Gap opening in the zeroth Landau level in gapped graphene: pseudo-Zeeman splitting in an angular magnetic field

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Abstract
We present a theoretical study of gap opening in the zeroth Landau level in gapped graphene as a result of pseudo-Zeeman interaction. The applied magnetic field couples with the valley pseudospin degree of freedom of the charge carriers leading to the pseudo-Zeeman interaction. To investigate its role in transport at the charge neutrality point (CNP), we study the integer quantum Hall effect in gapped graphene in an angular magnetic field in the presence of pseudo-Zeeman interaction. Analytical expressions are derived for the Hall conductivity using the Kubo–Greenwood formula. We also determine the longitudinal conductivity for elastic impurity scattering in the first Born approximation. We show that pseudo-Zeeman splitting leads to a minimum in the collisional conductivity at high magnetic fields and a zero plateau in the Hall conductivity. Evidence for activated transport at CNP is found from the temperature dependence of the collisional conductivity.

1. Introduction

In recent years, the experimental realization of a stable single layer of carbon atoms [1, 2] has stimulated much interest in the studies of its unusual properties [3, 4]. This material, known as graphene, is a tightly packed honeycomb lattice of carbon atoms. A graphene monolayer is a gapless semiconductor with conical touching of electron and hole bands. The charge carriers in this system obey a linear dispersion relation near the Dirac point, which endows it with unique electronic properties. This difference in the nature of the quasiparticles in graphene from conventional two-dimensional (2D) electronic systems has given rise to a host of new and unusual phenomena. Besides the fundamental interest in understanding the electronic properties of graphene there are also serious efforts to build nanoelectronic devices from graphene [5–7].

The quantum Hall measurements in graphene were one of the key tools providing evidence that the quasiparticles in graphene are chiral, massless fermions known as Dirac fermions [8–13]. A key difference in the integral quantum Hall effect in graphene compared to the standard effect in conventional two-dimensional electron gas (2DEG) systems is the occurrence of a zeroth Landau level (LL) state. There have been several experimental as well as theoretical studies of transport at the CNP which required analysis of the role of the zeroth LL state [14–19]. The nature of the splitting of the electronic states at the CNP at present remains unclear, whether this splitting is due to Zeeman interactions, electron– electron or electron–phonon interactions, an asymmetric gap, gapless edge states or due to valley splitting is still an open question. The results obtained in [16] were explained on the basis of field dependent splitting of the zeroth Landau level. Breakdown of the QHE in graphene leading to two insulating regimes was analyzed in [17, 18]. On the theoretical side [15] addressed the role of the zeroth LL in the QHE in graphene using Laughlin’s gauge argument. The role of disorder in addition to the LL structure was discussed in detail in [19]. In [14], the splitting of the zeroth LL was observed and it was attributed to lifting of the sublattice and spin symmetry.

We consider gapped graphene in the presence of an external magnetic field. Due to the breaking of sublattice symmetry a gap opens in the energy spectrum at the
Dirac points. One of the mechanisms that can lead to sublattice symmetry breaking is through a local asymmetric chemical or electrical environment provided by a substrate, such as epitaxial graphene on SiC or BN substrate. Band gaps of various magnitudes can be induced depending on the substrate [20, 21]. This symmetry breaking can have important consequences for transport at CNP as it can lead to pseudo-Zeeman splitting of the zeroth level when contributions of both the valleys are considered. It has been shown in [23, 30–33, 40, 43, 45] that if Berry phase effects are taken into account, for crystals with broken spatial inversion symmetry, the electrons acquire an orbital magnetic moment as a result of the self-rotation of the Bloch electron wavepacket. This applies to Dirac fermions in graphene with staggered sublattice potential which breaks inversion symmetry where the orbital magnetic moment is associated with the valley index and can lead to the valley QHE. In addition, various mechanisms for valley filtering and valley polarization have been discussed in relation to electronic devices [33, 40–43].

Our focus is on electron transport at CNP in gapped graphene in a tilted magnetic field when the sublattice symmetry of graphene is broken resulting in an energy gap at the Dirac point. This requires that we consider the valley QHE which has been discussed earlier in [22, 33, 40] and more recently in [23]. In [22], the authors relate the heights of the plateaus in the Hall conductivity and the peaks in the diagonal conductivity to the size of the bandgap and the amount of disorder in the system. A semiclassical presentation of the valley QHE in graphene is given in [23]. Here, we present a full quantum mechanical transport theory for the valley QHE and analyze the effects of the external tilted magnetic field on the transport at CNP at finite temperature in the presence of screened charged impurities. From the very beginning of our calculation, we explicitly introduce the Zeeman coupling of the external magnetic field with the valley pseudospin of the Dirac fermions and diagonalize the graphene Hamiltonian in its presence. Moreover, we consider an external angular magnetic field [14, 15] applied to the system in order to highlight the role of the out-of-plane to in-plane magnetic field in the splitting of the zeroth LL. Furthermore, the analysis of magnetotransport in this work is performed in the presence of elastic scattering due to charged impurities which are known to be the dominant scattering mechanism [24, 9, 25–29] in graphene on a substrate. In addition, this is a finite temperature study where the role of temperature in magnetotransport at CNP can be investigated. The electrical transport coefficients have been obtained from the standard Kubo formula in the self-consistent Born approximation [8, 9, 30].

