layers weakly coupled along the transverse direction and we denote by tc the interlayer tunneling parameter (figure 1). Each layer is a graphene-like system described by a triangular lattice with two atoms A and B per unit cell.

In the absence of lattice deformation, the Dirac points are in the points K and K’ at the corners of the first Brillouin zone (BZ) [17] (figure 2). By applying a uniaxial strain, along the y direction for example, the Dirac points leave the corners of the BZ and move in the same direction to merge in point M [18].

To describe the motion and the merging of Dirac cones in zero magnetic field, Montambaux et al [17] have proposed the following Hamiltonian (figure 1). Each layer is a graphene-like system described by a triangular lattice with two atoms A and B per unit cell.

\[ H = \sum_{\alpha} \frac{1}{2} t_{\alpha} \sum_{<ij>} C_{\alpha i}^{\dagger} C_{\alpha j} + \mu \sum_{\alpha} \sum_{i} \left( \psi_{\alpha i}^{\dagger} \psi_{\alpha i} - \frac{1}{2} \right) \]

\[ + \sum_{\alpha} \sum_{i,j} J_{\alpha}^{ij} \left( C_{\alpha i}^{\dagger} C_{\alpha j} + C_{\alpha j}^{\dagger} C_{\alpha i} \right) \]

\[ + \sum_{\alpha} \sum_{i} \left( \frac{\hbar}{2} \sum_{\beta} \sum_{j} V_{\alpha \beta}^{ij} C_{\alpha i}^{\dagger} C_{\beta j} \right) \]

\[ + \sum_{\alpha} \sum_{i} \left( \frac{e}{c} B_{\alpha} \sum_{j} \left( \psi_{\alpha i}^{\dagger} \sigma_{\alpha} \psi_{\alpha j} \right) \right) \]

where \( C_{\alpha i} \) and \( \psi_{\alpha i} \) are the annihilation operators for the Dirac electrons in the α layer at site i, \( J_{\alpha}^{ij} \) is the interlayer coupling, \( V_{\alpha \beta}^{ij} \) is the interlayer potential, \( e \) is the electron charge, \( c \) is the speed of light, and \( B_{\alpha} \) is the magnetic field.

Figure 1. Schematic representation of a multilayer system with magnetic field and current configuration. c denotes the interlayer distance and \( \theta \) is the out-of-plane angle of the magnetic field from the conducting layer.

Figure 2. (a) Deformation of the honeycomb lattice along the y direction. (b) Brillouin zone of undeformed graphene lattice. By applying a deformation, Dirac cones leave the K and K’ points and move in the same direction and eventually merge in point M [18].

1 For a review on Dirac cones in deformed graphene see [18].
following Hamiltonian, the so-called universal Hamiltonian:

\[
H_0(\vec{p}) = \begin{pmatrix}
0 & \Delta + \frac{p_x^2}{2m^*} - ic \gamma y

\Delta + \frac{p_x^2}{2m^*} + ic \gamma y & 0
\end{pmatrix},  \tag{1}
\]

where \( \vec{p} = (p_x, p_y) \) is the momentum measured relatively to the merging point \( D_0 \), \( c \gamma \) is the electron velocity along the \( y \) direction, \( m^* \) is an effective mass supposed to be positive and \( \Delta \) is the parameter governing the topological transition. This two-band Hamiltonian is written in the basis of the A and B site eigenstates (\( \psi_A, \psi_B \)).

The universal Hamiltonian of equation (1) describes a deformed graphene sheet in the presence of a uniaxial strain applied along the \( y \) axis [18]. The corresponding energy spectrum is

\[
\epsilon = \pm \sqrt{(\Delta + \frac{p_x^2}{2m^*})^2 + p_y^2 c \gamma^2}.  \tag{2}
\]

Equation (2) shows an hybrid character, called by Montambaux et al [17] a semi-Dirac spectrum, with a Schrödinger-like behavior along the \( x \) direction and a Dirac structure along the \( y \) axis.

The case of \( \Delta < 0 \) corresponds to two distinct Dirac points along the \( x \) axis at \( \pm p_x \) where \( p_D = \sqrt{-2m^* \Delta} \) whereas for \( \Delta = 0 \), the Dirac points merge at \( D_0 \).

For \( \Delta > 0 \), a gap of \( 2 \Delta \) opens in the energy spectrum and the system becomes an insulator.

To recover the full Dirac spectrum of undeformed graphene, the spectrum given by equation (2) can be linearized along the \( x \) axis in the vicinity of Dirac points [17].

