Bilayer graphene with long-range scatterers: Diamagnetism and weak-field Hall effect

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The diamagnetic susceptibility and the weak-field Hall conductivity are calculated for scatterers with nonzero range in bilayer graphene within a self-consistent Born approximation. The susceptibility exhibits a double-peak structure in the vicinity of zero energy. The Hall coefficient is given by the carrier concentration when the potential range is smaller or comparable to the Fermi wavelength, but becomes different when the range becomes larger than the Fermi wavelength. This deviation is not important in the case of charged impurities, but can become visible in the presence of environmental dielectric material.

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I. INTRODUCTION

Atomically thin graphenes consisting of a few layers of a monolayer graphite sheet are attracting much attention both theoretically and experimentally. Several reviews have already been published.\(^1\)\textsuperscript{--}\textsuperscript{4}\) Transport properties of graphenes were often studied in a self-consistent Born approximation assuming model short-range scatterers because of simplicity.\(^5\)\textsuperscript{--}\textsuperscript{11}\) Recently, such calculations were extended to the case of long-range scatterers in monolayer\(^1\textsuperscript{2}\)\textsuperscript{--}\textsuperscript{16}\) and bilayer graphenes.\(^1\textsuperscript{7}\) The purpose of this paper is to study the diamagnetic response and weak-field Hall effect in bilayer graphene in the presence of scatterers with nonzero range.

Intriguing electronic properties of graphene have been investigated mostly in flakes on SiO\(_2\) substrates with substantial disorder, exfoliated from bulk graphite.\(^1\textsuperscript{8}\) Quite recently, the quality of graphene was considerably improved by being suspended above substrates\(^1\textsuperscript{9}\)\textsuperscript{--}\textsuperscript{23}\) or transferred onto a boron nitride substrate.\(^2\textsuperscript{4}\)\textsuperscript{25}\) Further, graphenes grown on SiC\(^2\textsuperscript{6}\)\textsuperscript{--}\textsuperscript{30}\) or other substrates\(^3\textsuperscript{1}\)\textsuperscript{--}\textsuperscript{35}\) are now being intensively pursued for device applications and are subjected to various theoretical studies.\(^3\textsuperscript{6}\)\textsuperscript{37}\)

In graphenes, their electronic structure strongly varies with the change in the number of layers. The band structure of monolayer graphene is characterized by Dirac-like spectrum in which conduction and valence bands with linear dispersion stick at the \(K\) and \(K'\) points located at a Brillouin-zone corner.\(^1\)\textsuperscript{4}\textsuperscript{--}\textsuperscript{43}\) Bilayer graphene has a zero-gap structure, but with quadratic dispersion unlike monolayer, leading to nonzero density of states even at zero energy.\(^8\)\textsuperscript{,}\textsuperscript{10}\textsuperscript{,}\textsuperscript{44}\textsuperscript{--}\textsuperscript{49}\)

Various theoretical studies were reported on transport properties of bilayer graphene in different approximations.\(^4\textsuperscript{5}\)\textsuperscript{,}\textsuperscript{50}\textsuperscript{--}\textsuperscript{52}\) In this paper, we extend self-consistent Born approximation to the case of scatterers with nonzero range and study the diamagnetic response and the weak-field Hall effect. The approximation is known to work quite well although it breaks down when localization effects are dominant. We first consider scatterers with Gaussian potential to see explicit dependence on the potential range. In the case of charged impurities, we use the Thomas-Fermi approximation for screening.

The paper is organized as follows: In Sec. II, a brief review is given on the electronic states, a self-consistent Born approximation, formula for the diamagnetic susceptibility and the weak-field Hall conductivity, and the Boltzmann theory. In Sec. III model scatterers are introduced and some examples of numerical results are presented. The results are discussed in Sec. IV and short summary is given in Sec. V.

II. FORMULATION

A. Effective-mass description

We consider a bilayer graphene arranged in the AB (Bernal) stacking. Electronic states are described by the \(\mathbf{k}\cdot\mathbf{p}\) equation:\(^4\textsuperscript{4}\)

\[
\mathcal{H}_0(\mathbf{k})\mathbf{F}(\mathbf{r}) = \varepsilon \mathbf{F}(\mathbf{r}),
\]

with

\[
\mathcal{H}_0(\mathbf{k}) = \begin{pmatrix}
0 & \gamma \hat{k}_- & 0 & 0 \\
\gamma \hat{k}_+ & 0 & \Delta & 0 \\
0 & \Delta & 0 & \gamma \hat{k}_- \\
0 & 0 & \gamma \hat{k}_+ & 0
\end{pmatrix},
\]

and

\[
\hat{k}_\pm = \hat{k}_x \pm i\hat{k}_y,
\]

where \(\gamma\) is a band parameter, \(\mathbf{k} = (\hat{k}_x, \hat{k}_y) = -i\nabla\) is a wave-vector operator, and \(\Delta\) represents the inter-layer coupling between nearest-neighbor sites.