In section 2, we present the formulation of the problem and numerical discussion of density of states for different magnetic field strengths with varying tilt angle from out-of-plane to in-plane. Section 3 contains the derivation of the Hall conductivity as a function of the tilted magnetic field including discussion of numerical results, whereas in section 4 we evaluate the longitudinal conductivity as a function of tilt angle with discussion of results. In section 5, a summary of the work is given followed by an appendix.

2. Formulation

We consider Dirac fermions in graphene which is in the \(x-y\)-plane in the presence of a tilted magnetic field and pseudo-Zeeman interaction. The magnetic field \(\{B_x, B_z\} = (B \sin \theta, B \cos \theta)\) is applied at an angle \(\theta\) with the \(z\)-direction perpendicular to the graphene plane. The effective Hamiltonian for Dirac fermions in gapped graphene in a magnetic field [31–33] can be expressed as (the speed of light \(c = 1\) in the minimal substitution that follows)

\[
H^\tau_z = V_F \left( \begin{array}{cc} \Delta_z/V_F & p_x \tau_x - ip_y - i e A_y \\ p_x \tau_x + ip_y + i e A_y & -\Delta_z/V_F \end{array} \right) + \mathcal{H}_0^\tau_z.
\]  

(1)

Here \(\tau_z = \pm 1\) for valleys \(K\) and \(K'\), \((A_x, A_y)\) are the components of the vector potential, \(V_F\) characterizes the Fermi velocity of Dirac fermions. We identify \(\Delta_z = -\mu_B^B B_z\) as the pseudo-Zeeman term with \(B_z = B \cos \theta\), \(\sigma = \{\sigma_x, \sigma_y, \sigma_z\}\) are the Pauli matrices, the effective Bohr magneton is \(\mu_B^B = \frac{e h}{2m^*}\) with the effective mass \(m^*_z = 2\Delta h^2/3a^2\). The Bohr magneton and the effective mass are expressed in terms of the gap energy \(\Delta = 0.28\) eV (for graphene on SiC), the nearest neighbor hopping energy \(t = 2.82\) eV and the lattice constant \(a = 0.246\) nm with the result that the effective Bohr magneton \((\mu_B^B)\) can be 30 times larger than the free electron Bohr magneton \((\mu_B)\) [23, 33, 40]. This also allows us to ignore the real spin Zeeman term. The above Hamiltonian is the same as that obtained in [45, 46] in the absence of valley–orbit coupling.

The Hamiltonian \(H^\tau_z\) for the two valleys \((K, K')\) can be written as

\[
H^\tau_z = V_F \left( \begin{array}{cc} \Delta_z/V_F & p_x \tau_x - ip_y - i e A_y \\ p_x \tau_x + ip_y + i e A_y & -\Delta_z/V_F \end{array} \right) + \mathcal{H}_0^\tau_z
\]  

(2)

where the diagonal terms \(\Delta_z = \pm \mu_B^B B_z\) represent the potential asymmetry between A and B lattice sites, which opens an energy gap at the CNP. We have employed the Landau gauge and expressed the vector potential as \(A = (0, B_z z - B_x x, 0)\). The last term in the Hamiltonian given in equation (1) is regarded as the pseudospin Zeeman term \((\Delta_z = \mu_B^B B_z)\) [23, 30–33, 43], where the valleys \(K\) and \(K'\) serve as pseudospin up \((+1)\) and pseudospin down \((-1)\), respectively. Equation (2) is expressed as

\[
H^\tau_z = V_F \left( \begin{array}{cc} \Delta_z/V_F & p_x \tau_x - ip_y - i e (B_z x - B_x z) \\ p_x \tau_x + ip_y + i e (B_z x - B_x z) & -\Delta_z/V_F \end{array} \right)
\]  

(3)

To obtain the energy eigen solutions of the above equation, one can use the eigenvalue equation for a given spinor

\[
\Psi (\mathbf{r}) = \begin{pmatrix} \phi_1 (\mathbf{r}) \\ \phi_2 (\mathbf{r}) \end{pmatrix},
\]  

(4)

as

\[
H \begin{pmatrix} \phi_1 (\mathbf{r}) \\ \phi_2 (\mathbf{r}) \end{pmatrix} = E \begin{pmatrix} \phi_1 (\mathbf{r}) \\ \phi_2 (\mathbf{r}) \end{pmatrix}.
\]  

(5)
It yields the following equations

\[ \Delta_c \phi_1(r) - iV_F (p_x \tau_x + p_y + e(B_x x - B_y z)) \times \phi_1(r) = E \phi_1(r) \]

\[ iV_F (-i p_x \tau_x + p_y + e(B_x x - B_y z)) \phi_1(r) - \Delta_v \phi_2(r) = E \phi_2(r). \]

(6)

We try the ansatz

\[
\begin{pmatrix}
\phi_1(r) \\
\phi_2(r)
\end{pmatrix} = \frac{1}{\sqrt{L_y}} \exp[i k_y] \begin{pmatrix}
\psi_1(r) \\
\psi_2(r)
\end{pmatrix},
\]