Let us now focus on the case where the deformed system is in the presence of a magnetic field

\[ \vec{B}(x) = B \cos \theta \cos \phi, B_y = B \cos \theta \sin \phi, B_z = B \sin \theta. \]

The Hamiltonian given by equation (1) can be written, using the Peierls substitution \( \vec{p} \rightarrow \vec{p} + e \vec{A} \), as

\[
H(\vec{p}) = \begin{pmatrix}
0 & \Delta + \frac{\pi_x^2}{2m^*} - ic \gamma \pi_y

\Delta + \frac{\pi_x^2}{2m^*} + ic \gamma \pi_y & 0
\end{pmatrix},  \tag{3}
\]

where the effective momentum is given by \( \vec{p} = (\pi_x = p_x + e z B_x, \pi_y = p_y - e z B_y, 0) \) within the gauge \( \vec{A} = (z B_y - y B_z, 0) \). \( \pi_x \) and \( \pi_y \) satisfy the commutation relation \( [\pi_x, \pi_y] = -ie \hbar c \gamma B_z \).

To derive the eigenfunctions and the energy spectrum of the Hamiltonian given by equation (3), we consider for simplicity, as in [17], the squared Hamiltonian \( H_{\text{eff}} \). The eigenproblem reduces to

\[
H_{\text{eff}} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = E_n^2 \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix},  \tag{4}
\]

which may be written as

\[
\left\{ \left( \Delta + \frac{\pi_x^2}{2m^*} \right)^2 + c \gamma \pi_y^2 + ic \sqrt{2m^*} \pi_x, \pi_y \right\} \psi_{A,B} = E_n^2 \psi_{A,B},  \tag{5}
\]

where \( s = \pm \) corresponds respectively to the A and the B sites. Equation (5) takes the form

\[
[c \gamma \pi_y^2 + (\Delta + \frac{\pi_x^2}{2m^*})^2 + ic \sqrt{2m^*} \pi_x, \pi_y] \psi_{A,B} = E_n^2 \psi_{A,B}.  \tag{6}
\]

The potential \( V(Y) \) is given by

\[
V(Y) = \left( \frac{e^2 B_y^2}{2m^*} \right)^2 (\delta + Y^2)^2 + \frac{c \gamma e^2 B_z^2}{m^*} \sqrt{\delta}.  \tag{7}
\]

Here \( Y = s y_0 - y, y_0 = \frac{p_y + e z B_y}{e B_x} \) and we introduce, as in [17], the parameter \( \delta = \frac{2m^*}{e B_x^2} \Delta \).

\( V(Y) \) has two minima at \( Y_0 = \pm \sqrt{\delta} \) separated by a distance of \( 2 \sqrt{\delta} \) which decreases as the transverse component \( B_y \) of the magnetic field increases.

\( V(Y) \) can be described by a double independent well potential for large \( |\delta| \) corresponding to the case where Dirac cones are far from the merging point. In this case, an expansion of \( V(Y) \) around \( Y_0 \) yields

\[
V(Y) \sim V(u) = 4 \left( \frac{e^2 B_y^2}{2m^*} \right)^2 |\delta|^2 + s \frac{\hbar^2 c \gamma e^2 B_z^2}{m^*} \sqrt{\delta}.  \tag{8}
\]

Here \( u = Y - Y_0 \) and \( |u| \ll \sqrt{\delta} \). The eigenvalues of equation (6) are then

\[
E_n = \pm \frac{\sqrt{2} \hbar c \gamma}{l} \sqrt{n},  \tag{9}
\]

where \( l = \left( \frac{\hbar^2 c \gamma}{2m^* e B_x^2} \right)^{\frac{1}{2}} \).

\( E_n \) can be written in the form [17] \( E_n = \pm \sqrt{2} \hbar c \gamma c e B_x n \) as found by Himura et al [19] in \( \alpha - (BETD)\text{I}_3 \) in the case of nontilted Dirac cones.

In the limit of large negative \( \delta \), and using the notation of [9], the eigenstates of equation (6) corresponding to the layer position \( z_i \) take the following form.

For the zero mode \( (n = 0) \):

\[
F_{0, y_0, z_i}(\vec{r}) = \begin{pmatrix} 0 \\ h_{0, y_0, z_i}(\vec{r}) \end{pmatrix},  \tag{10}
\]

where

\[
h_{n, y_0, z_i}(\vec{r}) = \frac{1}{\sqrt{L}} \exp \left( \frac{i e z B_x}{\hbar} y \right) \times \exp \left[ \frac{e B_z}{\hbar} \left( \frac{B_y}{B_z} \pm \sqrt{|\delta| - y_0} \right) x \right] \times u_n(y - y_0) \delta(z_i).  \tag{11}
\]
Here $L$ is the layer length along the $x$ direction, $y_0$ is the center coordinate of the harmonic oscillator and $u_n(y-y_0)$ is the corresponding eigenfunction.

We now introduce the interlayer hopping Hamiltonian $\Delta H = -2t_c \cos \frac{q_y}{4}$ as a perturbation [9]. $c$ denotes the interlayer distance.

