Graphene magnetoresistance in a parallel magnetic field: Spin polarization effect

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We develop a theory for graphene magnetotransport in the presence of carrier spin polarization as induced, for example, by an application of an in-plane magnetic field \( (B) \) parallel to the 2D graphene layer. We predict a negative magnetoresistance \( \sigma \propto B^2 \) for intrinsic graphene, but for extrinsic graphene we find a non-monotonic magnetoresistance which is positive at lower magnetic fields (below the full spin-polarization) and negative at very high fields (above the full spin-polarization). The conductivity of the minority spin band \( (-) \) electrons does not vanish as the minority carrier density \( (n_-) \) goes to zero. The residual conductivity of \( (-) \) electrons at \( n_- = 0 \) is unique to graphene. We discuss experimental implications of our theory.

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Carrier transport properties of gated 2D graphene monolayers have been of active current interest \([1, 2, 3, 4, 5, 6, 7, 8]\), both for fundamental and technological reasons. From a fundamental perspective, understanding the mechanisms controlling graphene conductivity in experimental samples is of obvious importance. Such an understanding could lead to improvement in graphene mobilities, which in turn would help its eventual technological applications. The graphene chiral linear electron-hole capabilities, which in turn would help its eventual technologi-
der could either increase or decrease in the presence of spin-polarization. Remembering that graphene conductivity in the Boltzmann theory is given by \( \sigma \propto D_F \tau \), where \( \tau \) and \( D_F \propto \sqrt{g_s} \) are respectively the scattering time and the density of states at the Fermi level we conclude that if \( \tau \propto k_F^{-1} \) (i.e. if the disorder is independent of spin-polarization), then \( \sigma \propto g_s \), and it will always decrease (i.e. a positive magnetoresistance) in the presence of spin-polarization. When the disorder is spin-polarization dependent (either through the modification of \( k_F \) and/or \( q_F \)), the magnetoresistance could be either positive or negative. In particular, for the unscreened long-range disorder potential, \( V(q) \sim 1/q^n \), we have \( \sigma \propto g_s^{1-n} \). Note that for the bare Coulomb disorder \( (n = 1) \sigma \) remains a constant and does not depend on the spin polarization, implying no magnetoresistance.

Below we develop a detailed quantitative theory for the graphene parallel-field magnetoresistance in the presence of disorder arising from random charged impurity centers. This is because the screened charged impurity mobility is almost universally considered to be the dominant scattering mechanism in limiting graphene carrier mobility in currently available samples.

We find that the conductivity of intrinsic (i.e. undoped with \( E_F(B = 0) \) precisely at the Dirac point) graphene increases (i.e. negative magnetoresistance) with the applied magnetic field. For extrinsic graphene we find a positive magnetoresistance for \( B < B_s \) due to the magnetic field induced changes of the screening properties of graphene, where \( B_s \) is the field needed for full spin-polarization, and for \( B > B_s \) we find a negative magnetoresistance due to the depopulation of electrons in the valence band. This negative magnetoresistance in extrinsic graphene for \( B > B_s \), arising out of magnetic depopulation of the valence band, is the same qualitative effect which controls the negative magnetoresistance we find in intrinsic graphene.

We use the Boltzmann transport theory including only the effect of resistive scattering by random charged impurities [7]. The density of the random charged impurity centers is the only unknown parameter in our model, which sets the scale of the overall resistivity without affecting the \( \rho(B) \) dependence of interest in the problem. The Boltzmann conductivity of graphene at \( T = 0 \) is given by \( \sigma = e^2 v_F^2 D_F \tau(E_F)/2 \) where \( v_F \) is the Fermi velocity, \( D_F = g_s g_v \gamma^2 / (\hbar v_F) \) is the density of states at Fermi energy \( (g_s \text{ and } g_v \text{ are spin and valley degeneracy, respectively}) \), \( \tau(E_F) \equiv \tau \) is the transport relaxation time, and \( E_F = \gamma k_F \) the Fermi energy. The relaxation time is calculated in the Boltzmann theory as [11]

\[
\frac{1}{\tau(E_F)} = 4\pi n_i r_s^2 k_F \int_0^1 dx \frac{\sqrt{1-x^2}}{\epsilon(2k_Fx)^2},
\]