(8)

where \( L_y \) is the dimensions of the graphene monolayer in the y-direction. From equations (6)–(8) we obtain the eigenvalues of the nth LL as

\[
E_{n,0}^z = -\tau_z \Delta_z, \quad n = 0
\]

\[
E_{n,\pm}^z = \sqrt{\hbar^2 c_2^2 |n| + (\tau_z \Delta_z)^2}, \quad n \neq 0
\]

with \( s = \pm \) for electrons and holes. The corresponding eigenfunction is

\[
\psi_{z,n,k_y}(r) = \frac{e^{i k_y r}}{\sqrt{L_y}} \begin{pmatrix}
s c_1 \psi_{|n|-1} \left( \frac{(x + x_0)}{l} \right) \\
c_2 \psi_{|n|} \left( \frac{(x + x_0)}{l} \right)
\end{pmatrix}.
\]

(10)

The \( n = 0 \) Landau level (the zeroth LL) requires separate treatment. It lies just at the top of the valence band and its amplitude is only at B sites with energy \( E_0^z = -\Delta_z \), \( c_1 = 0 \) and \( c_2 = 1 \). In the above equation \( - \) is for holes and + for electrons, with \( x_0 = \vec{F} \cdot \vec{r}, \ \vec{l} = \sqrt{\frac{\hbar}{e B \cos \theta}}, \ c_1 = \sin(\alpha/2) \) with \( \sin(\alpha) = -\frac{\sinh \sqrt{2 |n|}}{\sqrt{\hbar^2 c_2^2 |n| + (\tau_z \Delta_z)^2}} \), \( c_2 = \cos(\alpha/2) \) with \( \cos(\alpha) = \frac{s \Delta}{\sqrt{\hbar^2 c_2^2 |n| + (\tau_z \Delta_z)^2}} \). The coefficients \( c_1 \) and \( c_2 \) are normalized such that \( |c_1|^2 + |c_2|^2 = 1 \). \( \varphi_n = \psi_{0,0}(x,y) = \sqrt{\frac{1}{\sqrt{2} \sqrt{\pi}}} H_n \left( \frac{x+y}{\sqrt{2}} \right) \exp \left[ -\frac{l^2}{2} \left( \frac{x+y}{\sqrt{2}} \right)^2 \right] \), \( H_n(x) \) are the Hermite polynomials, \( \omega_D = V_F \sqrt{\frac{e B \cos \theta}{\hbar}} \) is the cyclotron frequency of Dirac fermions and \( n \) is an integer.

Similarly, for the \( K' \) valley \( \phi_{n,k_y} \), the Hamiltonian yields the same eigenvalues as given in equations (9) with eigenfunctions

\[
\psi_{z,n,k_y}(r) = \frac{e^{i k_y r}}{\sqrt{L_y}} \begin{pmatrix}
s' c_1' \psi_{|n|-1} \left( \frac{(x + x_0)}{l} \right) \\
c_2' \psi_{|n|} \left( \frac{(x + x_0)}{l} \right)
\end{pmatrix},
\]

(11)

where \( s' = \pm \) for electrons and holes, \( c_1' = \sin(\alpha'/2) \) with \( \sin(\alpha') = -\frac{\sinh \sqrt{2 |n|}}{\sqrt{\hbar^2 c_2^2 |n| + (\tau_z \Delta_z)^2}} \), \( c_2' = \cos(\alpha'/2) \) with \( \cos(\alpha) = \frac{s \Delta}{\sqrt{\hbar^2 c_2^2 |n| + (\tau_z \Delta_z)^2}} \). The energy of the \( n = 0 \) LL for the \( K' \) valley is \( E_{0,0}^z = 0 \). In this case, the LL \( n = 0 \) lies just at the bottom of the conduction band and its amplitude is only at the A sites.

The density of states (DOS) is defined as

\[
D(\varepsilon) = \frac{A}{\pi l^2} \sum_{n,z,<,\tau_z} \delta(\varepsilon - E_{n,\tau_z}^z), \quad n \neq 0,
\]

(12)

and for \( n = 0 \), the above equation at CNP is written as

\[
D_{\text{CNP}}(\varepsilon) = \frac{A}{\pi l^2} \sum_{\tau_z} \delta(\varepsilon - E_{0,\tau_z}^z),
\]

where \( E_{0,\tau_z}^z = \pm \Delta_z \) for \( K \) and \( K' \) valleys respectively, and \( A \) is the area of the sample. Assuming a Gaussian broadening of width \( \Gamma \), the DOS at CNP is expressed as

\[
D_{\text{CNP}}(\varepsilon) = \frac{2}{\pi l^2} \sum_{\tau_z} \frac{1}{\Gamma} \frac{1}{\sqrt{2\pi}} \exp \left[ -\frac{(\varepsilon - E_{0,\tau_z}^z)^2}{2\Gamma^2} \right],
\]

(13)

where \( \Gamma \) is the Gaussian distribution broadening width of zero shift. Similarly, one can evaluate the DOS for the other valley \( (K') \).