From Kubo formula, and to the lowest order in $t_c$, the interlayer conductivity $\sigma_{zz}$ is given by

$$\sigma_{zz}(\omega) = \frac{i\hbar}{V} \sum_{\alpha} \sum_{\tilde{n} \tilde{n}_0} \sum_{\tilde{m}} f(E_{\alpha'}) - f(E_{\alpha}) |\langle \tilde{n}', \tilde{m}', \tilde{J}_z |n, \tilde{n}_0, \tilde{z}_i \rangle|^2 \frac{E_{\alpha'} - E_n}{\hbar \omega + i\tau + E_n - E_{\alpha'}}$$

(12)

where $\tilde{J}_z$ is the interlayer current density $\tilde{J}_z = \frac{\tilde{\tau}}{\pi}[z, \Delta H]$ and $\tau$ is the relaxation time.

In the quantum limit, the mixing of Landau levels could be neglected and the relevant contribution to the interlayer conduction is due to the zero-mode Landau level $n = 0$. The matrix element of the $\tilde{J}_z$ can be expressed in terms of the effective interlayer hopping parameter $\tilde{t}_c$ [9]:

$$\langle 0, \tilde{y}_0, \tilde{z}_i | \tilde{J}_z | 0, y_0, z_i \rangle = \frac{-ie\hbar}{\tilde{t}_c} \left[ \delta_{\tilde{z}_i z_i} + \delta_{\tilde{y}_0, y_0} + \frac{\hbar}{\tilde{t}_c} \right],$$

(13)

where

$$\tilde{t}_c = t_c \exp \left[ \frac{eB_y}{\hbar} (\tilde{y}_0 + y_0) \right] \exp \left[ -\frac{eB_z}{4\hbar} \left( \frac{c_y B_y^2}{c_x} + \frac{c_x B_x^2}{c_y} \right) \right].$$

(14)

The interlayer DC conductivity $\sigma_{zz} = \text{Re}(\sigma_{zz}(\omega = 0))$ can then be written as [9]:

$$\sigma_{zz} = 2C e^2 \tau c t_c |B_c| \frac{\pi \hbar}{\hbar} \exp \left[ -\frac{e^2}{2\hbar B_c} \frac{1}{\sqrt{2}} \left( \frac{1}{c_x} B_x^2 + \frac{1}{c_y} B_y^2 \right) \right]$$

(15)

where the factor $C$ given in [9] could be considered as a constant as far as the relaxation time is assumed to be fixed independent [9].

We denote by $\alpha$ the parameter measuring the amplitude of the strain: $\alpha = \sqrt{\frac{c_x}{c_y}}, c_x = \sqrt{-\frac{2\Delta}{m}}$. The same parameter has been introduced by Himura et al [19] as a measure of the anisotropy strength. In our calculation, based on the universal Hamiltonian, this parameter describes the proximity of Dirac cones to the merging point. The smaller $\alpha$, the closer the merging.

In equation (15), the proportionality of the prefactor to $B_c$ is due to the Landau level degeneracy $\frac{1}{2\pi \hbar^2} = \frac{\sqrt{2}}{2\pi \hbar}$. Equation (15) is similar to the interlayer conductivity expression obtained by Osada [9] if one takes the case of the undeformed graphene-like system $\alpha = 1$.

It is worth noting that the expression of $\sigma_{zz}$ given by equation (15) is reminiscent of that obtained by Himura et al [19] in $\alpha$-(BEDT)$_2$TTF in the case of nontilted Dirac cones.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure3}
\caption{Dependence of the anisotropy parameter $\alpha = \sqrt{\frac{c_x}{c_y}}$ as a function of the hopping parameter ratio $\frac{t'}{t}$. At the merging, $\alpha$ vanishes.}
\end{figure}

If the hopping integrals are limited to the first neighboring atoms, the universal Hamiltonian parameters, in the case of fixed $\Delta$ and $c_y$, take the form [17]

$$\Delta = t' - 2t, \quad c_x = \sqrt{\frac{3a_0}{\hbar}} \sqrt{\frac{r^2 - r_r^2}{4}},$$

(16)

and

$$c_y = \frac{3a_0}{2\hbar}.$$

where $r'$ is the hopping parameter along the $y$ direction which is different from the other first neighbor hopping parameter $t$ regarding the effect of the uniaxial strain (figure 2). $a_0$ is the distance between the two atoms of the unit cell. The dependence of $\alpha$ on the hopping parameter $r'$ is represented in figure 3. At the merging, $t' = 2t$, $\alpha$ vanishes.

To derive the interlayer conductivity given by equation (15), we have assumed a large negative $\Delta$ so that the two valleys of the double well potential $V(Y)$ (equation (7)) could be considered as independent. The two Dirac cones are far from the merging point $D_0$. This assumption can be justified as long as $\alpha$ is not close to zero. One needs to define a criterion to fix the critical value of $\alpha$ below which the two potential valleys start to interact. This point will be discussed later.