The parameters \(\gamma\) and \(\Delta\) are related to tight-binding parameters \(\gamma_0\) and \(\gamma_1\) through \(\gamma = (\sqrt{3}/2)a\gamma_0\) and \(\Delta = \gamma_1\), where \(a\) is the lattice constant given by \(a = 2.46\ \text{Å}\), \(\gamma_0 \approx 3.16\ \text{eV}\),\(^5\textsuperscript{3}\) and \(\gamma_1 \approx 0.39\ \text{eV}\).\(^5\textsuperscript{4}\) Couplings between vertically neighboring atoms are known to cause trigonal warping and four band touching points at zero energy in
the energy scale of a few meV.\textsuperscript{8,44} Such a structure can easily be washed out in actual bilayer graphenes with disorder\textsuperscript{8} and will be neglected in the following.

The states are specified by the set of quantum numbers \((j, k)\), with \(k\) wave vector and \(j = 1, 2, 3, 4\) specifying bands in the order of increasing energy. The wave function is written as
\[
F_{jk}(r) = \frac{1}{L} \exp(ik \cdot r)U[\theta(k)]F_{jk},
\]
where \(L^2\) is the area of the system, \(k = |k|, k_x = k \cos \theta(k), k_y = k \sin \theta(k),\) and
\[
U(\theta) = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & e^{i\theta} & 0 & 0 \\
0 & 0 & e^{2i\theta} & 0 \\
0 & 0 & 0 & e^{3i\theta}
\end{pmatrix}.
\]
Then, \(F_{jk}\) satisfies
\[
\mathcal{H}_0(k)F_{jk} = \varepsilon_j(k)F_{jk},
\]
with
\[
\mathcal{H}_0(k) = \begin{pmatrix}
0 & \gamma_k & 0 & 0 \\
\gamma_k & 0 & \Delta & 0 \\
0 & \Delta & 0 & \gamma_k \\
0 & 0 & \gamma_k & 0
\end{pmatrix}.
\]
The density of states becomes
\[
D(\varepsilon) = \frac{g_v g_s e^2}{2\pi^2 \varepsilon^2 \Delta^2} \left[ \frac{\Delta}{2} + \varepsilon + \theta(\varepsilon - \Delta) \left| \varepsilon - \frac{\Delta}{2} \right| \right],
\]
where the spin and valley degeneracies are given by \(g_s = 2\) and \(g_v = 2\), respectively, and \(\theta(t)\) is the step function defined by
\[
\theta(t) = \begin{cases}
1 & (t > 0); \\
0 & (t < 0).
\end{cases}
\]

\section*{B. Self-consistent Born approximation}

Let us consider Green’s function defined by
\[
\hat{G}(k, \varepsilon) = \begin{pmatrix}
\frac{1}{\varepsilon - \bar{H}} \\
\varepsilon - \mathcal{H}_0(k) - \hat{\Sigma}(k, \varepsilon)
\end{pmatrix}^{-1},
\]
with
\[
\bar{H} = \mathcal{H}_0 + \sum_j v(r - r_j),
\]
where \(\langle \cdot \cdot \cdot \rangle\) denotes average over impurity configurations, \(\hat{\Sigma}(k, \varepsilon)\) is the self-energy matrix, and \(v(r)\) is the potential of scatterers. We consider scatterers with isotropic potential
\[
v(r) = \int \frac{dq}{(2\pi)^2} v(q) e^{iq \cdot r},
\]
where \(v(q) = v(q)\) with \(q = |q|\). Within the self-consistent Born approximation, we have
\[
\hat{\Sigma}(k, \varepsilon) = n_i \int \frac{dk'}{(2\pi)^2} v(k - k') \hat{G}(k', \varepsilon) v(k' - k),
\]
where \(n_i\) is the impurity concentration per unit area.

\section*{C. Diamagnetic susceptibility}

A theoretical scheme to calculate the diamagnetic susceptibility was developed by Fukuyama.\textsuperscript{55} It gives the following expression valid in bilayer graphene within the \(k\-\mathbf{p}\) scheme.\textsuperscript{9,50,56,57}
\[
\chi = \int_{-\infty}^{\infty} d\varepsilon \left( - \frac{\partial J(\varepsilon)}{\partial \varepsilon} \right) \chi(\varepsilon),
\]
\[
\chi(\varepsilon) = \int_{-\infty}^{\varepsilon} d\varepsilon' \left( - \frac{1}{\pi} \right) \text{Im} F(\varepsilon + i0),
\]
with
\[
F(\varepsilon) = \frac{g_v g_s e^2}{2h^2L^2} \text{Tr} \left( \frac{1}{\varepsilon - \bar{H}} \hat{H}_s \hat{H}_y \hat{H}_s \frac{1}{\varepsilon - \bar{H}} \hat{H}_y \frac{1}{\varepsilon - \bar{H}} \hat{H}_s \frac{1}{\varepsilon - \bar{H}} \hat{H}_y \right),
\]
where
\[
\hat{H}_x = \frac{\partial \bar{H}}{\partial k_x} = \gamma \hat{v}_x, \quad \hat{H}_y = \frac{\partial \bar{H}}{\partial k_y} = \gamma \hat{v}_y.
\]