The above expression for the DOS at CNP is plotted in figure 1 as a function of the Fermi energy (gate voltage) as the magnetic field strength is varied to see the splitting of the zeroth LL. The applied magnetic field is perpendicular to the graphene plane, the tilt angle \( \theta = 0 \). The magnetic field is varied from \( 5 \) T (solid line), \( 10 \) T (dashed line), \( 20 \) T (dotted line) to \( 30 \) T (dashed line) for fixed values of angle \( (0^\circ) \) and temperature \( (T = 0) \).
strength at 30 T. The tilt angle is varied from 0° to 90° (dotted line), 60° (dotted line) to 90° (dashed line) at zero temperature (T = 0).

In figures (1 and 2) the following parameters were employed: $g = 60$ [31, 32]. The broadening of the LLs generally depends on the magnetic field strength, the temperature, LL index and the scattering parameters. This requires a self-consistent calculation usually performed numerically. In order to carry out a tractable analytical calculation we have chosen a constant level width $\Gamma = 10$ meV [9, 25, 34–36].

In the presence of a magnetic field, there are two contributions to magnetoconductivity [37, 38]: the collisional (hopping) contribution and the Hall contribution. The former is the localized state contribution which carries the effects of SdH oscillations. The Hall contribution is the nondiagonal contribution. In order to calculate the electrical conductivity in the presence of pseudo-Zeeman interactions and a tilted magnetic field we will follow the formulation of [39], which is derived from the general Liouville equation [37, 38] and more recently in graphene [39], and references therein.

3. Hall conductivity

The Hall conductivity $\sigma_{xy}$ is obtained from the nondiagonal elements of the conductivity tensor, given by [37–39]

$$
\sigma_{xy} = \frac{2i\hbar e^2}{\Omega} \sum_{\xi \neq \xi'} f_{\xi}(1 - f_{\xi'}) \langle \xi | v_x | \xi' \rangle \langle \xi' | v_y | \xi \rangle \times \frac{(1 - e^{\beta(E_\xi - E_{\xi'})})}{(E_\xi - E_{\xi'})^2}.
$$

Since $f_{\xi}(1 - f_{\xi'}) (e^{\beta(E_\xi - E_{\xi'})}) = f_{\xi}(1 - f_{\xi'})$ and $\Omega \rightarrow S_0 \equiv L_y$, we obtain

$$
\sigma_{xy} = \frac{2i\hbar e^2}{S_0} \sum_{\xi \neq \xi'} (f_{\xi} - f_{\xi'}) \langle \xi | v_x | \xi' \rangle \langle \xi' | v_y | \xi \rangle \frac{(E_\xi - E_{\xi'})}{(E_\xi - E_{\xi'})^2}.
$$

(15)

Since the x and y components of the velocity operator are $v_x = \frac{\partial H}{\partial p_x}$ and $v_y = \frac{\partial H}{\partial p_y}$ where $H = V_F [\sigma_x \tau_z + \sigma_y (p_y + eA_y)] + \Delta, \sigma_z$, therefore, $v_x = V_F \sigma_x \tau_z$ and $v_y = V_F \sigma_y$. Hence

$$
\langle \xi | v_x | \xi' \rangle = c_1 c_2 V_F (\delta_{\eta, -1'} + \delta_{\eta, -1})
$$

(16)

and

$$
\langle \xi | v_y | \xi' \rangle = -ic_1 c_2 V_F (\delta_{\eta, -1'} - \delta_{\eta, -1}).
$$

(17)

Since $| \xi \rangle \equiv | n, s, \tau_x, \tau_y \rangle$, there will be one summation over $k_y$ which, with periodic boundary conditions for $k_y$, will give

$$
\sum_{k_y} \rightarrow \frac{L_y}{2\pi} \int_{L_y/2}^{L_y/2} dk_y = \frac{S_0}{2\pi \Gamma^2}.
$$

(18)

Substituting the values of the matrix elements of velocity in equation (15) yields

$$
\sigma_{xy} = \frac{2 \times 2(c_1 c_2)^2 \hbar e^2 V_F^2}{2\pi \Gamma^2} \sum_{\xi \neq \xi'} (f_{\xi} - f_{\xi'}) \frac{(\delta_{\eta, -1'} - \delta_{\eta, -1})}{(E_\xi - E_{\xi'})^2}.
$$

(19)

Here the factor of 2 is due to spin degeneracy. Since $E_\xi \equiv E_{\xi, n} = \sqrt{\hbar^2 \omega_D^2 |n| + (\tau_x \Delta_z)^2}$ we obtain

$$
(E_\xi - E_{\xi'})^2 = \left[ \sqrt{2\hbar^2 \omega_D^2 |n| + (\tau_x \Delta_z)^2} \right]^2.
$$

(20)

Substituting equation (20) in (19) we obtain the Hall conductivity

$$
\sigma_{xy} = \frac{2(c_1 c_2)^2 \hbar e^2 V_F^2}{2\pi \Gamma^2 \hbar^2 \omega_D^2} \sum_{x', y', n', \tau_x', \tau_y'} \left\{ f_{x', n'} \frac{(f_{x, n}' - f_{x', n'})^2}{(\delta_{n, n'} - 1)} - \delta_{n, n'} \Delta_z \right\} \left\{ \left[ \frac{\sqrt{|n| + (\tau_x \Delta_z)^2 / 2\hbar^2 \omega_D^2}}{\sqrt{|n'| + (\tau_x' \Delta_z)^2 / 2\hbar^2 \omega_D^2}} \right]^{-1} \right.
$$