where \( k_F \) is the Fermi wave vector, \( n_i \) is the background random charged impurity density and \( r_s = e^2/\kappa \gamma \) (\( \kappa \) being the background dielectric constant) is the graphene fine-structure constant, and \( \epsilon(q) = 1 + v(q) \Pi(q) \) is the RPA dielectric function of the system, where \( v(q) = 2\pi e^2/\kappa q \) is the electron-electron 2D Coulomb interaction and \( \Pi(q) \) the 2D irreducible finite wave vector polarization function. When the system is spin unpolarized with a 2D carrier density, \( n \), the polarizability function becomes \( \Pi(q) = D_F P(q/k_F) \) [12], where

\[
P(x) = \begin{cases} 
1 & \text{if } x \leq 2 \\
1 + \frac{x^2}{8} - \frac{1}{2}\sqrt{1-\frac{4}{x^2}} - \frac{\pi}{4} \sin^{-1} \left( \frac{x}{2} \right) & \text{if } x > 2
\end{cases}
\]

Then the conductivity becomes

\[
\sigma = \frac{e^2 n}{h} n_i \frac{1}{2\pi n_i I(2\tau)}
\]

where \( I(x) \) is calculated to be [11]

\[
I(x) = \frac{\pi}{4} - \frac{d}{dx} \left[ x^2 g(x) \right]
\]

with

\[
g(x) = \frac{\pi}{2} x - 1 + \sqrt{1-x^2} \left\{ \begin{array}{ll} 
\text{sech}^{-1}(x) & \text{if } x \leq 1 \\
\sec^{-1}(x) & \text{if } x > 1
\end{array} \right.
\]

When the parallel magnetic field is applied, the carrier densities \( n_\pm \) for spin up/down are not equal. Note that the total density \( n = n_+ + n_- \) is fixed by the external gate. The spin-polarized densities themselves are obtained from the relative shifts (i.e. the spin-splitting) in the spin up and down bands introduced by the Zeeman splitting associated with the applied field \( B \). In this case the polarizability function becomes

\[
\Pi(q) = D_F^+ P(q/k_F^+) + D_F^- P(q/k_F^-)
\]

where \( D_F^+ \) and \( k_F^+ \) are the density of states at Fermi energy and the Fermi wave vector of spin up (down) state, respectively. Note that \( g_v (= 2 \text{ in the } B = 0 \text{ graphene case}) \) is not lifted, but the spin degeneracy, by definition, is lifted by the in-plane field \( B \). The usual unpolarized \( B = 0 \) paramagnetic state has \( k_F^- = k_F^+ = k_F \); \( n_+ = n_- = n/2 \).

By defining the spin-polarization parameter given by \( \xi = (n_+ - n_-)/n \) we can calculate the irreducible polarizability function in the case of unequal population of \( n_\pm \). (Eqs. (1)–(3) above apply to the \( \xi = 0 \) unpolarized situation.) In Fig. [11] we show the irreducible polarizability of the system for different spin-polarization parameter values. For unpolarized graphene (i.e. \( \xi = 0 \)) we have \( n_+ = n/2 \) and \( k_F^+ = \sqrt{2\pi n_+} = \sqrt{n} = k_F \). In this case the polarizability \( \Pi(q) \) is constant up to \( q = 2k_F \) and then increases with \( q \). For fully spin polarized system (i.e. \( \xi = 1 \)) we have \( n_+ = n \) and \( n_- = 0 \); \( k_F^+ = \sqrt{2\pi n} = \sqrt{2}k_F \) and \( k_F^- = 0 \). In this case \( \Pi(q)/D_F \) increases linearly up to \( q = 2k_F^+ \) with a slope \( (\pi/8)(k_F/k_F^-) = \pi\sqrt{2}/16 \) and
has a kink at $q = 2k_F^\pm$. For the partially polarized system, $0 < \xi < 1$, $\Pi(q)$ has two distinct kink points at $q = 2k_F^\pm$.

Now we calculate the conductivity in the presence of a parallel magnetic field for screened Coulomb disorder. In the presence of the magnetic field the total conductivity can be expressed as a sum of conductivities of spin up/down carriers, i.e., $\sigma = \sigma_+ + \sigma_-$, where $\sigma_\pm$ is the conductivity of the (±) spin subband, since the two spin channels are simply parallel transport channels as Coulomb scattering conserves the spin quantum number and therefore inter-spin-channel scattering is not allowed. The conductivities $\sigma_\pm$ are given by $\sigma_\pm = e^2v_F^2D_F^\pm(\varepsilon_F^\pm)/2$. In calculating the scattering times $\tau(\varepsilon_F^\pm)$ we have to use the two component polarizability given in Eq. (4). The total carrier resistivity $\rho$ is defined by $\rho = 1/\sigma$.

