Valley Hall Conductivity in Graphene: Effects of Higher-Order Scattering

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(Dated: February 1, 2018)

The valley Hall conductivity, having opposite signs between the K and K’ valleys, is calculated in monolayer and bilayer graphenes with nonzero gap in the presence of short-range scatterers within a single-site approximation. In the case of small disorder, the Hall conductivity is quantized into \( \pm e^2/2h \) and \( \pm e^2/h \) in the monolayer and bilayer graphene, respectively, in the gap region, while it is enhanced over the results in the absence of scatterers in the band region. With the increase in the strength of each impurity potential, large asymmetry between the conduction and valence band appears. For scatterers with attractive potential, the disorder parameter is effectively enhanced and reduced in the conduction and valence band, respectively. The behavior is opposite for repulsive scatterers.

Effects of skew scattering causing asymmetry in the scattering direction remain small and do not play significant role.

Keywords: impurity scattering, skew scattering, topological Hall effect, topological current

I. INTRODUCTION

Graphenes are attracting much attention as discussed in several reviews.\(^1\)–\(^6\) The electron motion in monolayer graphene is described by Weyl’s equation for a neutrino or the Dirac equation in the relativistic limit.\(^7\)–\(^11\) When graphene is placed on a certain substrate material, potential difference appears between two sublattice points, giving rise to band-gap opening.\(^12\)–\(^17\) Bilayer graphene has a zero-gap structure, but with quadratic dispersion unlike monolayer.\(^18\)–\(^20\) A gap is opened in a perpendicular electric field due to a gate voltage.\(^21\)–\(^24\) In the presence of a gap, the Hall conductivity in each of the K and K’ valleys becomes nonzero even in the absence of a magnetic field, although its sign is opposite between the valleys and the total Hall conductivity vanishes.\(^25\)–\(^35\) The purpose of this paper is to study this valley Hall conductivity in disordered graphenes, taking into account effects of higher order scattering.

Recent experiments succeeded in detection of valley Hall currents in monolayer graphene on boron-nitride substrate\(^36\) and gated bilayer graphene.\(^37,38\) A zero-field Hall voltage was observed in MoS\(_2\) monolayers in the presence of valley polarization induced by illumination of circularly polarized light.\(^39\) Similar Hall voltage should be observed in graphene in a perpendicular electric field due to a gate voltage. In the presence of a gap, the Hall conductivity in each of the K and K’ valleys becomes nonzero even in the absence of a magnetic field, although its sign is opposite between the valleys and the total Hall conductivity vanishes.\(^25\)–\(^35\) The purpose of this paper is to study this valley Hall conductivity in disordered graphenes, taking into account effects of higher order scattering.

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II. MONOLAYER GRAPHENE

In a graphene sheet, a unit cell contains two carbon atoms, usually denoted by A and B, and the conduction and valence bands consisting of \( \pi \) orbitals cross at K and K’ points of the Brillouin zone, where the Fermi level is located.\(^54,55\) Electronic states of the \( \pi \)-bands near a K point are described by the \( \mathbf{k} \cdot \mathbf{p} \) equation.\(^7\)–\(^11\)

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

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

with \( \mathbf{k}_\pm = k_x \pm ik_y \), where \( \mathbf{F}(\mathbf{r}) \) is a two-component wave function, \( \varepsilon \) is energy, \( \mathbf{k} = (k_x, k_y) = -i \nabla \) is a wave-vector operator, and \( \gamma \) is a band parameter, given by \( \gamma = (\sqrt{3}/2)a\gamma_0 \) with \( a \) the lattice constant (2.46 Å) and \( \gamma_0 \) the nearest-neighbor hopping integral (\( \sim 3 \) eV).

In the above matrix Hamiltonian, the bases are the Bloch functions of the K point localized at the A and B sites of a unit cell and the diagonal terms \( \pm \Delta \) represent potential asymmetry between the A and B sites, which opens an energy gap \( 2|\Delta| \) at \( \mathbf{k} = 0 \).\(^27,56\) We can safely assume \( \Delta \geq 0 \) without loss of generality. The energy bands are

\[
\varepsilon_s(\mathbf{k}) = s\sqrt{\gamma^2 k^2 + \Delta^2},
\]

in this paper, effects of higher order scattering on the valley Hall conductivity are studied in graphenes with short-range scatterers.