(21)

The above equation can be further simplified and the final result for the angular Hall conductivity (see appendix for details) is

$$
\sigma_{xy} = \frac{2(c_1 c_2)^2 \hbar}{\pi \hbar} \sum_{n, j} \left[ n + \left( \frac{\Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 + \frac{1}{2} \right]
$$

$$
\times \left( f_{+, n}^j - f_{+, n+1}^j + f_{-, n}^j - f_{-, n+1}^j \right)
$$

(22)
where we have introduced the sum over \( j = \pm 1 \) for a concise final expression. The effect of the tilted magnetic field can be seen in the distribution function through \( \eta_D = V_F \sqrt{\frac{e B \cos \theta}{h}} \) as

\[
J_{n,s} = f(E_{n,s}) = \left[ \exp \left( \frac{\left( \frac{\Delta c}{\hbar} \frac{\Delta c}{\hbar} 2 |\mu| + \left( \frac{\Delta c}{\hbar} \right)^2 - E_F \right)}{k_B T} \right) + 1 \right]^{-1}.
\]

The Hall conductivity at CNP is written as

\[
\sigma_{yx} = \frac{2(e/c)(z)^2}{\pi \hbar} \sum_{n \neq 0} \left( \left( \frac{\Delta c}{\hbar} \right)^2 + \frac{1}{2} \right) \times \left[ f_{+0} - f_{+1} + f_{-0} - f_{-1} \right]
\]

where \( J_{n,s} = f(E_{n,s}) = \left[ \exp \left( \frac{\left( \frac{\Delta c}{\hbar} \frac{\Delta c}{\hbar} 2 |\mu| + \left( \frac{\Delta c}{\hbar} \right)^2 - E_F \right)}{k_B T} \right) + 1 \right]^{-1} \). The limit when the tilt angle (\( \theta = 0 \)) and the pseudo-Zeeman term vanish (\( \Delta c = \mu B \approx 0 \)), and we consider the transport contribution from a single valley only, the results obtained are consistent with previous works in the literature [1–3, 8–10, 37].

Elements of the resistivity tensor \( \rho_{\mu\nu} \) (\( \mu, \nu = x, y \)) can be determined from those of the conductivity tensor \( \sigma_{\mu\nu} \), obtained above, using the expressions: \( \rho_{xx} = \sigma_{yy}/S \), \( \rho_{yy} = -\sigma_{xx}/S \) and \( \rho_{xy} = -\sigma_{yx}/S \) where \( S = \sigma_{xx} \sigma_{yy} - \sigma_{xy} \sigma_{yx} \) with \( S \approx \frac{\sigma_{xx}^2}{h^2} = \frac{\pi e^2}{B^2 \cos^2 \theta} \).

The Hall conductivity, as a function of the Fermi energy, for different values of the temperature is shown in figure 3. In this figure, we have shown results for different values of temperature 5 (solid line), 25 (dotted line), 75 (dashed line) and 125 K (dot-dashed line). The step around the CNP disappears completely at 125 K. The magnetic field is 5 T. \( g = 60 \).

This shows that in order to observe pseudo-Zeeman splitting of the zeroth LL one needs to be in the regime of high magnetic fields such that the thermal energy does not wash out the splitting of the zeroth LL. Here, we have not considered the electron–phonon interaction which can affect the results at high temperatures. That is intended for future work. Furthermore, as the tilt angle of the magnetic field is increased, the perpendicular component of the magnetic field becomes smaller and the plateaus in the Hall conductivity disappear. We find that at a temperature of 5 K and magnetic field 5 T, \( \theta = 80^\circ \), the steps disappear completely which is consistent with the discussion of the DOS in section 2.

### 4. Collisional conductivity

To obtain the collisional contribution to conductivity, we assume that electrons are elastically scattered by randomly distributed charged impurities as it has been shown that charged impurities play a key role in the transport properties of graphene near the Dirac point. This type of scattering is dominant at low temperature. The collisional conductivity when spin degeneracy is considered is given by [37–39]

\[
\sigma_{xx}^{\text{col}} = \frac{\beta e^2}{S_0} \sum_{\xi, \xi'} (f(E) - f(E')) W_{\xi\xi'}(E, E')(x_\xi - x_{\xi'})^2
\]

where \( f(E) = (\exp \frac{E - E_F}{k_B T} + 1)^{-1} \) is the Fermi–Dirac distribution function with \( f(E) = f(E') \) for elastic scattering, \( k_0 \) is the Boltzmann constant and \( \beta \) is the chemical potential. \( W_{\xi\xi'} \) is the transmission rate between the one-electron states in states \( \xi \) and \( \xi' \), \( S_0 \) the volume of the system, and \( e \) the electron charge.

Conduction occurs by transitions through spatially separated states from \( x_\xi \) to \( x_{\xi'} \), where \( x_\xi = \langle \xi | x | \xi \rangle \) is the mean value of the \( x \) component of the position operator when the electron is in state \( \xi \). This is the well known hopping type formula for transport in the presence of a constant external magnetic field.