The Feynman diagrams for the susceptibility are shown in Fig. 1. The contributions of diagrams (a), (b), and (c) are denoted by \(F^{(a)}, F^{(b)},\) and \(F^{(c)}\), respectively. Then, we have
\[
F(\varepsilon) = F^{(a)}(\varepsilon) + F^{(b)}(\varepsilon) - F^{(c)}(\varepsilon) = 2F^{(a)}(\varepsilon) - F^{(c)}(\varepsilon),
\]
where use has been made of \(F^{(a)} = F^{(b)}\) in the second equality.

The contribution of diagram (a) of Fig. 1 becomes
\[
F^{(a)}(\varepsilon + i0) = \frac{g_v g_s e^2}{2h^2} \int \frac{dk}{(2\pi)^2} \text{Tr} \hat{G}(k, \varepsilon + i0) \times \hat{J}_x(k, \varepsilon + i0, \varepsilon + i0) \hat{J}_y(k, \varepsilon + i0, \varepsilon + i0)
\]
\[
\times \hat{G}(k, \varepsilon + i0) \hat{J}_x(k, \varepsilon + i0, \varepsilon + i0) \hat{J}_y(k, \varepsilon + i0, \varepsilon + i0),
\]
in terms of current vertices \(\hat{J}_x\) and \(\hat{J}_y\) and double-current vertex \(\hat{J}_{xy}\), satisfying a Bethe-Salpeter-type equation shown in Fig. 1. Further, we have
\[
F^{(c)}(\varepsilon + i0) = \frac{g_v g_s e^2}{2h^2} \int \frac{dk}{(2\pi)^2} \text{Tr} \hat{G}(k, \varepsilon + i0) \times \hat{J}_x(k, \varepsilon + i0, \varepsilon + i0) \hat{J}_y(k, \varepsilon + i0, \varepsilon + i0)
\]
\[
\times \hat{G}(k, \varepsilon + i0) \hat{J}_x(k, \varepsilon + i0, \varepsilon + i0) \hat{J}_y(k, \varepsilon + i0, \varepsilon + i0),
\]
\[
\chi(\varepsilon) = \frac{g_v g_s e^2}{4\pi h^2 c^2} \left( \Delta - |\varepsilon| - \frac{1}{3} \right).
\]
It satisfies
\[ \int_{-\infty}^{\infty} \chi(\varepsilon) d\varepsilon = -g_0g_{\varepsilon}e^2c^2/3\pi\hbar^2c^2, \] (23)
i.e., twice as large as that in monolayer graphene. This sum rule is shown to be satisfied even in the presence of disorder by making arguments similar to those in the mono-layer graphene. In fact, it is satisfied by numerical results shown below within sufficient accuracy.

**D. Weak-field Hall conductivity**

A theoretical scheme to calculate the weak-field Hall conductivity proportional to applied magnetic field was also developed by Fukuyama. In the present system, it is given by
\[ \sigma_{xy} = \int \left( -\frac{\partial f(\varepsilon)}{\partial \varepsilon} \right) \sigma_{xy}(\varepsilon) d\varepsilon, \] (24)
with
\[ \sigma_{xy}(\varepsilon) = \sigma'_{xy}(\varepsilon) + \sigma''_{xy}(\varepsilon), \] (25)
where
\[ \sigma'_{xy} = \frac{g_0g_{\varepsilon}e^2}{\pi\hbar^2} H_{xy}(\varepsilon), \] (26)
\[ \sigma''_{xy} = \frac{g_0g_{\varepsilon}e^2}{\pi\hbar^2} 2 \int_{0}^{\varepsilon} H'_{xy}(\varepsilon) d\varepsilon'. \] (27)