The paper is organized as follows: In Sect. II, the method of calculations and some examples of numerical results are presented in monolayer graphene after a brief discussion on the appearance of small ‘skew scattering’. In Sect. III, results for bilayer graphene are presented. A short discussion and summary are given in Sect. IV. A brief discussion is made on broad resonance for strong scatterers in Appendix A.
where $k = |k|$ and $s = +1$ and $-1$ for the conduction and valence band, respectively, and the wave functions are

$$F_{+k}(r) = \begin{pmatrix} \cos \varphi_k \\ e^{i\theta_k} \sin \varphi_k \end{pmatrix} e^{ikr}, \quad (4)$$

$$F_{-k}(r) = \begin{pmatrix} -\sin \varphi_k \\ e^{i\theta_k} \cos \varphi_k \end{pmatrix} e^{ikr}, \quad (5)$$

with $k = k(\cos \theta_k, \sin \theta_k)$ and $\tan(2\varphi_k) = \gamma k/\Delta$. The corresponding density of states is given by

$$D(\varepsilon) = \frac{g_v g_s |e|}{2\pi\gamma^2} \theta(\varepsilon^2 - \Delta^2), \quad (6)$$

where $g_v (=2)$ is the valley degeneracy associated with the K and K' valleys, $g_s (=2)$ is the spin degeneracy, and

$$\theta(t) = \begin{cases} 1 & \text{if } t > 0; \\ 0 & \text{if } t < 0. \end{cases} \quad (7)$$

Let us consider a scatterer with a delta-potential

$$\hat{V}(r) = u \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \delta(r), \quad (8)$$

with strength $u$. This model potential corresponds to a scatterer with potential range larger than the lattice constant but shorter than the effective electron wavelength.\(^5\) In the vicinity of zero energy, the wavelength is infinitely large and the model can describe most of dominant scatterers including charged impurities.\(^5\)

When the range is smaller than the lattice constant, as in the case of lattice defects, the diagonal elements become different, but, at the same time, intervalley scattering between the K and K' points plays significant roles.\(^6\) The corresponding $T$ matrix satisfies

$$\hat{T}(\varepsilon) = \hat{V} + \hat{V} \frac{1}{\varepsilon - \hat{H}_0 + i0} \hat{T}(\varepsilon). \quad (9)$$

In the wave-vector space, $(2,2)$ matrix $\hat{T}_{kk'}(\varepsilon)$ becomes independent of $k$ and $k'$ and

$$\hat{T}(\varepsilon) = u \begin{pmatrix} 1 - u & 1 \\ (2\pi)^2 (\varepsilon - \hat{H}_0 + i0)^{-1} \end{pmatrix}^{-1} \begin{pmatrix} u_1(\varepsilon) & 0 \\ 0 & u_2(\varepsilon) \end{pmatrix}, \quad (10)$$

where

$$u_1(\varepsilon) = \frac{u}{1 - u} G^{(0)}_{11}(\varepsilon), \quad u_2(\varepsilon) = \frac{u}{1 - u} G^{(0)}_{22}(\varepsilon). \quad (11)$$

Here, we have introduced cutoff energy $\varepsilon_c$, roughly corresponding to the maximum energy where the band can approximately be regarded as a linear function of $k$.

The scattering strength between states $k$ and $k'$ in the conduction band ($s = +1$), having a same energy, becomes

$$|\langle k' | \hat{T}(\varepsilon) | k \rangle|^2 = |u_1|^2 \cos^2 \varphi + |u_2|^2 \sin^2 \varphi + \frac{1}{2} |\text{Re}(u_1 u_2^*) \cos \theta - \text{Im}(u_1 u_2^*) \sin \theta|^2 \sin^2 2\varphi, \quad (14)$$

with $\varphi \equiv \varphi_k = \varphi_{k'}$ and $\theta = \theta_{k'} - \theta_k$. We can define the various components of the effective scattering strength,

$$T_{00}^2 \equiv \langle \langle k' | \hat{T}(\varepsilon) | k \rangle \rangle^2 \theta, \quad (15)$$

$$T_{01}^2 \equiv \langle \langle k' | \hat{T}(\varepsilon) | k \rangle \rangle^2 (1 - \cos \theta) \theta, \quad (16)$$

$$T_{22}^2 \equiv 2 \langle \langle k' | \hat{T}(\varepsilon) | k \rangle \rangle^2 \sin^2 \theta \theta, \quad (17)$$

where $\langle \cdot \cdot \rangle_\theta$ represents the average over the scattering angle $\theta$. $T_{00}^2$ corresponds to the level broadening, $T_{01}^2$ to the transport relaxation time, and $T_{22}^2$ to the intensity of skew scattering, giving asymmetry between $\theta > 0$ and $\theta < 0$.

