Optical Hall conductivity of gapped graphene

Antonio Hill, Andreas Sinner and Klaus Ziegler
Institut für Physik, Universität Augsburg, Universitätsstraße 1, D–86159 Augsburg, Germany

Abstract. We calculate the optical Hall conductivity for mono– and bilayer graphene within the Kubo formalism and demonstrate that the ratio of the jump in the Hall conductivity in bilayer graphene is twice the corresponding value of monolayer graphene. Furthermore, we find a characteristic logarithmic singularity as the frequency approaches the gap energy. The optical Hall conductivity is almost unaffected by thermal fluctuations and disorder in monolayer graphene. Only for bilayer graphene disorder has a stronger effect on transport properties.

PACS numbers: 81.05.ue, 72.80.Vp, 78.67.Wj

Monolayer graphene (MLG) is a monoatomic sheet of carbon atoms arranged in a honeycomb lattice with unique transport properties. This is a consequence of the two–dimensional nature of the material and due to the band structure which consists of two separate bands touching one another at isolated nodal points. In the vicinity of the nodal points quasiparticles exhibit a linear spectrum. The main difference between MLG and bilayer graphene (BLG) is that the low–energy excitations of the latter have a quadratic spectrum [1, 2]. For the longitudinal conductivity this difference causes a factor of 2 for the DC conductivity [3] and also for the optical conductivity [4]. This leads to the question how a change of the low–energy spectrum affects the quantum Hall properties of few layer graphene.

An intriguing phenomenon in graphene is the quantum Hall effect (QHE) which was already observed in the first experiments on graphene [5]. It exhibits a rather unexpected anomalous behavior. In contrast to the QHE in a two–dimensional electron gas of a semiconductor, the Hall plateaux appear antisymmetrically around zero carrier density [1]. Additionally, the magnitude of the Hall conductivity of the first plateau is for BLG twice the corresponding value of MLG [1]. This doubling of the Hall conductivity is similar to the above mentioned effect found for the longitudinal conductivity. An open question is whether or not the doubling appears also for the optical Hall conductivity. This shall be studied in the rest of this paper using the Kubo formalism.

It is widely accepted that the QHE occurs in semimetals as a consequence of a gap opening and broken time reversal symmetry. Usually, this is achieved by applying a magnetic field perpendicular to the 2D plane, whereas the gap opening alone can be obtained by hydrogenation of MLG [6] or by a double gate in the case of BLG [2].
Since the broken time reversal symmetry implies a broken symmetry between the two nodal points in MLG or BLG, we can study the QHE by assuming the absence of intervalley scattering and focusing only on one nodal point. Such a situation can be created by applying a periodic magnetic field \[7\] or a spin texture \[8\].

In the following we calculate the Hall conductivity for low–energy quasiparticles near a nodal point with a uniform gap and a power–law spectrum with an integer exponent. Then the low–energy Hamiltonian, describing electrons in graphene–like systems with a uniform gap \(\Delta = 2m\), reads in Fourier representation as

\[
H = \begin{pmatrix}
\frac{m}{(k_x + ik_y)^n} (k_x - ik_y)^n \\
-m
\end{pmatrix},
\]

where \(n = 1\) should be associated with MLG and \(n = 2\) with BLG. For general \(n\) the eigenvalues of the Hamiltonian are

\[
E_l = (-1)^l E, \quad E = \gamma \sqrt{m^2 + k^{2n}},
\]

where \(l = 0\) (\(l = 1\)) refer to the upper (lower) band, respectively. The corresponding eigenvectors are

\[
\psi^\pm_k (r) = \sqrt{\frac{E \mp m}{2E}} \left(\frac{(k_x - ik_y)^n}{\pm E - m} \right) \exp(i k \cdot r).
\]

The band parameter \(\gamma\) for MLG is \(\gamma = v_F\) \[9\] and for BLG \(\gamma = v_F^2/\gamma_1\) \[10\], where \(v_F\) is the Fermi velocity and \(\gamma_1 \approx 0.4eV\) is the interlayer coupling constant. To simplify the notation we drop indices for spin– and valley degeneracy and put \(\gamma\) equal to unity.