Here, we have defined
\[ H_{xy}(\varepsilon) = \frac{1}{L^2} \text{Im} \text{Tr} \left[ \hat{H}_x \hat{G}(\varepsilon + i0) \hat{H}_x \hat{G}(\varepsilon + i0) \right], \] (28)
and \( l \) is the magnetic length given by \( l = \sqrt{\hbar/\varepsilon B} \), where \( B \) is the strength of magnetic field \( \mathbf{B} \) perpendicular to the system. Figure 2 shows the diagrams for (a) \( H_{xy}(\varepsilon) \) and (b) \( H'_{xy}(\varepsilon) \). We have
\[ H_{xy}(\varepsilon) = H_{xy}^{(a)}(\varepsilon) + H_{xy}^{(b)}(\varepsilon) - H_{xy}^{(c)}(\varepsilon), \] (30)
\[ H'_{xy}(\varepsilon) = H'_{xy}^{(a)}(\varepsilon) + 2H'_{xy}^{(b)}(\varepsilon) + 2H'_{xy}^{(c)}(\varepsilon) - H'_{xy}^{(f)}(\varepsilon) \]
\[ -2H'_{xy}^{(g)}(\varepsilon) - 2H'_{xy}^{(h)}(\varepsilon) + H'_{xy}^{(k)}(\varepsilon), \] (31)
where use has been made of \( H_{xy}^{(e)} = H_{xy}^{(a)} \), \( H_{xy}^{(d)} = H_{xy}^{(c)} \), \( H_{xy}^{(i)} = H_{xy}^{(g)} \), and \( H_{xy}^{(j)} = H_{xy}^{(h)} \).

For example, we have
\[ H_{xy}^{(a)}(\varepsilon) = \gamma^4 \int \frac{dk}{(2\pi)^2} \text{Im} \text{Tr} \left[ \hat{G}(k, \varepsilon - i0) \hat{J}_x(k, \varepsilon - i0) \hat{G}(k, \varepsilon + i0) \hat{J}_x(k, \varepsilon + i0) \hat{G}(k, \varepsilon + i0) \hat{J}_y(k, \varepsilon + i0, \varepsilon + i0) \hat{G}(k, \varepsilon + i0) \hat{J}_y(k, \varepsilon + i0, \varepsilon + i0), \right. \] (32)
and have similar expressions for \( H_{xy}^{(b)} \) and \( H_{xy}^{(c)} \). Further, we have
\[ H_{xy}^{(a)}(\varepsilon) = \gamma^4 \int \frac{dk}{(2\pi)^2} \text{Im} \text{Tr} \hat{G}(k, \varepsilon + i0) \hat{J}_x(k, \varepsilon + i0) \hat{G}(k, \varepsilon + i0, \varepsilon + i0) \hat{J}_x(k, \varepsilon + i0, \varepsilon + i0) \hat{G}(k, \varepsilon + i0) \hat{J}_y(k, \varepsilon + i0, \varepsilon + i0), \] (33)
and
where vertex $\tilde{J}_1$ satisfies the following Bethe-Salpeter-type equation:
\[
\tilde{J}_1(k, \varepsilon, \varepsilon') = 1 + n_1 \int \frac{dk'}{(2\pi)^2} \left( \hat{v}(k - k') \tilde{G}(k', \varepsilon) \tilde{J}_1(k', \varepsilon, \varepsilon') \times \tilde{G}(k', \varepsilon') \hat{v}(k' - k) \right)
\]
Similar expressions can be written down for other terms of $H'_{xy}$. The diagonal conductivity is written as
\[
\sigma = \int d\varepsilon \left( -\frac{\partial f}{\partial \varepsilon} \right) \sigma(\varepsilon),
\]
with
\[
\sigma(\varepsilon) = -\frac{g_v e^2 \gamma^2}{4\pi\hbar} \sum_{s,s'=\pm 1} \int \frac{dk}{(2\pi)^2} \text{Tr} \hat{v}_s \tilde{G}(k, \varepsilon + is0) \times \tilde{J}_s(k, \varepsilon + is0) \tilde{G}(k, \varepsilon + is'0).
\]
The Hall coefficient is given by
\[
R_H = \frac{\sigma_{xy}}{B \sigma_z}.
\]

\section{Boltzmann Hall conductivity}

Let us define $g_{jk}$ as deviation of the distribution function of states $(j, k)$ to the lowest order in applied electric field $E$. Then, the Boltzmann equation is given by
\[
(-e)E \cdot v_{jk}(\varepsilon) \left( -\frac{\partial f}{\partial \varepsilon(\varepsilon)} \right) = \sum_j \int \frac{dk'}{(2\pi)^2} \frac{2\pi}{\hbar} |V_{j'k'}| \delta(\varepsilon - \varepsilon'(k)) \left[ (g_{jk} - g_{j'k'}) - \frac{e}{\hbar} (v_{jk} \times B) \frac{\partial g_{jk}}{\partial k} \right],
\]
where $V$ is the impurity potential and $v_{jk}$ is the group velocity $v_{jk} = (k/k)\epsilon_j$ with
\[
v_j = \frac{\partial \varepsilon_j(k)}{\hbar \partial k}.
\]
First, we shall write
\[
g_{jk} = (-e)\tau_j(\varepsilon) v_{jk} \cdot \left( \alpha_j E + \beta_j \frac{B}{B} \times E \right) \left( -\frac{\partial f}{\partial \varepsilon_j(k)} \right),
\]
with relaxation time $\tau_j$ and appropriate dimensionless coefficients $\alpha_j$ and $\beta_j$, to be determined in the following.
In the absence of a magnetic field, we have $\beta_j = 0$, and setting $\alpha_j = 1$,