We have

$$T_{22}^2 = -\frac{1}{2} \text{Im}(u_1 u_2^*) \sin^2 2\varphi. \quad (18)$$

In the lowest Born approximation, $T_{22}^2 = 0$ because $u_1 = u_2 = u$. The skew scattering becomes nonzero only when higher order processes are considered. In the absence of a gap, i.e., $\Delta = 0$, we have $u_1 = u_2 \uparrow$ up to the higher order because of $G^{(0)}_{11} = G^{(0)}_{22}$, showing

$$|\langle k' | \hat{T}(\varepsilon) | k \rangle|^2 = \frac{1}{2} |u_1|^2 (1 + \cos \theta). \quad (19)$$

The above shows the absence of backscattering (vanishing scattering for $\theta = \pi$). $T_{00}^2 = T_{01}^2 = 0$, and $T_{22}^2 = 0$.

Let us consider the case of weak scattering potential and the energy region close to the conduction-band bottom, i.e., $\varepsilon \gtrsim \Delta$. Then, we have $G^{(0)}_{11} \gg G^{(0)}_{22}$ and

$$u_1 \approx u_{11} \approx u_1 + u_1 G^{(0)}_{11}, \quad u_2 \approx u_1, \quad (20)$$

$$T_{22}^2 \approx -\frac{1}{2} u^3 \text{Im} G^{(0)}_{11} \sin^2 2\varphi. \quad (21)$$

Furthermore, we have

$$\text{Im} G^{(0)}_{11} \approx -\frac{2\pi \Delta}{4\pi \gamma^2}, \quad \sin 2\varphi \approx \sqrt{\frac{2(\varepsilon - \Delta)}{\Delta}}, \quad (22)$$

giving

$$T_{22}^2 \approx \frac{u^3 (\varepsilon - \Delta)}{2\gamma^2}. \quad (23)$$

This shows that the skew scattering changes its direction depending on the sign of $u$.\(^6\)
Then, we have $\theta_j = 0$. Furthermore, because scatterers are assumed to cause no intervalley scattering and also to be not so strong, we have $d > a$ and $u_0 \ll \gamma_0$. Then, the parameter should not be too large, i.e., $|u_0| \lesssim 1$.

Figure 1(a) shows some examples of the scattering strength $|\langle \mathbf{k}'|\tilde{T}(\varepsilon)|\mathbf{k}\rangle|^2$ as a function of the scattering angle $\theta$ in the case of $\tilde{u} = -1$. The cutoff energy is chosen as $\Delta/\varepsilon_c = 0.005$. The results are dependent on $\Delta/\varepsilon_c$ only weakly, i.e., logarithmically. The scattering strength is larger in the conduction band than in the valence band. The reason lies in the fact that $u < 0$ corresponds to an impurity with attractive potential for the conduction band and to that with repulsive potential for the valence band. For an attractive potential, the electron wave function tends to have large amplitude at the impurity due to higher order perturbations, enhancing the scattering strength, while the hole wave function becomes smaller, reducing the scattering strength.

The scattering for $\theta < 0$ is slightly larger than for $\theta > 0$ in the conduction band ($\varepsilon > 0$), in agreement with Eq. (23), while the behavior is opposite in the valence band ($\varepsilon < 0$). In the whole energy region $-2.5 < \varepsilon/\Delta < 2.5$, the asymmetry between $\theta > 0$ and $\theta < 0$, i.e., the skew scattering, remains very small.