Collisional conductivity arises as a result of migration of the cyclotron orbit due to scattering by charge impurities. The scattering rate \( W_{\xi\xi'} \) is given by

\[
W_{\xi\xi'}(E, E') = \frac{2\pi N_I}{S_0 \hbar} \sum_q |U_q|^2 |F_{\epsilon'\epsilon}(u)|^2 \delta(E - E') \delta_{k_\xi, k_{\xi'} + q_\epsilon}.
\]

The Fourier transform of the screened impurity potential is

\[
U_q = U_0/\sqrt{q^2 + k_0^2},
\]

where \( U_0 = e^2/4 \pi e 0 \varepsilon ; k_0 \) is the screening wavevector, \( \varepsilon \) is the static dielectric constant of the material and \( e_0 \) is the dielectric permittivity. \( F_{\epsilon'\epsilon}(u) \) are the form factors, \( \langle \xi | e^{iq^\xi} | \xi' \rangle \) with \( u = \vec{q}^2(q^x + q^y)^2/2 = \frac{q^2}{2} \) with \( q^2 = (q_x^2 + q_y^2) \). \( N_I \) is the impurity density and the wavefunction is \( \langle \xi | x | \xi \rangle = \langle n, s, t, k_\xi \rangle \). In the situation studied here the diffusion contribution is zero because the diagonal elements of the velocity operators vanish. Noting that \( \sigma_{xx}^{\text{col}} = \sigma_{xx}^{\text{col}} \) for screened impurity scattering such that \( k_0 \gg q \), we can ignore the \( q \) dependence in equation (25).

Here \( \langle \xi | x | \xi \rangle = x_\xi \) is the expectation value of the position with \( (x_\xi - x_{\xi'})^2 = (l^2 q_\xi)^2 \) and \( q_\xi = q_\perp \sin \xi \). Since the
The collisional conductivity at CNP given by equation (32) is crucial, the collisional conductivity is expressed as

\[ \sigma_{xx}^{\text{col}} \propto \sum_{\tau_z} \beta f(E_{\tau_z}^c) \left( 1 - f(E_{\tau_z}^c) \right) \]

(32)

The collisional conductivity at CNP given by equation (32) is shown graphically in figure 4 as a function of the Fermi energy for a fixed magnetic field at \( \theta = 0 \) tilt angle as the temperature \( (T) \) is varied: \( T = 5 \) K (solid line), 25 K (dotted line), 75 K (dashed line) and 125 K (dot-dashed line) for fixed values of the magnetic field (5 T) and tilt angle (0°).

![Figure 4. Gap opening in the collisional conductivity as a function of the Fermi energy at low temperature. Temperature is varied from 5 K (solid line), 25 K (dotted line), 75 K (dashed line), to 125 K (dot-dashed line) for fixed values of the magnetic field (5 T) and tilt angle (0°).](image)

3 \times 10^{15} \text{ m}^{-2}, \ k_f = 10^{-7} \text{ m}^{-1}, \ V_F = 10^6 \text{ m s}^{-1}, \text{ magnetic field is 5 T and } U_0 = e^2/4\pi\epsilon_0\epsilon. \text{ We take } \epsilon = 4 \text{ (graphene on a SiO}_2 \text{ substrate) and } \epsilon_0 \text{ the dielectric permittivity of free space, with } k_F = (\pi n_k)^{1/2} \text{ being the Fermi wavenumber. In figure 4, as the temperature is decreased, the collisional conductivity exhibits a gap around CNP due to splitting of the zeroth LL. This splitting at CNP is due to the pseudo-Zeeman interaction as discussed earlier in the context of the DOS at CNP. With an increase in temperature, at 195 K, the splitting is completely eradicated and there is only a single peak at CNP. Furthermore, equation (32) in the limit of low temperatures or high magnetic fields, yields the temperature dependence of the collisional conductivity as } \sigma_{xx}^{\text{col}} \text{ (at CNP) } \propto \beta e^{-\beta \Delta_c}, \text{ which represents an activated type of behavior of the conductivity at the CNP.}

In the limit of zero temperature \( (T = 0) \), equation (32) can be expressed as

\[ \sigma_{xx}^{\text{col}} \text{ (at CNP) } \propto \sum_{\tau_z} \delta(\epsilon - E_{\tau_z}^c), \]

(33)

which can then be written in terms of the Gaussian DOS as derived and discussed in section 2. The effect of the angular magnetic field on the collisional conductivity follows the discussion presented in section 2 for the DOS. Further, the results for the DOS at CNP are consistent in the limit of no Zeeman interactions and a perpendicular magnetic field (for \( \theta = 0 \)) with the experimental as well as theoretical results of [34–36].