First, we consider intrinsic (i.e. undoped or un gated, with $n$ and $E_F$ both being zero) graphene where the conduction band is empty and the valence band fully occupied at $B = 0$. Applying a parallel magnetic field to intrinsic graphene would cause a shift of the chemical potential from the Dirac point, and therefore the spin polarized (+) electrons induced from the valence band will start to occupy the empty conduction band, leaving holes created in the valence band. (The situation is not dissimilar from what happens at $T \neq 0$.) The created intrinsic electron density, $n_-$, is the same as the intrinsic hole density, $n$, in the valence band, and the total density is proportional to the applied magnetic field ($B$), i.e. $n = p = g_v/(16\pi)(\Delta/\gamma)^2$, where $\Delta = g^*\mu_B B$ (with $g^*$ is electron spin g-factor and $\mu_B$ the Bohr magneton) being the Zeeman energy. Since both carriers contribute to the conductivity and $n = p$, we can calculate the total conductivity as $\sigma = e^2h\frac{n}{n_+}\frac{1}{I(2\pi\tau)}$. Since $n \propto B^2$, the calculated conductivity of intrinsic graphene increases quadratically with the applied magnetic field. Note that for this negative magnetoresistance phenomenon in intrinsic graphene as induced by the applied parallel field, spin-polarization itself does not play any role – the physics is dominated by the field-induced creation of electron-hole pairs which can then carry current.

In the case of extrinsic graphene (where $E_F(n \neq 0)$ an applied magnetic field produces different numbers of spin up (+) and down (−) electrons in the conduction band (or, for holes in the valence band) and we find

$$n_\pm = \frac{g_v}{4\pi\gamma^2}(\mu \pm \Delta/2)^2$$

where $\mu$ is the chemical potential, which is determined by conserving the total number of electrons, $n = n_+ + n_-$. Then we have $\mu(B) = \gamma\sqrt{\pi n}/1 - \delta^2/4$, where $\delta = \Delta/E_F$ and $E_F = \gamma k_F = \gamma\sqrt{\pi n}$ is the Fermi energy at $B = 0$ (unpolarized system). When $B = 0$ ($\Delta = 0$) we have $\mu = E_F$. We can relate the spin-polarization parameter $\xi$ to the applied magnetic field as $\xi = \delta/\sqrt{1 - \delta^2/4}$. At $\delta = \sqrt{2}$ the system is fully spin polarized (i.e. $\xi = 1$). Thus, the so-called saturation (or the spin-polarization) field for complete spin-polarization is given by $B_s = \sqrt{2}E_F/(g^*\mu_B)$, which is smaller by a factor of $\sqrt{2}$ than $B_s = 2E_F/(g^*\mu_B)$ for a 2D parabolic band dispersion. The conductivity of the partially polarized system can be calculated as

$$\sigma = \frac{e^2}{h}\frac{1}{n_+}\frac{1}{2\pi^2}\left[\frac{n_+}{I_+} + \frac{n_-}{I_-}\right],$$

where

$$I_{\pm} = \int_0^1 dx \frac{\sqrt{1 - x^2}}{e(2k_F^\pm x)^2}.$$

In Fig. 2 we show the calculated resistivity, $\rho = 1/\sigma$, as a function of spin polarization for $r_s = 0.85$ and 2.2 which correspond to graphene on SiO$_2$ substrate and vacuum. Note that we can represent the Fermi wave vectors as a function of the spin polarization, $k_F^\pm = k_F\sqrt{1 \pm \xi}$. The total resistivity increases as the spin polarization (or magnetic field) increases because of overall suppression of screening. At $\xi = 1$ (or $B = B_s$) we have

$$I_+ = \frac{1}{(1 + \pi r_s/4)^2}I\left(\frac{r_s}{1 + \pi r_s/4}\right),$$

and as $\xi \rightarrow 1$

$$I_- = \frac{1}{16\pi r_s^2}I_-.\frac{1}{n_-}.$$

Thus, as $\xi \rightarrow 1$, $n_\rightarrow 0$ and the scattering time of spin (−) electrons diverges as $1/n_\rightarrow$ because $\tau_\rightarrow \propto 1/I_\rightarrow$. This means that the conductivity of spin (−) electrons, $\sigma_\rightarrow n_-/I_\rightarrow$, is finite at $\xi = 1$ even though there is no spin down carrier. That is, we have $\sigma_\rightarrow(B_s) = \frac{e^2}{h}\frac{n_8}{2}$.
where \( \rho(0) \) is the resistance at \( B = 0 \). Inset shows the conductivities of each spin state. Note that the conductivity \( \sigma_- \) does not vanish at \( \xi = 1 \) (or \( B = B_1 \)). (b) Magnetoresistance at \( B_s \), \( \rho(B_s)/\rho(0) \), as a function of interaction parameter \( r_s \). (Note that \( r_s > 2.2 \) is not a physical regime.)