$$\sum_{j'} \Gamma_{j j'}^{(0)}(\epsilon) - \Gamma_{j j'}^{(1)}(\epsilon) \tau_j(\epsilon) = \sum_{j' \neq j} \Gamma_{j j'}^{(1)}(\epsilon) \frac{\nu_{j' \tau j'}}{\nu_{j'}} \tau_j(\epsilon) = 1. \quad (41)$$

with

$$\Gamma_{j j'}^{(n)}(\epsilon) = \int \frac{dk'}{(2\pi)^2} \frac{2\pi}{\hbar} |V_{j'k',jkl}|^2 \delta[\epsilon - \epsilon_{\tau j'}(k')] \cos(n\theta_{kk'}), \quad (42)$$

where $\theta_{kk'}$ is the angle between $k'$ and $k$. Formally, we can solve the above equations as

$$\tau_j = \sum_{j'} \left[ \hat{\Omega}(\epsilon)^{-1} \right]_{jj'}, \quad (43)$$

with

$$\left[ \hat{\Omega}(\epsilon) \right]_{jj'} = \begin{cases} \sum_{j'} \Gamma_{j j'}^{(0)}(\epsilon) - \Gamma_{j j'}^{(1)}(\epsilon) & (j' = j); \\ -\Gamma_{j j'}^{(1)}(\epsilon) \frac{\nu_{j' \tau j'}}{\nu_{j'}} & (j' \neq j). \end{cases} \quad (44)$$

In magnetic field, we have

$$\sum_{j'} \Omega_{jj'}(\epsilon) \tau_j(\epsilon) \omega_j + \omega_j \tau_j \beta_j = 1, \quad (45)$$

$$\sum_{j'} \Omega_{jj'}(\epsilon) \tau_j(\epsilon) \omega_j - \omega_j \tau_j \alpha_j = 0, \quad (46)$$

where we have defined the cyclotron frequency:

$$\omega_j = \frac{eH \nu_j}{\hbar} k_j. \quad (47)$$

with $\epsilon_{\tau j}(k_j) = \epsilon$. Let us define a diagonal matrix $\hat{\omega}(\epsilon) = (\omega_j)$. Then, we have formally

$$\tau_j \alpha_j = \sum_{j'} \left[ \hat{\Omega} + \hat{\omega} \hat{\Omega}^{-1} \hat{\omega} \right]_{jj'}, \quad (48)$$

$$\tau_j \beta_j = \sum_{j'} \left[ \hat{\Omega} - \hat{\omega} \hat{\Omega}^{-1} \hat{\omega} \right]_{jj'}. \quad (49)$$

The conductivity tensor becomes

$$\sigma_{xx}(\epsilon) = \frac{g_e g_h}{2} \sum_{j} D_j(\epsilon) e^2 \tau_j(\epsilon) \alpha_j(\epsilon) v_j(\epsilon)^2, \quad (50)$$

$$\sigma_{xy}(\epsilon) = -\frac{g_e g_h}{2} \sum_{j} D_j(\epsilon) e^2 \tau_j(\epsilon) \beta_j(\epsilon) v_j(\epsilon)^2. \quad (51)$$

with partial density of states for band $(j,k)$

$$D_j(\epsilon) = \int \frac{dk}{(2\pi)^2} \delta[\epsilon - \epsilon_j(k)]. \quad (52)$$

To the lowest order in the strength of the magnetic field, we have

$$\alpha_j = 1, \quad \tau_j \beta_j = \sum_{j'} \left[ \hat{\Omega}^{-1} - \hat{\omega} \hat{\Omega}^{-1} \hat{\omega} \right]_{jj'}, \quad (53)$$

$$\tau_j \beta_j \beta_j = \sum_{j'} \left[ \hat{\Omega}^{-1} \hat{\omega} \hat{\Omega}^{-1} \hat{\omega} \right]_{jj'}. \quad (54)$$

giving the zero-field diagonal conductivity and the weak-field Hall conductivity.