Figure 1(b) shows some examples of the components of the effective scattering strength as a function of the energy. The asymmetry of $T_2^2$ and $T_1^2$ between the conduction and valence bands becomes more and more prominent with the increase of $|\tilde{u}|$. Furthermore, with the increase of $|\varepsilon|$ the skew scattering component becomes larger than Eq. (23) in the conduction band and smaller in the valence band. The results for $u > 0$ can be obtained by replacing $\varepsilon$ with $-\varepsilon$, i.e., by the mirror reflection with respect to $\varepsilon = 0$. The direction of the skew scattering is closely related to the enhancement and the reduction of the effective scattering strength in higher orders as will be discussed in Sect. IV.

As can clearly be seen for $\tilde{u} = -2$ in Fig. 1(b), the absolute values of $T_0^2$, $T_1^2$, and $T_2^2$ increases with energy for $\varepsilon/\Delta \gg 1$. This corresponds to the appearance of a very broad resonance similar to that discussed previously for

![Diagram](image-url)
lattice defects. This will be briefly discussed in Appendix A. Similar calculations for the K’ point show that the scattering strength is given by Eq. (14) except that θ is replaced with −θ. Therefore, T₀^3 and T₁^3 are the same, but the skew scattering is exactly opposite between the K and K’ points.

We consider a disordered system with scatterers:

$$\mathcal{H} = \sum_i \hat{V}(r-r_i),$$

where $\hat{V}(r)$ is defined in Eq. (8) and $r_i$ represents the position of $i$th impurity. As already mentioned above, the model describes most of dominant scatterers in the vicinity of zero energy, where we are interested in. Within a single-site approximation or self-consistent t-matrix approximation, we consider the diagrams shown in Fig. 2 for (2, 2) matrix self-energy $\Sigma(k, \varepsilon)$ of (2, 2) matrix Green’s function $\hat{G}(k, \varepsilon)$.

FIG. 2: A diagrammatic representation of (a) the self-energy in a single-site approximation for scatterers with short-range potential and (b) the Bethe-Salpeter-type equation for the vertex function. $v_\mu$ can be one of $v_x, v_y, v_\perp$, and 1.

The self-energy becomes independent of $k$ and becomes

$$\hat{\Sigma}(\varepsilon) = n_i u \left[ 1 - u \int \frac{dk'}{(2\pi)^2} \hat{G}(k', \varepsilon) \right]^{-1},$$

with

$$\hat{G}(k, \varepsilon) = [\varepsilon - \hat{H}_0(k) - \hat{\Sigma}(\varepsilon)]^{-1} \equiv \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix},$$

where $n_i$ is the impurity concentration. In this approximation, effects of higher order scattering at a single impurity are exactly taken into account. Obviously, the self-energy becomes diagonal and is written as

$$\hat{\Sigma}(\varepsilon) = \begin{pmatrix} \Sigma_0(\varepsilon) + \Sigma_1(\varepsilon) & 0 \\ 0 & \Sigma_0(\varepsilon) - \Sigma_1(\varepsilon) \end{pmatrix}.$$  (29)

The self-consistency equations are

$$\Sigma_0 = \frac{1}{2} \left[ \frac{n_i u}{1 - u G_{11}} + \frac{n_i u}{1 - u G_{22}} \right],$$

$$\Sigma_1 = \frac{1}{2} \left[ \frac{n_i u}{1 - u G_{11}} - \frac{n_i u}{1 - u G_{22}} \right].$$  (30)
FIG. 4: The diagrammatic representation of the valley Hall conductivity $\sigma'_{xy}(\varepsilon)$, $\sigma''^{(a)}_{xy}(\varepsilon)$, and $\sigma''^{(b)}_{xy}(\varepsilon)$ in the single-site approximation.

The vertex functions satisfy Bethe-Salpeter type equations shown in Fig. 2(b). Following the procedure previously described, the solutions are obtained as

$$J_\pm(\varepsilon, \varepsilon') = J_\pm(\varepsilon, \varepsilon') \tilde{v}_\pm, \quad (42)$$

where $J_\pm(\varepsilon, \varepsilon')$ satisfies

$$J_+(\varepsilon, \varepsilon') = 1 + J_+(\varepsilon, \varepsilon') \frac{n_1 u^2 \mathcal{G}_{11,22}(\varepsilon, \varepsilon')}{[1 - u \mathcal{G}_{11}(\varepsilon)][1 - u \mathcal{G}_{22}(\varepsilon')]} \quad (43)$$

$$J_-(\varepsilon, \varepsilon') = 1 + J_-(\varepsilon, \varepsilon') \frac{n_1 u^2 \mathcal{G}_{22,22}(\varepsilon, \varepsilon')}{[1 - u \mathcal{G}_{22}(\varepsilon)][1 - u \mathcal{G}_{11}(\varepsilon)']} \quad (44)$$