The Hall conductivity can be calculated as the off–diagonal element of the Kubo conductivity tensor \[4\]:

\[
\sigma_{\mu\nu} = \lim_{\alpha \to 0} \frac{i}{\hbar} \int \sum_{l,l'} \langle E_l|j_\mu|E_{l'}\rangle \langle E_{l'}|j_\nu|E_l\rangle \frac{f(E_{l'} - E_F) - f(E_l - E_F)}{E_l - E_{l'}} \frac{d^2k}{E_l - E_{l'} + \omega - i\alpha} \frac{1}{(2\pi)^2},
\]

where \(E_F\) represents the Fermi energy, \(f(E) = 1/(1 + \exp(\beta E))\) the Fermi–Dirac distribution at the inverse temperature \(\beta\) and \(\omega\) the frequency of the external field. The current operator

\[
j_\mu = ie[H, r_\mu]
\]

has vanishing diagonal elements. This is due to the fact that for \(\omega \neq 0\) the excitations \(E_l, E_{l'}\) satisfy \(|E_l - E_{l'}| = \omega\), and it is also reflected by vanishing intraband matrix elements. First we calculate current matrix elements defined in \(4\). Due to rotational symmetry of the model, the use of polar coordinates is more convenient. Since the angular variable enters only the current matrix elements, the corresponding integration can be carried out separately. Then we obtain for the intraband matrix elements

\[
\int_0^{2\pi} \langle \pm E|j_x| \pm E\rangle \langle \pm E|j_y| \pm E\rangle d\varphi = \\
4e^2 \int_0^{2\pi} n^2 k^{4n-2} \frac{\cos(\varphi) \sin(\varphi)}{4E^2} d\varphi = 0.
\]
The nonvanishing interband contribution of the matrix elements reads
\[
\int_0^{2\pi} \langle \pm E | j_x | \mp E \rangle \langle \mp E | j_y | \pm E \rangle d\varphi = \pm 2e^2 i\pi n^2 k^{2n-2} \frac{m}{E}.
\] (7)

In contrast to the calculation of the longitudinal optical conductivity in [4], the current matrix elements are now imaginary. In order to obtain the real part \(\sigma'_{\mu\nu}\) of \(\sigma_{\mu\nu}\) we have to evaluate a Cauchy principal value integral
\[
\sigma'_{\mu\nu} = \frac{i}{\hbar} \int \sum_{\nu \neq l} 2e^2 i\pi n^2 k^{2n-2} \frac{m}{E_l} \frac{1}{E_l - E_{l'}} \times \frac{f(E_{l'} - E_F) - f(E_l - E_F)}{E_l - E_{l'} + \omega} \frac{k dk}{(2\pi)^2}.
\] (8)

Substituting the \(k\) integration by an integration over the energy \(E = \sqrt{m^2 + k^{2n}}\), the corresponding Jacobian becomes
\[
J = \left( \frac{\partial E}{\partial k} \right)^{-1} = \frac{E}{nk^{2n-1}}.
\] (9)

All powers of \(k\) in the integrand cancel each other, such that the real part of the Hall conductivity reduces to the simple expression
\[
\sigma'_{xy} = \frac{ne^2}{\pi\hbar} \int_{|m|}^{\infty} \frac{f(-E - E_F) - f(E - E_F)}{4E^2 - \omega^2} dE.
\] (10)

The imaginary part is given by
\[
\sigma''_{xy} = \frac{ne^2}{\pi\hbar} \int_{|m|}^{\infty} \frac{f(-E - E_F) - f(E - E_F)}{2E} \times [\delta(2E + \omega) - \delta(2E - \omega)] dE.
\] (11)

In the limits \(T \to 0\) and \(E_F \to 0\) we obtain
\[
\sigma'_{xy} = \frac{n}{2} \frac{e^2 m}{\hbar} \ln \left| \frac{2m + \omega}{2m - \omega} \right|,
\] (12)
\[
\sigma''_{xy} = -\frac{ne^2}{\hbar} \frac{\omega}{\omega} \theta(\omega - 2m),
\] (13)

which reduces in the DC limit \(\omega \to 0\) to
\[
\sigma'_{xy} = \text{sgn}(m) \frac{n}{2} \frac{e^2}{\hbar}, \quad \sigma''_{xy} = 0.
\] (14)

This result was also found by Semenoff for \(n = 1\) [11]. Hence, the DC Hall conductivity is a nonzero constant proportional to the spectral power exponent \(n\). We would like to emphasize once again that the time reversal symmetry breaking is crucial for observing the QHE. If we had considered a second nodal point (i.e. with time reversal symmetry), the Hall conductivities from both cones would cancel each other.