### III. NUMERICAL CALCULATIONS

#### A. Scatterers with Gaussian potential

In order to see the explicit dependence on the potential range, we first assume scatterers with Gaussian potential

$$v(r) = \frac{\epsilon_0}{4\pi d^2} \exp \left(-\frac{r^2}{d^2}\right), \quad (55)$$

with range $d$. We define a dimensionless parameter characterizing the scattering strength

$$W = \frac{\nu_0 \epsilon_0^2}{4\pi \gamma^2}. \quad (56)$$

where $n_i$ is the concentration of scatterers per unit area. This parameter is the same as that defined previously for short-range scatterers with $d \to 0$ ($W = \gamma^{-1}$ in Refs. 5–7)

For such scatterers with isotropic potential, the dependence on the direction of the wave vector can be eliminated by a unitary matrix (5) as has previously been shown. Therefore, the self-consistency equation for the self-energy and Bethe-Salpeter-type equations can be written only for the absolute value $k$ of the wave vector $k$. These equations can be solved by discretizing $k$ and by introducing cutoff energy $\epsilon_c$ and wave vector $k_c$ with $\epsilon_c = \gamma k_c$. Details are described in Ref. 17. The cutoff energy $\epsilon_c$ and wave vector $k_c$ through $\epsilon_c = \gamma k_c$ is chosen as $\epsilon_c \approx \gamma_0$ ($\approx 3$ eV), corresponding to the region where the linear dispersion is approximately valid. Further, we choose $\Delta/\epsilon_c = 0.1$ and introduce wave vector $k_0$ characterizing the energy difference between the lowest and excited conduction band such that

$$\gamma k_0 = \Delta. \quad (57)$$

Is should be noted that the actual value of cutoff $\epsilon_c$ is irrelevant as long as it is sufficiently larger than typical energy scale $\Delta$ because states with higher energy do not contribute to physical quantities for long-range scatterers.

#### B. Charged scatterers

We consider charged impurities with screening effect included in a Thomas-Fermi approximation. The potential is

$$v(q) = \frac{2\pi e^2}{\kappa(q + q_s)}, \quad (58)$$

where $\kappa$ is the static dielectric constant, which is chosen to be 2.5 in the following, and $q_s$ is the Thomas-Fermi screening constant given by

$$q_s = \frac{2\pi e^2}{\kappa} D(\epsilon_F), \quad (59)$$
at zero temperature. The scattering strength is a function of the density of states at the Fermi level and therefore should be determined in a self-consistent manner for each Fermi level. Further, in order to obtain the carrier concentration, we have to calculate the density of states below the Fermi level for each Fermi level. To characterize the impurity concentration, we introduce

$$n_{\Delta} \equiv \frac{g_s g_v \Delta^2}{2\pi \gamma^2}, \quad (60)$$

which corresponds to the electron concentration in the lowest conduction band for the Fermi level at $\Delta$, i.e., the bottom of the excited conduction band.

### C. Diamagnetic susceptibility

Some examples of calculated diamagnetic susceptibility and density of states for scatterers with Gaussian potential are shown in Fig. 3. Here, the unit of the susceptibility is chosen as

$$\chi_{\Delta} \equiv \frac{e^2 \gamma^2}{c^2 h^2 \Delta}, \quad (61)$$

One important feature is that the peak at zero energy slightly splits into two. The behavior is essentially independent of the potential range. The amount of the splitting becomes smaller corresponding to the fact the peak itself becomes sharper with the decrease of disorder $W$, but does not disappear even for $W = 0.01$, although not shown here. A possible origin of the splitting will be discussed in a next section.

In the case of long-range potential $dk_0 > 1$, effects of scattering are important only in the vicinity of zero

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**FIG. 3:** An example of calculated diamagnetic susceptibility (solid lines) and density of states (dotted lines) for scatterers with Gaussian potential. (a) $W = 0.02$ and (b) $W = 0.05$.

**FIG. 4:** (Color online) Calculated diamagnetic susceptibility (solid lines) and density of states (dotted lines) for charged scatterers screened in the Thomas-Fermi approximation.
energy and the bottom of the excited conduction band. As a result, the susceptibility becomes different from the ideal case only in these energy regions. In the short-range case \( \Delta k_0 < 1 \), on the other hands, states are almost equally affected independent of the energy and the susceptibility has a long tail for \( |\epsilon| > \Delta \). The results show that the sum rule (23) is satisfied within numerical accuracy.

Figure 4 shows the susceptibility and the density of states for charged scatterers screened in the Thomas-Fermi approximation. Because the screening becomes stronger and the disorder becomes weaker with the increase of the Fermi energy, the double-peak feature near zero energy is enhanced, but the susceptibility quickly vanishes for \( |\epsilon| > \Delta \) in agreement with the ideal result. A double-peak feature was also obtained in monolayer graphene. The sum rule (23) is not satisfied and the integral becomes smaller with the impurity concentration, because the effective scattering strength strongly varies as a function of the Fermi level.