Here, we have defined

$$\mathcal{G}_{ijk}(\varepsilon, \varepsilon') = \int \frac{dk}{(2\pi)^3} G_{ij}(k, \varepsilon) G_{kl}(k, \varepsilon'), \quad (45)$$

where $i, j, k, l$ are either 1 or 2. In terms of $J_\pm$, the conductivity is diagrammatically given by Fig. 3. It is explicitly calculated as

$$\sigma(\varepsilon) = \frac{g_0 e^2 \varepsilon}{\pi \hbar} \text{Re} \left[ J_+(\varepsilon, \varepsilon') \mathcal{G}_{22,22}(\varepsilon, \varepsilon') \right] \quad (46)$$

where $J_+(\varepsilon, \varepsilon') = J_+(\varepsilon + i0, \varepsilon - i0)$, etc., for simplicity.

The formal expression of the valley Hall conductivity has been given in a previous paper. Within the single-site approximation, it is written as

$$\sigma_{xy}(\varepsilon) = \sigma'_{xy}(\varepsilon) + \sigma''^{(a)}_{xy}(\varepsilon), \quad (47)$$

$$\sigma_{xy}''(\varepsilon) = \sigma''^{(a)}_{xy}(\varepsilon) + \sigma''^{(b)}_{xy}(\varepsilon), \quad (48)$$

where each term is represented by diagrams shown in Fig. 4. In the clean-limit with sufficiently small disorder, $\sigma'_{xy}$ gives the quantized value $-e^2/2h$ in the gap and a vanishingly small contribution in the band continuum, while $\sigma''_{xy}$ remains nonzero only outside the gap. The diagram $\sigma''^{(b)}_{xy}$, explicitly depending on the sign of $u$ as the skew scattering, appears only when effects of higher order scattering are included.

The Hall conductivity for electrons near the K' point is given by the same expression as the K point except that the sign is opposite. Therefore, the total Hall conductivity vanishes as expected, when the K and K' points are equally populated by electrons, i.e., without valley polarization.

The vertex function $J_0(\varepsilon) \equiv J_0(\varepsilon + i0, \varepsilon - i0)$ is written as

$$J_0(\varepsilon) = \begin{pmatrix} J_1(\varepsilon) & 0 \\ 0 & J_2(\varepsilon) \end{pmatrix}, \quad (49)$$

with

$$\begin{pmatrix} J_1(\varepsilon) \\ J_2(\varepsilon) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{n_1 u^2 \mathcal{G}_{11,11}}{[1 - u \mathcal{G}_{11}(\varepsilon)]} \begin{pmatrix} J_1(\varepsilon) \\ J_2(\varepsilon) \end{pmatrix} + \frac{n_1 u^2 \mathcal{G}_{12,21}}{[1 - u \mathcal{G}_{11}(\varepsilon)]} \begin{pmatrix} J_1(\varepsilon) \\ J_2(\varepsilon) \end{pmatrix} \quad (50)$$

The final formulas for the Hall conductivity are given by

$$\sigma'_{xy}(\varepsilon) = \frac{g_0 e^2 \varepsilon}{\hbar} \text{Im} \left[ J_+(\varepsilon, \varepsilon') \mathcal{G}_{22,22}(\varepsilon, \varepsilon') \right] \quad (51)$$

$$\sigma''^{(a)}_{xy}(\varepsilon) = \frac{2g_0 e^2 \varepsilon}{\hbar} \int_{-\infty}^{\infty} d\varepsilon' \text{Im} \left[ J_+(\varepsilon, \varepsilon') \mathcal{G}_{11,22}(\varepsilon, \varepsilon') \right] \quad (52)$$

$$\sigma''^{(b)}_{xy}(\varepsilon) = \frac{2g_0 e^2 \varepsilon}{\hbar} \int_{-\infty}^{\infty} d\varepsilon' \text{Im} \left[ J_+(\varepsilon, \varepsilon') \mathcal{G}_{11,22}(\varepsilon, \varepsilon') \right] \quad (53)$$

with

$$\mathcal{G}_{ijk}(\varepsilon, \varepsilon') = \int \frac{dk}{(2\pi)^3} G_{ij}(k, \varepsilon) G_{kl}(k, \varepsilon') G_{mn}(k, \varepsilon), \quad (54)$$

where $i, j, k, l, m, n$ are either 1 or 2.