According to equation (15), $\sigma_{zz}$ increases linearly with the field amplitude for a normal field as found in the undeformed case [9].

In the presence of an inplane field component $B_{||}$, the increase of $\sigma_{zz}$ is reduced compared to the undeformed case. This decrease is due to the Gaussian decay of the effective interlayer tunneling amplitude $\tilde{t}_c$ (equation (14)) and is more pronounced as $\alpha$ decreases.

The inplane component $B_{||}$ generates a positive magnetoresistance effect since it induces an inplane Lorentz force. The latter reduces the interlayer tunneling giving rise to a positive magnetoresistance.

In figure 4, we plot the dependence of the interlayer resistivity $\rho_{zz}$ as a function on the magnetic field amplitude
to equation (15), renormalization of the inplane field component sign change of the magnetoresistance is due to a strain component, along the direction of Dirac point motion, renormalizes the inplane field component: the effective field decay giving rise to a positive magnetoresistance. This $B$ is renormalized as $\alpha$. The latter is found to decrease as $B$. Here $\alpha$ is a robust effect which survives under uniaxial strain. Feature predicted in multilayer Dirac electron systems [9, 19]

Calculations are done for $\theta = \frac{\pi}{4}$ and $\phi = \frac{\pi}{4}$ and the field is expressed in the unit of $\frac{2\pi}{\sqrt{3}}$.

$B. \rho_{zz}$ is given by [7, 9, 19]

$$\rho_{zz} = \frac{A}{B_0 + |B_z| \exp \left[ -\frac{1}{2} \frac{e^2}{\hbar c} \left( \frac{1}{2} r^2 + \alpha^2 B_x^2 \right) \right]}.$$ (17)

Here $B_0 = 0.1$ T is a fitting parameter [9] and $A = \frac{\pi h^2}{2e^2r e\sqrt{3}}$.

Figure 4 shows a negative magnetoresistance for $\alpha$ close to unity. It turns out that the negative magnetoresistance feature predicted in multilayer Dirac electron systems [9, 19] is a robust effect which survives under uniaxial strain.

However, as $\alpha$ decreases, the Gaussian exponential decay in $\sigma_{zz}$ (equation (15)) overcomes the linear increase with $B_2$ and a crossover from negative to positive interlayer magnetoresistance takes place at a critical field value $B_{cr}(\alpha)$. The latter is found to decrease as $\alpha$ is reduced. This sign change of the magnetoresistance is due to a strain renormalization of the inplane field component $B_z$. According to equation (15), $B_I$ is responsible of the Gaussian exponential decay giving rise to a positive magnetoresistance. This effect is enhanced in the presence of the anisotropy which renormalizes the inplane field component: the effective field component, along the direction of Dirac point motion, $B_\parallel$ is renormalized as $B_\parallel = \frac{B_z}{\alpha}$ which gets larger as the merging is approached ($\alpha$ decreases).

Numerical results obtained from equation (15) show that the maximum of the resistivity is, as in undeformed graphene layers [9], for an inplane magnetic field ($\theta = 0$). The results show that the peak for an inplane field is broadened as $\alpha$ decreases, reflecting the enhancement of the inplane Lorentz force. This behavior is found to be unchanged by varying the azimuthal angle $\Phi$.

The azimuthal angle dependence of the interlayer resistivity for different values of $\alpha$ is depicted in figure 5 which shows that the motion of Dirac cones ($\alpha \neq 1$) gives rise to the $\Phi$ dependence of $\rho_{zz}$. The maximum of the resistivity corresponds to $\Phi = 0$ where the inplane magnetic field component is aligned perpendicular to the strain direction $y$. Morinari et al [7] ascribed the $\Phi$ dependence of $\rho_{zz}$ in $\alpha$-(BEDT)$_2$I$_3$ to the tilt of Dirac cones rather than to the anisotropy of Fermi velocity. We propose that a $\Phi$ dependent interlayer magnetoresistance could be a signature of Dirac cone motion. The question is how to distinguish experimentally between the $\Phi$ dependence due to the anisotropy of Fermi velocities (or the tilt of Dirac cones) and that induced by Dirac point motion? Fermi surface probes may be a key issue to unveil this question.

To summarize, the magnetoresistance shows, in the case of independent Dirac valleys, a $\phi$ dependence for deformed honeycomb lattice and a possible sign change in the presence of an inplane field component. The latter gives rise to an inplane Lorentz force which gets enhanced as the strain amplitude increases ($\alpha$ decreases). This enhancement results from a strain renormalization of the field component along the direction perpendicular to the deformation axis.

At this point a natural question arises: below which value of $\alpha$ does our assumption of independent Dirac valleys break down? In the following section, we try to bring some answers.