D. Weak-field Hall effect

First, we show in Fig. 5 the comparison between \( \sigma'_{xy}(\epsilon) = \sigma'_{xy}(\epsilon) + \sigma''_{xy}(\epsilon) \) and \( \sigma'_{xy}(\epsilon) \) (dotted lines) for scatterers with Gaussian potential with disorder \( W = 0.05 \). The unit of the Hall conductivity is chosen as \( W^2 \sigma^\Delta_{xy} \) with

\[
\sigma^\Delta_{xy} = \frac{\gamma_0 e^2}{2\pi \hbar} \left( \frac{2\pi}{k_{\text{F}}} \right)^2 .
\]

FIG. 5: (Color online) Comparison between \( \sigma_{xy}(\epsilon) = \sigma'_{xy}(\epsilon) + \sigma''_{xy}(\epsilon) \) (solid lines) and \( \sigma'_{xy}(\epsilon) \) (dotted lines) for scatterers with Gaussian potential. \( W = 0.05 \). ‘\( \times 4 \)’ and ‘\( \times 40 \)’ mean that the actual results should be multiplied by 4 and 40, respectively. Contributions of \( \sigma''_{xy}(\epsilon) \) can practically be neglected.

FIG. 6: (Color online) Calculated weak-field Hall conductivity (solid lines) compared with the Boltzmann result for scatterers with Gaussian potential. \( W = 0.05 \).

FIG. 7: (Color online) The inverse Hall coefficient \( R_{H}^{-1} \) (solid lines) as a function of the carrier concentration for scatterers with Gaussian potential. The dotted lines represent corresponding Boltzmann results.
The figure shows that contributions of $\sigma^\prime_{xy}(\varepsilon)$ can practically be neglected and that $\sigma_{xy}$ is determined by $\sigma^\prime_{xy}(\varepsilon)$ which is given by the Green’s function and current vertex functions at the Fermi level. This feature is independent of potential range $d$ and $W$, and considerably simplifies actual calculations of the Hall conductivity. In the following, therefore, we shall show only $\sigma_{xy} \approx \sigma^\prime_{xy}$, completely neglecting $\sigma^\prime\prime_{xy}$.

Figure 6 shows the comparison with the Boltzmann result. It is interesting to note that the absolute value lies smaller than the Boltzmann results. This difference becomes larger with the potential range and with the increase in the Fermi level. This feature is quite in contrast to the diagonal conductivity calculated in Ref. 17, which is enhanced over the Boltzmann conductivity.

Figure 7 shows the inverse Hall coefficient $R_H^{-1}$ as a function of the carrier concentration. It is approximately in proportion to the carrier concentration except in the very vicinity of zero energy with a coefficient close to unity for short-range scatterers and becoming larger with the potential range. This tendency is closely related to the enhancement of the diagonal conductivity and the reduction in the absolute value of the Hall conductivity in comparison with the Boltzmann conductivities, as mentioned above. Possible origins of such behavior are discussed in the next section.

Figure 8 shows some examples of weak-field Hall conductivity (solid lines) and diagonal conductivity (dotted lines) for charged scatterers screened in the Thomas-Fermi approximation. The unit of the carrier concentration is chosen as $n_\Delta$ introduced in Eq. (60). When the Fermi level lies in the lowest conduction band, both the diagonal conductivity and the absolute value of the Hall conductivity are enhanced over the corresponding Boltzmann results. When the Fermi level goes into the excited conduction band, on the other hand, the Hall conductivity is reduced, while the diagonal conductivity remains enhanced, although the deviations from the Boltzmann results are smaller.

Figure 9 shows the corresponding inverse Hall coefficient $R_H^{-1}$ as a function of the carrier concentration. It is well approximated by the carrier concentration except in the vicinity of zero energy. When the energy is lowered from the positive direction toward zero energy, $R_H^{-1}$ takes a maximum, then decreases, and diverges to negative infinity. The electron concentration corresponding to the maximum increases roughly in proportion to the impurity concentration.

**IV. DISCUSSION**

In monolayer graphene, the susceptibility becomes a singular delta-function at zero energy in the absence of disorder.\cite{38,63-65}\ In bilayer graphene, the delta-function is broadened into a logarithmic function within the energy region $-\Delta < \varepsilon < +\Delta$. Because the energy integral is twice of that in monolayer graphene, the susceptibility approaches a delta function twice as large as in monolayer in the limit $\Delta \to 0$. In monolayer graphene,
peak splitting appears only when the disorder is sufficiently large for scatterers with Gaussian potential and always appears for charged impurities mainly due to self-consistent screening. In bilayer graphene, on the other hand, the susceptibility seems to exhibit a double-peak structure independent of kinds of scatterers. The splitting is not reproduced when a simple energy-independent relaxation time is introduced.