Our results for both the Hall conductivity and the collisional conductivity are relevant to transport measurements performed at the CNP on epitaxial graphene grown on substrates such as SiC or BN where a band gap arises as a result of interaction with the substrate. In this regard, we have shown that one possible source of the opening of the gap in the DOS of the zeroth LL is the pseudo-Zeeman interaction which leads to the observed behavior of a plateau in the Hall conductivity and a dip in the collisional conductivity at CNP. In gapless graphene, such as graphene on SiO\(_2\) substrate, opening of a gap in the DOS of the zeroth LL can
also occur due to valley splitting of the LLs. In this case it can occur due to the inherent crystallographic symmetries of graphene [44]. The main difference in terms of realization in real physical systems is that in gapped graphene the effective Bohr magneton or the effective dipole moment that couples with the external magnetic field is much larger which leads to larger valley splitting compared to gapless graphene for the same magnetic field. For an energy gap of 0.28 eV for graphene on SiC substrate, the effective dipole moment is about 30 times larger than the free electron spin magnetic moment. Therefore far smaller magnetic fields are required to observe the valley splitting in gapped graphene as against gapless graphene.

5. Summary

In this work, we have investigated the coupling of an external magnetic field with the valley pseudospin of Dirac fermions and its effects on electron transport in gapped graphene. Specifically, we have analyzed the splitting of the zeroth LL due to this pseudo-Zeeman interaction and its effects on the collisional and Hall conductivity at the CNP. To understand the role of the pseudo-Zeeman interaction we have obtained analytic expressions and have plotted the results for the DOS at CNP in the presence of an external magnetic field whose tilt angle is varied. These results show that the pseudo-Zeeman interaction causes splitting of the zeroth LL which vanishes when the magnetic field is aligned along the graphene plane. We find that the collisional conductivity at CNP shows activated behavior when the pseudo-Zeeman interaction is taken into account. Furthermore, we are able to show that as the temperature is increased for a fixed magnetic field, the closing of the gap in the zeroth LL occurs.

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Appendix

Equation (21) is written as

\[
\sigma_{yx} = \frac{2(\zeta c z^2 \hbar^2 \omega_D^2)}{2\pi \ell^2 h^2 \omega_D^2} \sum_{n,n',\tau_1,\tau_2} (f_{\tau_1 n}^{\tau_2} - f_{\tau_2 n+1}^{\tau_1}) [\delta_{n,n'-1} \\
- \delta_{n-1,n'}] \left( s\sqrt{|n| + (\tau_1 \Delta z)^2/2h^2\omega_D^2} \\
- s'\sqrt{|n'| + (\tau_2 \Delta z)^2/2h^2\omega_D^2} \right)^{-1}. \tag{A.1}
\]

For \( s, s' = +, + \) and \( s, s' = +, - \), the summation in the above equation for \( n' = n + 1 \) is written as

\[
= \sum_{n,n',\tau_1,\tau_2} \left( f_{\tau_1 n}^{\tau_2} - f_{\tau_2 n+1}^{\tau_1} \right) \left( \frac{1}{\sqrt{n + (\tau_1 \Delta z)^2/2h^2\omega_D^2}} - \frac{1}{\sqrt{n + (\tau_2 \Delta z)^2/2h^2\omega_D^2}} \right) \left( f_{\tau_1 n}^{\tau_2} - f_{\tau_2 n+1}^{\tau_1} \right). \tag{A.2}
\]

Note that the \( n' = n - 1 \) contribution vanishes as this corresponds to transition to filled states. Equation (A.2) can be simplified to yield

\[
= \sum_{n,n',\tau_1,\tau_2} \left( \sqrt{n + (\tau_1 \Delta z)^2/2h^2\omega_D^2} - \sqrt{n + (\tau_2 \Delta z)^2/2h^2\omega_D^2} \right) \left( f_{\tau_1 n}^{\tau_2} - f_{\tau_2 n+1}^{\tau_1} \right) \left( n + (\tau_1 \Delta z)^2/2h^2\omega_D^2 \right) \left( n + (\tau_2 \Delta z)^2/2h^2\omega_D^2 \right) \left( f_{\tau_1 n}^{\tau_2} - f_{\tau_2 n+1}^{\tau_1} \right). \tag{A.3}
\]

For \( s, s' = -, + \) and \( s, s' = -, - \), the summation on the right-hand side of equation (A.1) is expressed as

\[
= \sum_{n,n',\tau_1,\tau_2} \left( f_{\tau_1 n}^{\tau_2} - f_{\tau_2 n+1}^{\tau_1} \right) \left( \frac{1}{\sqrt{n + (\tau_1 \Delta z)^2/2h^2\omega_D^2}} - \frac{1}{\sqrt{n + (\tau_2 \Delta z)^2/2h^2\omega_D^2}} \right) \left( f_{\tau_1 n}^{\tau_2} - f_{\tau_2 n+1}^{\tau_1} \right). \tag{A.4}
\]

Equation (A.4) can be simplified to yield

\[
= \sum_{n,n',\tau_1,\tau_2} \left( \frac{1}{\sqrt{n + (\tau_1 \Delta z)^2/2h^2\omega_D^2}} - \frac{1}{\sqrt{n + (\tau_2 \Delta z)^2/2h^2\omega_D^2}} \right) \left( f_{\tau_1 n}^{\tau_2} - f_{\tau_2 n+1}^{\tau_1} \right). \tag{A.5}
\]
Considering the numerator of equation (A.3), we obtain

\[
+ \left( -\sqrt{n} + \left( \frac{\tau_1 \Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \right) - \sqrt{n+1} + \left( \frac{\tau'_1 \Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \\
\times (f^+_{-,n} - f'_{+,n+1}) \bigg/ \left\{ -\sqrt{n} + \left( \frac{\tau_1 \Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \\
+ \sqrt{n+1} + \left( \frac{\tau'_1 \Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \right\} \\
- \sqrt{n+1} + \left( \frac{\tau'_1 \Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \bigg\}.
\]