2.2. Interacting Dirac valleys

Regarding the double-well structure of the potential $V(Y)$ (equation (7)), the Landau levels are doubly degenerate in the case where $\alpha$ is close to unity (large $\Delta$). However, by approaching the merging (reducing $\alpha$), the degeneracy is removed due to the tunneling between the Dirac valleys. The $E_{\ell=0}$ level splits into two levels separated by a gap. The system undergoes a crossover from a semi-metallic state, where $E_{\ell=0}$ is degenerate, to a semi-conducting state where the degeneracy is lifted. This is expected to result in a change from a negative to a positive interlayer magnetoresistance since the carrier density of the lowest energy level is reduced.

The valley degeneracy could also be removed, at a fixed value of $\Delta$, by increasing the magnetic field amplitude:
the distance between the potential minima (equation (7)) decreases with increasing the magnetic field ($2\gamma_0 \propto \sqrt{l_0|B|}$). A crossover from a negative to a positive magnetoresistance is expected at a critical field $B_{c,cr}(\alpha)$ for a given value of the parameter $\alpha$.

As the merging is approached ($\alpha$ decreases), the two potential valleys are no longer independent and a small field value could remove the valley degeneracy. The closer the merging, the smaller $B_{c,cr}$.

It is worth emphasizing that the idea of a sign change in magnetoresistance, resulting from removing the degeneracy of the zero Landau level by increasing the magnetic field or by approaching the merging, is consistent with the numerical results of Montambaux et al [17] (see figure 6 of [17]). The latter show that the degeneracy of the Landau energies is lifted as the merging parameter $\delta \propto \frac{A}{B_{c,cr}^2}$ is increased.

The crossover from the negative to the positive interlayer magnetoresistance observed by Tajima et al [8] in $\alpha$-(BEDT)T$_2$I$_3$ has been ascribed by Osada [9] to the Zeeman energy effect. Morinari and Tohyama [20] proposed that the sign change of the magnetoresistance in $\alpha$-(BEDT)T$_2$I$_3$ is due to a Landau level mixing effect which depends on the level broadening.

In the following we argue that, in deformed multilayer Dirac electron systems, such crossover may be induced by a tunneling between Dirac valleys which takes place at high magnetic field or close to the merging. We do not claim that this scenario is responsible of the sign change of the magnetoresistance of $\alpha$-(BEDT)T$_2$I$_3$ since the merging of Dirac cones has not yet been observed in this material [11]. However, this does not rule out the idea of a field induced interaction between Dirac valleys in $\alpha$-(BEDT)T$_2$I$_3$ which may generate, in addition to the Zeeman splitting, a crossover from negative to positive magnetoresistance.

Montambaux et al [17] have estimated the gap $\Delta E_n$ between the two energy levels obtained when the valley degeneracy of a Landau level $E_n$ is lifted. They found that

$$\Delta E_n \sim e^{-\frac{\gamma B}{l_0^2}}.$$

Since $\alpha^2 = \frac{c_s}{c_y} = \sqrt{\frac{2A}{m^*c_y^2}}$, $\Delta E_n$ takes the form

$$\Delta E_n \sim e^{-\sqrt{\frac{2mc_s c_y^2}{\pi^2}m^*}}a^6. \quad (18)$$

The expressions of $m^*$ and $c_y$ for fixed $m^*$ and $\Delta$ are given by [17]

$$m^* = \frac{2\hbar^2}{3m_0^2}, \quad c_y = \frac{3mc_0}{\hbar},$$

where $m_0$ is the distance between neighboring atoms of the honeycomb lattice.

$\Delta E_n$ can then be written as

$$\Delta E_n \sim e^{-\sqrt{\frac{2mc_s c_y^2}{\pi^2}m^*}}a^6. \quad (19)$$

where the dimensionless field is $\tilde{B}_c = \frac{B_c c_y^2}{\hbar}$.

The critical field $B_{c,cr}$ at which the gap $\Delta E_n$ opens should scale, according to equation (19), as

$$\ln B_{c,cr} \sim 6\ln \alpha. \quad (20)$$

The energy gap around the $n = 0$ Landau level was also calculated by Esaki et al [21] who found the same exponential behavior as Montambaux et al [17].

To take into account the interaction between the Dirac valleys inducing the degeneracy lifting of the Landau level, we adopt a perturbative approach. We consider the first-order correction to the Landau energy. The corresponding wave functions are those given in the previous section, being the zeroth-order correction in terms of the perturbation.