Figure 5 shows some examples of numerical results for $u < 0$, corresponding to attractive and repulsive potential for the conduction and valence band, respectively. As shown in Figs. 5(a) for $W = 0.02$, (c) for $W = 0.05$, and (e) for $W = 0.09$, the conductivity exhibits large asymmetry between the conduction and valence bands with
FIG. 5: (Color online) Some examples of numerical results in monolayer graphene for $\Delta / \varepsilon_c = 0.005$. The density of states and the conductivity are shown in (a), (c), and (e), and the valley Hall conductivity in (b), (d), and (f). The results in the self-consistent Born approximation are denoted by $\bar{u} = 0$. (a) and (b) $W = 0.02$. (c) and (d) $W = 0.05$. (e) and (f) $W = 0.09$. The origin of the vertical axis is shifted depending on $\bar{u} \equiv u \varepsilon_c / (4 \pi \gamma^2)$. 
the increase of \( |\tilde{u}| \). In fact, the conductivity is reduced in the conduction band and enhanced in the valence band in comparison with the results in the self-consistent Born approximation denoted by \( \tilde{u} = 0 \). On the other hand, the density of states is slightly enhanced in the conduction band and reduced in the valence band, although not so apparent for the clean case of \( W = 0.02 \) shown in (a).

The valley Hall conductivity shown in Figs. 5(b), (d), and (f) also exhibits some asymmetry between the conduction and valence bands. In fact, the enhancement over the ideal result outside the band-gap region is slightly reduced from that in the Born approximation in the conduction band and enhanced in the valence band for \( W = 0.02 \), as shown in (b). The asymmetry becomes less obvious with the increase of \( W \) as shown in (d) and (f). For large \( W = 0.09 \) shown in (f), for which the gap has disappeared, the valley Hall conductivity near zero energy becomes smaller than the ideal result, but the enhancement persists for sufficiently large \( |\tilde{u}| \), although not shown in the figure.

The numerical results show that the contribution of \( n^{(0)}_{xy}(\epsilon) \) in the band continuum is smaller than the line width of total \( \sigma_{xy}(\epsilon) \) in Fig. 5. The reason is likely to lie in the fact that \( n^{(0)}_{xy} \) itself has vanishingly small contribution in the band region as mentioned before and that the skew-scattering component is small as shown in Fig. 1. Roughly speaking, effects of higher order scattering can be understood in terms of effective enhancement and reduction of disorder parameter \( W \) in the conduction and valence band, respectively, depending on \( |\tilde{u}| \) for \( u < 0 \). Therefore, effects of skew scattering are not important in the range of parameter \( \tilde{u} \) considered here.

The skew scattering may become important for larger \( |\tilde{u}| \), for which resonance-like features appear even in the band continuum, as discussed in Appendix A. However, the present model using the \( \mathbf{k} \cdot \mathbf{p} \) Hamiltonian may be insufficient for strong scatterers, and effects of such resonance will not be discussed here.

### III. BILAYER GRAPHENE

In bilayer graphene, electronic states in the vicinity of the K point are described by the Hamiltonian\(^{18-20}\)

\[
H_0 = \begin{pmatrix}
\epsilon F d/2 & \gamma k_- & 0 & 0 \\
\gamma k_+ & \epsilon F d/2 & \gamma_1 & 0 \\
0 & \gamma_1 & -\epsilon F d/2 & \gamma k_- \\
0 & 0 & \gamma k_+ & -\epsilon F d/2
\end{pmatrix}, \quad (55)
\]

where \( \gamma_1 \approx 0.4 \, \text{eV} \) represents the strength of the interlayer coupling,\(^{71} \) \( F \) is the effective electric field between the layers, and \( d \) is the interlayer distance. In asymmetric bilayer graphene with nonzero \( F \), a gap is opened and the lowest conduction band and the highest valence band exhibit a dispersion like a Mexican hat near \( k = 0 \).