(A.5)

The denominator of equations (A.3) and (A.5) is

\[
\left( -\sqrt{n} + \left( \frac{\tau_1 \Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \right) - \sqrt{n+1} + \left( \frac{\tau'_1 \Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \\
\times (f^+_{-,n} - f'_{+,n+1}) + \left[ 2n + \left( \frac{\tau_1 \Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \\
+ \left( \frac{\tau'_1 \Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \right] + 2 \sqrt{n+1} + \left( \frac{\tau'_1 \Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \\
\times (f^+_{-,n} - f'_{+,n+1}) \\
\bigg\}.
\]

(A.7)

The denominator of equations (A.3) and (A.5) is

\[
\left( -\sqrt{n} + \left( \frac{\tau_1 \Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \right) - \sqrt{n+1} + \left( \frac{\tau'_1 \Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \\
\times (f^+_{-,n} - f'_{+,n+1}) + \left[ 2n + \left( \frac{\tau_1 \Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \\
+ \left( \frac{\tau'_1 \Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \right] + 2 \sqrt{n+1} + \left( \frac{\tau'_1 \Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \\
\times (f^+_{-,n} - f'_{+,n+1}) \\
\bigg\}.
\]

(A.8)

One may notice that grouping terms such as \( +, + \) and \( +, - \)
for \( s \) and \( s' \) that contain \( f^+_{+,n} \) leads to the cancellation of
the following factor (2 \( n + \left( \frac{\tau_1 \Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \)) in equation (A.6). The same holds for the \( -, - \) and \( -, + \) terms in equation (A.7). Now using equations (A.3), (A.5)--(A.8) in
(A.1), we arrive at the result

\[
\sigma_{yx} = \frac{(c_1 c_2)^2 e^2}{\pi h} \sum_{n, \tau, \tau'} \left[ \left( n + \frac{1}{2} \left( \frac{\tau_1 \Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \right) \\
+ \frac{1}{2} \left( \tau'_1 \Delta_z \right)^2 \right] \delta_{+,n} - f'_{+,n+1} \\
+ f^+_{-,n} - f'_{-,n+1} \right] / (\tau^2_z - \tau'^2_z - 1)^2.
\]

(A.9)

Performing the summation over \( \tau \) and \( \tau' \) for \( +, + \) and \( +, - \)
respectively, equation (A.9) is simplified to yield

\[
\sigma_{yx} = \frac{(c_1 c_2)^2 e^2}{\pi h} \left\{ \sum_{n} \left[ \left( n + \frac{1}{2} \left( \frac{\Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \right) \\
+ \frac{1}{2} \left( \frac{\Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \right] \delta_{+,n} - f'_{+,n+1} \\
+ f^+_{-,n} - f'_{-,n+1} \right] + \sum_{n} \left[ \left( n + \frac{1}{2} \left( \frac{\Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \right) \\
+ \frac{1}{2} \left( \frac{\Delta_z}{\hbar \omega_D \sqrt{2}} \right)^2 \right] \delta_{-,n} - f'_{-,n+1} \\
+ f^+_{-,n} - f'_{-,n+1} \right] \}
\]

(A.10)
After simplifying the above equation we get
\[
\sigma_{yx} = \frac{(c_1 c_2)^2 e^2}{\pi \hbar} \sum_n \left[ n + \left( \frac{\Delta_z}{\hbar v_F \sqrt{2}} \right)^2 + \frac{1}{2} \right] \times \delta \left( f_{+n} - f_{+n+1} + f_{-n} - f_{-n+1} \right) - \left( f_{+n+1} + f_{-n+1} \right). \tag{A.11}
\]
Similarly performing the summation over \( \tau \) and \( \tau \) for \( \tau = + \) and \( \tau = - \), equation (A.9) is simplified to yield
\[
\sigma_{yx} = \frac{(c_1 c_2)^2 e^2}{\pi \hbar} \sum_n \left[ n + \left( \frac{\Delta_z}{\hbar v_F \sqrt{2}} \right)^2 + \frac{1}{2} \right] \times \delta \left( f_{+n} - f_{+n+1} + f_{-n} - f_{-n+1} \right) - \left( f_{+n+1} + f_{-n+1} \right). \tag{A.12}
\]
Finally combining equations (A.11) and (A.12), we arrive at the final result for the Hall conductivity
\[
\sigma_{yx} = \frac{2(c_1 c_2)^2 e^2}{\pi \hbar} \sum_{n,j} \left[ n + \left( \frac{\Delta_z}{\hbar v_F \sqrt{2}} \right)^2 + \frac{1}{2} \right] \times \delta \left( f_{+n} - f_{+n+1} + f_{-n} - f_{-n+1} \right). \tag{A.13}
\]
with \( j = \pm 1 \). In the limit \( \Delta_z = 0 \), the above result reduces to that of [39] exactly.

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