It is likely that the splitting is related to the strong energy dependence of the broadening near zero energy. In the vicinity of zero energy, the electron wavelength becomes much larger than the range of the impurity potential and therefore scatterers are essentially regarded as of short-range. Then, the energy-dependence of the broadening is determined by that of the density of states. As shown in the insets in Fig. 3, the deviation of the density of states from that in the ideal bilayer graphene shows ‘singular’ dependence on the energy, roughly corresponding to the double-peak structure of the susceptibility.

As has been discussed in the previous section, there is the clear tendency that, for long-range scatterers with Gaussian potential, the absolute value of the Hall conductivity is smaller than the Boltzmann result, while the diagonal conductivity becomes larger. There can be various reasons causing this feature. First, the present system consists of conduction and valence bands degenerate at zero energy corresponding to $k = 0$ even when the Fermi level lies below the first excited conduction band. Therefore, we cannot a priori expect that the Boltzmann result based on a single-band picture is valid. Further, there remain significant amounts of interband elements for the vector potential associated with magnetic field, and therefore, the effect of the magnetic field cannot be fully incorporated in the form of the Lorentz force determined by the velocity expectation value. In fact, the singular orbital susceptibility is not described by such semi-classical approach at all and requires a full quantum-mechanical treatment of off-diagonal interband terms.

Another plausible reason lies in the big difference between the lifetime and transport relaxation time. For long-range scatterers, there remains considerable energy broadening due to scattering near the forward direction almost independent of energy, while the transport relaxation time, determined dominantly by backward scattering, becomes very long and increases rapidly with energy.

Because of considerable broadening, there can be wide distribution of states contributing to the current in applied electric field for a fixed Fermi level. In fact, states with higher $k$ in the field direction within the broadened spectrum significantly contributes to the current because of smaller backward scattering probability. As a result, the conductivity becomes larger than the Boltzmann conductivity when the Fermi wavelength becomes smaller than the potential range.

In the presence of magnetic field, such states are slightly deflected in the direction perpendicular to the electric field due to the Lorentz force. However, this perpendicular motion is easily pushed back by near-forward
scattering by long-range scatterers. As a result, those states making extra contributions to the diagonal conductivity do not contribute to the Hall current, leading to the reduction of the Hall conductivity.

For more realistic charged impurities, the Hall coefficient is essentially determined by the carrier concentration, in agreement with experiments. For the Coulomb scattering, its potential range is always comparable to the Fermi wavelength because of screening except that the effective potential range becomes larger than the Fermi wavelength due to the reduction of the screening constant. In the presence of dielectric environment material, however, the effective potential range remains smaller than the Fermi wavelength due to the reduction of the screening constant. There have been experimental reports in which graphene is covered by liquid with high dielectric constant, but the results remain controversial and further it is likely that extra sources of scattering are induced by highly polarizable liquid.

One important feature of bilayer graphene is that the band structure can be strongly modified due to opening of a band gap by applied electric field. The present formulation is also applicable to bilayer graphene with nonzero gap, as has been used for calculations of the density of states and the conductivity. The application to the present problem, requiring considerable computation time due to the fact that the effective potential range remains smaller than the Fermi wavelength, is left for a future work.

V. SUMMARY

The diamagnetic susceptibility and the weak-field Hall conductivity have been calculated for scatterers with nonzero range in the self-consistent Born approximation. The self-energy and current vertex functions explicitly depend on the wave vector and become (4,4) matrices. Corresponding self-consistent equations have been numerically solved for scatterers with Gaussian potential with varying range and for charged impurities with screened Coulomb potential within the Thomas-Fermi approximation.

For scatterers with Gaussian potential, the diamagnetic susceptibility is close to that of an ideal bilayer graphene except in the vicinity of zero energy and the bottom of the excited conduction band. Important feature is the peak splitting near zero energy. The behavior is essentially independent of the potential range and the amount of the splitting becomes smaller with the decrease of disorder W. For charged impurities, this peak splitting is enhanced due to the self-consistent determination of the screening constant within the Thomas-Fermi approximation.

For long-range scatterers with Gaussian potential, the absolute value of the Hall conductivity becomes smaller than the Boltzmann result in contrast to the diagonal conductivity becoming larger. As a result, the Hall coefficient deviates from $-n_e e c$ for long-range scatterers. For charged impurities, such deviation is not appreciable because the effective potential range remains smaller than the Fermi wavelength due to screening effect. In the presence of dielectric environment material, however, the deviation becomes appreciable because of the reduction in the screening constant.

FIG. 12: (Color online) Calculated inverse Hall coefficient for charged scatterers in the presence of dielectric material on top of bilayer graphene.
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