The energy difference in the Kubo formula of the conductivity in the quantum limit ($n = n' = 0$) (equation (12)) is then replaced by $\Delta E_n$:

$$\sigma_{zz}(\omega) \sim \frac{i\hbar}{V} \sum_{\text{spin}} \sum_{\text{states}} \frac{d}{dE} \left| \langle 0 | \hat{J}_z | 0 \rangle \right|^2 \left( \frac{\hbar}{2} \right)^2 \Delta E_n \left( \frac{\hbar}{eB_c} \right)^2 \exp \left[ \frac{1}{2} \frac{e^2}{\hbar B_c} \left( \frac{1}{\alpha^2 B_c^2 + \alpha^2 B_c^2} \right) \right]. \quad (21)$$

The DC conductivity then takes the form

$$\sigma_{zz} = \frac{|B_z|}{A} \frac{1}{1 + \frac{\hbar^3}{2mc_y^2}} \exp \left[ -\frac{\hbar B_c}{2mc_y} \left( \frac{1}{\alpha^2 B_c^2 + \alpha^2 B_c^2} \right) \right]. \quad (22)$$

where $A = \frac{\pi \hbar^3}{2mc_y^2 e^2}$ as given in section 2.1.

The interlayer resistivity is then given by

$$\rho_{zz} = \frac{B_0 + \rho_{zz}}{1 + \frac{\hbar^2 \Delta E_n}{2mc_y^2}}.$$

(23)

For a rough estimation of the effect of the energy gap $\Delta E_n$ on the conductivity, we make the following approximation for the correction term:

$$\frac{1}{1 + \frac{\hbar^2 \Delta E_n}{2mc_y^2}} \sim 1 - e^{-4\sqrt{\frac{\pi}{2}mc_y^2}},$$

where we have replaced the energy gap $\Delta E_n$ by its expression given by equation (19).

In figure 6 we plot the field dependence of the interlayer resistivity $\rho_{zz}$ (equation (23)) in the case of a transverse magnetic field. The results show a change in the behavior of $\rho_{zz}$ at a critical field $B_{c,cr}$ which decreases with decreasing $\alpha$. $B_{c,cr}$ marks the departure from the $1/B_c$ behavior expected for undeformed material ($\alpha = 1$).

Obviously, the interlayer resistivity does not show a sign change even close to the merging. An inplane field component is needed to induce such a crossover as we show in what follows.

The dependence of $B_{c,cr}$ on $\alpha$ is shown in figure 7 according to which $\ln B_{c,cr} \sim 0.3 \ln \alpha$ which is in good agreement with the value estimated by Montambaux et al [17] (equation (20)). This agreement support the approximation of the first-order energy correction we introduced in the Kubo formula (equation (21)) to account for the contribution of the Dirac valley tunneling to the magnetotransport.
Interlayer resistivity \(\rho_{zz}\) as a function of the field amplitude \(B\) for different values of the parameter \(\alpha\). The solid (broken) lines correspond to the results with interacting (independent) Dirac valleys.

In the presence of a coupling between Dirac valleys which gets more pronounced as the magnetic field increases (independent) Dirac valleys.

The conclusion of this section is that the crossover from negative to positive magnetoresistance could be induced by a coupling between Dirac valleys which gets more pronounced by approaching the merging or by increasing the magnetic field amplitude.

In the following, we focus on the behavior of the interlayer magnetoresistance at the merging and see how the field and the angle dependences of \(\rho_{zz}\) are affected.

3. Interlayer magnetoresistance: merging of Dirac cones

The diagonalization of the universal Hamiltonian for \(\Delta=0\) and in the gauge \(\bar{A}=(zB_y-yB_z,-zB_x,0)\) reduces to

\[
\left(\frac{\hbar c_y}{\gamma}\right)^2 \left[\bar{\Phi}^2 + \bar{Y}^4 - 2s\bar{Y}\right] \psi_{A,B} = E_n^2 \psi_{A,B},
\]

where we take, for simplicity, the squared Hamiltonian. The dimensionless operators \(\bar{\Phi}\) and \(\bar{Y}\) are given by \(\bar{\Phi} = \frac{\gamma}{\bar{B}}\pi_x\), \(\bar{Y} = \frac{\gamma}{\bar{B}}, Y = y_0 - Y, y_0 = \frac{p_\gamma + eB_z}{\bar{B}}\) and \(\pi_x = p_y - ezB_c\). \(\gamma\) is written as \([17]\)

\[
\gamma = \left(\frac{2\hbar c_n m^{\frac{1}{2}}}{e^2 B_c^2}\right)^{\frac{1}{2}}.
\]

\(\bar{\Phi}\) and \(\bar{Y}\) satisfy the commutation relation \([\bar{Y}, \bar{\Phi}_1] = -i\)

The eigenfunction of equation (24) is of the form

\[
\psi(\bar{Y}) \sim e^{i\epsilon_1} e^{i\epsilon_2 Y} \phi(\bar{Y}),
\]

where \(c_1 = \frac{eB_y}{\bar{B}} (\bar{Y}_0 - \frac{\bar{B}Y}{\bar{B}})\) and \(c_2 = \frac{eB_z}{\bar{B}}\). \(\phi(\bar{Y})\) is the eigenfunction of anharmonic quartic oscillator and \(\bar{Y}_0\) is the corresponding center coordinate. \(\phi(\bar{Y})\) is the eigenfunction of

\[
H_{anh} = \left(\frac{\hbar c_y}{\gamma}\right)^2 \left[\bar{\Phi}^2 + \bar{Y}^4 - 2s\bar{Y}\right].
\]
We will consider in what follows the case of \( s = 1 \) since \( s = \pm 1 \) corresponds to a symmetric problem as a function of \( \bar{y} \).