For large \(\omega\) the optical Hall conductivity decays like \(\omega^{-1}\). Remarkable is the singularity at \(\omega = 2m\) in [12]. It appears when the external frequency \(\omega\) is equal to the gap of the electronic system. The latter means that there is an additional current contribution to the transport due to the excitation of states in the upper band. This
is a kind of resonance that disappears for higher frequencies. Moreover, instead of the singularity the longitudinal optical conductivity only jumps to a finite value at $\omega = 2m$. The singularity of the optical Hall conductivity could be used to determine the gap experimentally.

In figure 1 we show a plot of expression (10) as a function of $\omega$ and different temperatures. The Hall conductivity scales with $n$. This is in agreement with QHE experiments, where the plateau of BLG around zero carrier density is twice that of MLG. The temperature dependence is controlled by the energy scale of the corresponding system. In MLG, the relevant energy scale is the hopping parameter $t \approx 2.8eV$, which corresponds to a temperature $\approx 32.5 \times 10^3 K$. The relevant scale of BLG is even higher, since it is $\propto t^2/\gamma_1$. Therefore, expression (10) is insensitive over a wide range of temperatures $T \ll T_F$, as shown in figure 1. In particular, the gap singularity of the optical Hall conductivity survives. For very high temperatures, however, the Hall conductivity is reduced and goes eventually to zero. This is shown for fixed frequency $\omega$ in figure 2.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Temperature dependence of the Hall conductivity.}
\end{figure}

**Disorder:** We have seen that thermal fluctuations have almost no effect on the singularity at $\omega = 2m$. Since graphene is also subject to disorder effects (ripples, impurities, etc.), we study their influence on the singularity in the following. Returning to the Kubo formula (4), we can rewrite the conductivity as (cf. 13)

$$\sigma_{\mu\nu} = \lim_{\alpha \to 0} \frac{i}{\hbar} \int \int \frac{\langle Tr [j_\mu \delta(H_{dis} - \epsilon')j_\nu \delta(H_{dis} - \epsilon)] \rangle}{\epsilon - \epsilon' + \omega - i\alpha} \times f_\beta(\epsilon' - E_F) - f_\beta(\epsilon - E_F) d\epsilon d\epsilon', \quad (15)$$

where $\langle ... \rangle$ represents the disorder average. The latter can be approximated in the self-consistent Born approximation by replacing the Hamiltonian $H_{dis}$ by $\langle H_{dis} \rangle + i\eta$ 14. The average Hamiltonian $\langle H_{dis} \rangle$ is the same as the Hamiltonian in (1) and $\eta$ is the
Optical Hall conductivity of gapped graphene

Figure 2. Optical Hall conductivity near the singularity as a function of the inverse temperature $\beta$.

scattering rate caused by the disorder. This implies that we have to replace in (15) the Dirac delta functions by

$$\delta(H_{dis} - \epsilon) \rightarrow \delta_\eta(H - \epsilon) = \frac{i}{2\pi} \left[ (H - \epsilon + i\eta)^{-1} - (H - \epsilon - i\eta)^{-1} \right].$$  \hspace{1cm} (16)

In MLG the scattering rate is $\eta \propto \exp(\pi/g)$ \cite{15}, where $g$ is the variance of the random gap. In BLG, on the other hand, $\eta$ is proportional to the variance $g$, which implies that the influence of disorder on BLG is much stronger. Realistic fluctuations in graphene are less than a tenth of the hopping rate $g \approx 0.1$. This implies that a realistic scattering rate would be $\eta \approx 2 \times 10^{-14}$ (MLG) and $\eta \approx 0.1$ (BLG).