which is independent of the interaction parameter \( r_s \). This is a consequence of vanishing density of states of graphene as \( n \to 0 \) and the peculiarity of graphene screening properties, i.e. the contribution of interband transition to screening. We also show as an inset in Fig. 2 the calculated conductivities of each spin subband. As expected \( \sigma_- \) does not vanish as \( \xi \to 1 \). The result in Fig. 2(a) does not depend on the carrier density at \( B = 0 \). However, it is weakly dependent on the interaction parameter \( r_s \). The maximum magnetoresistance at \( B_s \) can be calculated as

\[
\frac{\rho(0)}{\rho(B_s)} = \frac{\sigma(B_s)}{\sigma(0)} = \frac{I_0}{I_+} + \frac{16\pi^2}{\pi} I_0,
\]

where \( I_0 = I(2r_s) \), and is shown in Fig. 2(b). As \( r_s \to 0 \) we have \( I_0, I_+ \to \pi/4 \), and the ratio becomes \( \rho(B_s)/\rho(0) \to 1 \). As \( r_s \to \infty \) \( I_0 \to 64r_s^2 \) and \( I_+ \to (16/\pi^2r_s^2)I(4/\pi) \), and the ratio becomes \( \rho(B_s)/\rho(0) \approx 1.22 \). Thus we always have positive magnetoresistance in extrinsic graphene as the applied in-plane magnetic field increases from 0 to \( B_s \). Note also that \( \rho(B_s)/\rho(0) \) has a shallow maximum at \( r_s \approx 0.5 \).

As the magnetic field increases beyond \( B_s \), i.e. \( B > B_s \), the number density of spin (+) state is given by

\[
n_+ = n + p = n + n \frac{1}{2} \frac{\delta^2}{\delta^2} \left( \frac{\delta^2}{2} - 1 \right)^2,
\]

where \( p \) is the induced hole density created in the valence band due to the magnetic field. In Fig. 3 we show the calculated resistivity of graphene as a function of magnetic field. A very interesting feature is the sharp decrease of resistivity for \( B > B_s \), which is unexpected, when compared with ordinary 2D systems where the resistivity saturates (or increases) for \( B > B_s \). In graphene, however, for \( B > B_s \), the calculated conductivity increases as \( B^2 \). This increasing conductivity for \( B > B_s \) in extrinsic graphene has exactly the same physical origin as the negative magnetoresistance we find for intrinsic graphene.

Given the nontrivial (and surprising) magnetoresistive behavior of graphene we predict in a parallel magnetic field, namely, negative magnetoresistance \( (\sigma(B) \sim B^2) \) in intrinsic graphene and positive magnetoresistance \( (\rho(B \ll B_s) \sim B^2) \) as well as negative magnetoresistance \( (\sigma(B \gg B_s) \sim B^2) \) for extrinsic graphene, a question naturally arises about the experimental observability of our predicted phenomenon. We believe that our predictions should be observable at low temperatures \((< 1K)\) in high-mobility graphene samples provided reasonable values of spin-polarization \((e.g. \xi = 0.5 \) or above) are achieved. Using \( g^* = 2 \) for graphene we find \( \Delta \approx 0.12B \) meV where \( B \) is measured in tesla. This leads to \( B_s(T) \approx 140\sqrt{n} \) where \( n \) is the graphene carrier density measured in unit of \( 10^{10} \) cm\(^{-2}\). Thus, for \( n = 10^8 \) cm\(^{-2}\), \( B_s \approx 14T \), which should enable a direct verification of our theory close to the charge neutrality point.

We anticipate \( g^* \) to be enhanced by electron-electron interaction effects, perhaps as much as by a factor of 2 for
\( r_s = 2.2 \), and therefore the necessary magnetic field values may be a factor 2 lower for free-standing graphene in vacuum than on a substrate. It seems that a verification (or falsification) of our predicted magnetoresistance behavior should be possible in high-mobility suspended graphene samples at low carrier densities \[13\]. This would help our understanding of the resistive mechanisms and the nature of disorder in graphene environment.

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