In \cite{22, 23}, the authors studied the eigenproblem of the following anharmonic quartic oscillator:

\[
H_{\pm} = -\frac{d^2}{dx^2} + g^2 x^4 \pm 2g|x|.
\]

The groundstate eigenfunction of the potential \( V_-(x) = g^2 x^4 - 2g|x| \) is of the form \( \phi_0^{-}(x) \sim e^{-x^{2/3}} \).

Therefore, the solution \( \phi(\bar{y}) \) of the anharmonic part of equation (24) can be written, for the lowest Landau level and for \( \bar{y} > 0 \), as

\[
\phi(\bar{y}) = \phi_0^{-}(\bar{y}) \sim e^{-\frac{1}{3} \bar{y}}. \tag{26}
\]

The eigenstate of the zero-mode level of equation (24) then takes the form

\[
F_{0,\tilde{y}_0,\tilde{z}_0}(\tilde{r}) = \begin{pmatrix} 0 \\ f_{0,\tilde{y}_0,\tilde{z}_0}(\tilde{r}) \end{pmatrix}, \tag{27}
\]

where

\[
f_{0,\tilde{y}_0,\tilde{z}_0}(\tilde{r}) \sim \exp \left[ \frac{iZe_B}{\hbar} \left( \tilde{y}_0 - \frac{\tilde{z}_0^2}{2} \right) \right] \times \exp \left[ \frac{i\sqrt{3}\tilde{C}}{\hbar} \right] \exp \left[ -\frac{(\tilde{y}_0 - \bar{y})^3}{3\gamma^3} \right]. \tag{28}
\]

The interlayer hopping matrix is given, as in section 2, by

\[
(F_{0,\tilde{y}_0,\tilde{z}_0}|\Delta H|F_{0,\tilde{y}_0,\tilde{z}_0}) = -\tilde{t}_c(\tilde{y}_0', \tilde{z}_0', \tilde{y}_0, \tilde{z}_0) \times \left[ \frac{\delta_{\tilde{z}^{'},-\tilde{z}} + \delta_{\tilde{z}^{'},\tilde{z}} - \sqrt{3} \tilde{\gamma}}{\gamma} + \frac{\delta_{\tilde{z}^{'},+\tilde{z}} - \delta_{\tilde{z}^{'},-\tilde{z}}}{\gamma} \right]. \tag{29}
\]

The effective interlayer hopping can then be written as

\[
\tilde{t}_c(\tilde{y}_0', \tilde{z}_0', \tilde{y}_0, \tilde{z}_0) \sim \tilde{t}_c \exp \left[ \frac{ieBz}{\hbar} \left( \frac{\tilde{y}_0 + \tilde{y}_0'}{2} \right) \right] \int_0^{\infty} dx \times \exp \left[ i\frac{c}{\hbar} \left( \tilde{z}_0' - \tilde{z}_0 \right) \right] \times \exp \left[ \frac{1}{3} \left( \frac{x + a}{\gamma} \right)^3 \right] \times \exp \left[ \frac{1}{3} \left( \frac{x - a}{\gamma} \right)^3 \right],
\]

with \( x = \bar{y} - \frac{\tilde{y}_0' + \tilde{y}_0}{2} \), \( a = \frac{\tilde{y}_0' - \tilde{y}_0}{2} = \frac{\tilde{z}_0' - \tilde{z}_0}{2} \), and \( \gamma \) is given by equation (25).

Using the Kubo formula, we obtain the interlayer conductivity to the lowest-order contribution of \( \tilde{t}_c \):

\[
\sigma_{zz} \sim \tilde{t}_c^2 |B_z| \int_0^{\infty} \exp \left[ \frac{ieB_z x}{\hbar} \right] f(x)^2,
\]

where \( c \) is the interlayer distance and \( f(x) \) is given by

\[
f(x) = \exp \left[ -\frac{1}{3} \left( \frac{c}{\gamma} \right)^3 \left( \frac{x + B_y}{c - 2B_z} \right)^3 \right] \times \exp \left[ -\frac{1}{3} \left( \frac{c}{\gamma} \right)^3 \left( \frac{x - B_y}{c - 2B_z} \right)^3 \right]. \tag{31}
\]

The normal field component \( B_z \) appearing in the prefactor of \( \sigma_{zz} \) in equation (30) is due to the degeneracy of the Landau level.