Now the trace can be expressed again in the diagonal representation as

$$\text{Tr} \left[ j_\mu \delta_\eta(H - \epsilon') j_\nu \delta_\eta(H - \epsilon) \right] =$$

$$\int \left\langle E_l | j_\mu | E_{l'} \right\rangle \left\langle E_{l'} | j_\nu | E_l \right\rangle \ \delta_\eta(E_l - \epsilon') \delta_\eta(E_{l'} - \epsilon) \frac{k \, dk}{(2\pi)^2}.$$

The angular integration can be carried out (cf. (7)) and transforming the $k$-integral to an energy integral gives

$$\sigma'_{xy} = \frac{e^2 \nu m}{2\pi \hbar} \int_{|\epsilon|}^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty \frac{f_\beta(\epsilon' - E_F) - f_\beta(\epsilon - E_F)}{\epsilon - \epsilon'} \frac{1}{\epsilon - \epsilon' + \omega}$$

$$\times \left[ \delta_\eta(E - \epsilon') \delta_\eta(-E - \epsilon) - \delta_\eta(-E - \epsilon') \delta_\eta(E - \epsilon) \right] d\epsilon d\epsilon' dE.$$

We evaluated expression (18) for $T = 0$ and $\mu = 0$ numerically for several values of $\eta$. The results are depicted for the real and imaginary part of the optical Hall conductivity in figures 3 and 4. One can see that the Hall plateaux remains nearly constant for all $\eta$ under consideration, whereas the singularity is broadened.

Conclusions: In this work we have studied the optical Hall conductivity of gapped graphene within a low–energy approximation. Our calculations indicate that the DC Hall conductivity in MLG and BLG only depends on the sign of the mass term and on
Figure 3. Real Part of the optical Hall conductivity for different values of the scattering rate $\eta$.

Figure 4. Imaginary part of the optical Hall conductivity for different values of the scattering rate $\eta$.

the exponent of the low–energy spectrum and it reproduces the experimentally observed factor of 2. Interesting is that the optical Hall conductivity is quite insensitive to thermal fluctuations over a wide range of temperatures. The effect of the curvature of the low–energy spectrum is also surprisingly simple: The optical Hall conductivity of MLG and BLG differ by a factor 2, as it was also found for the longitudinal optical conductivity. The same factor 2 appears in the visual transparency of MLG and BLG [12]. Interestingly, there is a logarithmic singularity in the optical Hall conductivity when the frequency $\omega$ of the external AC field becomes equal to the gap of the electronic system. The appearance of the singularity in our calculations is related to particle–hole excitations and can be interpreted as a resonance phenomenon. Although thermal fluctuations have no effect on this singularity, disorder may soften it in the case of
BLG, where the scattering rate can be large. In case of MLG, where the scattering rate is very small, the singularity of the optical Hall conductivity is almost unaffected. Consequently, the singularity could be used to determine the gap in MLG by measuring the optical Hall conductivity.

References

[1] Novoselov K S, McCann E, Morozov S V, Fal’ko V I, Katsnelson M I, Zeitler U, Jiang D, Schedin F and Geim A K 2006 Nat. Phys. 2 177
[2] Ohta T, Bostwick A, Seyller T, Horn K and Rotenberg E 2006 Science 313 951
[3] Cserti J 2007 Phys. Rev. B 75 033405
[4] Ziegler K and Sinner A 2010 arXiv:1001.3366v1
[5] Novoselov K S, Geim A K, Morozov S V, Jiang D, Zhang Y, Dubonos S V, Grigorieva I V and Firsov A A 2004 Science 306 666
[6] Elias D C, Nair R R, Mohiuddin T M G, Morozov S V, Blake P, Halsall M P, Ferrari A C, Boukhvalov D W, Katsnelson M I, Geim A K and Novoselov K S 2009 Science 323 610
[7] Haldane F D M 1988 Phys. Rev. Lett. 61 2015
[8] Hill A, Sinner A and Ziegler K 2011 New J. Phys. 13 035023
[9] Castro Neto A H, Guinea F, Peres N M R, Novoselov K S and Geim A 2009 Rev. Mod. Phys. 81 109
[10] McCann E and Fal’ko V I 2006 Phys. Rev. Lett. 96 086805
[11] Semenoff G W 1984 Phys. Rev. Lett. 53 2449
[12] Nair R R, Blake P, Grigorenko A N, Novoselov K S, Booth T J, Stauber T, Peres N M R and Geim A K 2008 Science 320 1308
[13] Ziegler K 2007 Phys. Rev. B. 75 233407
[14] Abergel D S L, Apalkov V, Berashevich J, Ziegler K and Chakraborty T 2010 Adv. Phys. 59 261
[15] Ziegler K 2009 Phys. Rev. B 79 195424