In a graphene-like system, at the merging (\( \Delta = 0 \)), \( m^* = \frac{m_e}{3\pi^2} \) and \( c_y = \frac{2m_0}{\hbar} \) where \( m_0 \) is the distance between the two atoms of the unit cell \cite{17}. We then obtain \( (\frac{c}{\gamma})^3 = \frac{a_0}{2c}B_z^2 \), where the dimensionless magnetic field is \( \bar{B}_z = \frac{\sqrt{c}}{\hbar}B_z \). We take for numerical calculations \( c = 1.75 \) nm and \( a_0 = 10 \) Å as in \( \alpha \) (BEDT-TTF).

The field dependence of the interlayer conductivity \( \sigma_{zz} \) for a transverse magnetic field is plotted in figure 9.

Contrary to the case of separated Dirac cones, \( \sigma_{zz} \) decreases at the merging by increasing the normal field amplitude. This decrease appears as the continuity of the positive interlayer magnetoresistance obtained beyond the crossover field \( B_{zz,cr} \) for vanishing \( \alpha \) in section 2. We can then conclude that the crossover from negative to positive magnetoresistance is due to Dirac cone motion. As \( \alpha = \sqrt{\bar{B}_z} \) decreases, Dirac cones get closer to the merging point and the interlayer conductivity is reduced.

We do not claim that our calculations provide a continuous description of the Dirac point motion from the zero gap to the gapped phase. But there is a sign change of the magnetoresistance, for a normal field \( (B = B_z) \), if the system moves from the independent Dirac valleys to the merging phase. In the former case, \( \sigma_{zz} \) is linear to \( B_z \) whereas in the latter case \( \sigma_{zz} \) decreases with increasing \( B_z \).

To obtain a continuous analytical description of the magnetotransport with the Dirac point motion, one needs to derive the expression of the eigenfunctions of the anharmonic quartic oscillator with the potential given by equation (7).
the best of our knowledge, these eigenfunctions have not been analytically determined. Skála et al [24] found solutions for the Schrödinger equation corresponding to the Hamiltonian

$$H = -\frac{d^2}{dx^2} + V(x),$$

where $V(x) = V_1x + V_2x^2 + V_3x^3 + V_4x^4$ with the condition $V_4 > 0$. The solution is of the form

$$\psi(x) = \exp(-g_0x - g_1x^2/2 - g_2x^3).$$

However, $\psi(x)$ diverges for $x \to \pm\infty$.

In figure 10 we present the field dependence of the interlayer conductivity $\sigma_{zz}$ in the presence of an inplane field component. $\sigma_{zz}$ shows a positive magnetoresistance as a function of the field amplitude.

Figures 11 and 12 show the field orientation dependence of the interlayer conductivity at the merging.

According to figure 12 the interlayer conductivity $\sigma_{zz}$ shows a maximum along the strain direction $y$ ($\Phi = \pi/2$). This behavior is found to be independent of the out-of-plane angle $\theta$ as in the case where Dirac cones are far from the merging (figure 5).

However, the dependence of $\sigma_{zz}$ on the out-of-plane angle $\theta$ is different from that found far from the merging. The maximum of the conductivity is no more for a transverse magnetic field ($\theta = \pi/2$) but is shifted towards $\theta = 0$ as the inplane field component $B_\parallel$ is turned along the strain direction $y$. This behavior could be used as an experimental probe for the merging of Dirac cones.

4. Concluding remarks

We have derived the expression of the interlayer magnetoresistance in a multilayer deformed Dirac electron system. We have discussed the signature of the motion and the merging of Dirac cones induced by the deformation.

In the case of independent Dirac valleys, the system shows a negative magnetoresistance for a normal magnetic field as in the undeformed case. However, a crossover from a negative to a positive magnetoresistance takes place in the presence of an inplane field component. The latter induces an inplane Lorentz force which reduces the interlayer tunneling. This effect is more pronounced as the amplitude of the deformation is increased.

The motion of Dirac cones, resulting from the deformation, gives rise to a dependence of the interlayer magnetoresistance on the azimuthal angle. However, the behavior of the interlayer resistivity with the out-of-plane angle $\theta$ is unchanged compared to the undeformed case.

We have argued that the sign change of the magnetoresistance could also result from a coupling between Dirac valleys which removes the degeneracy of the Landau level and, hence, reduces the density of carriers. This coupling is enhanced as the merging is approached or at high magnetic field. A criterion is proposed to define the range of validity of the independent Dirac valleys assumption.
These features may be observed in a stack of deformed graphene-like systems which can be simulated by optical lattices [14] or microwave experiments [16].

We suggest that, besides the Zeeman splitting, the effect of Dirac valley interaction should be taken into account to explain the sign change of the magnetoresistance in $\alpha$-(BEDT)$_2$I$_3$ at high magnetic field.

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