There are other parameters describing interlayer interactions. Most of them slightly modify the band structure except \( \gamma_3 \), which causes trigonal warping and four band touching points at zero energy in the energy scale of a few meV.\(^{18,19} \) Such a structure is easily washed out in the presence of large disorder.\(^{19} \) In the following, therefore, interlayer parameters other than \( \gamma_1 \) will be neglected. Then, except that the Hamiltonian becomes a \((4,4)\) matrix, calculations for the density of states, the conductivity, and the Hall conductivity are made exactly in the same manner as in the monolayer graphene.

Figure 6 shows some examples of numerical results for \( u < 0 \). Qualitative features of the results including the asymmetry between the conduction and valence bands are essentially the same as in the monolayer graphene. In fact, as shown in (a) for \( W = 0.03 \), (c) for \( W = 0.05 \), and (e) \( W = 0.1 \), the conductivity exhibits large asymmetry between the conduction and valence bands with the increase of \( |\tilde{u}| \). The density of states is slightly enhanced in the conduction band and reduced in the valence band.

As shown in (b) and (d), the enhancement of the valley Hall conductivity over the ideal result outside the band-gap region is slightly reduced from that in the Born approximation denoted by \( \tilde{u} = 0 \) in the conduction band and becomes larger in the valence band. Roughly speaking, effects of higher order scattering can be understood simply in terms of effective enhancement or reduction of \( W \) in the conduction and valence bands, respectively. The contribution of \( n^{(b)}_{xy}(\epsilon) \) is again smaller than the line width of total \( \sigma_{xy}(\epsilon) \) in Fig. 6, although not explicitly shown here. Therefore, effects of skew scattering are not important in the range of parameter \( \tilde{u} \) considered here, the same as in the monolayer graphene.

### IV. DISCUSSION AND SUMMARY

As has been discussed in previous papers,\(^{52,53} \) the origin of the valley Hall conductivity can be ascribed to a circular cyclotron motion present even in the absence of a magnetic field in graphene with a gap. In the monolayer graphene, for example, the effective magnetic field for the K valley causing this cyclotron motion is given by \( B_\text{eff} = \Delta / \mu_\text{B}^2 \) with \( \mu_\text{B} = e \hbar / (2m^* c) \) and \( m^* = h^2 / (2\Delta \gamma^2) \). The effective magnetic field has an opposite sign for the K’ valley. As is clear in Fig. 1, the skew scattering has the tendency to slightly increase the cyclotron radius or weaken the cyclotron motion in the conduction band and to slightly reduce the cyclotron radius or strengthen the cyclotron motion in the valence band for \( u < 0 \). This can be seen also in Eq. (23).

The case of \( u < 0 \) corresponds to an impurity with attractive potential for the conduction band and to that with repulsive potential for the valence band. For an attractive potential, the wave function tends to have large amplitude at the impurity due to higher order perturbations, enhancing the scattering strength over the result in the lowest Born approximation. For a repulsive potential, on the other hand, the wave function becomes smaller, reducing the scattering strength.

The skew scattering may be understood as scattering effects on the cyclotron motion itself. In the lowest Born approximation, the cyclotron motion is interrupted by...
FIG. 6: (Color online) Some examples of numerical results in bilayer graphene for $eFd/\gamma_1 = 0.5$. The density of states and the conductivity are shown in (a), (c), and (e), and the valley Hall conductivity in (b), (d), and (f). The results in the self-consistent Born approximation are denoted by $\tilde{u} = 0$. (a) and (b) $W = 0.03$. (c) and (d) $W = 0.05$. (e) and (f) $W = 0.1$. The origin of the vertical axis is shifted depending on $\tilde{u} \equiv u_c / (4\pi\gamma^2)$. 
FIG. 7: (Color online) Some examples of (a) the scattering strength for large $\tilde{u}$ and (b) $\tilde{G}_{11}(\varepsilon)$ and $\tilde{G}_{22}(\varepsilon)$ as a function of energy for $\Delta/\varepsilon_c = 0.005$ [see Eqs. (A3) and (A4)]. In (a), the solid, dotted, and dashed lines represent $T_2$, $T_1$, and $T_0$, respectively, and the arrows indicate resonance energies. The origin of the vertical axis is shifted depending on $\tilde{u} \equiv \hbar \varepsilon_c / (4\pi \gamma^2)$.

In summary, the valley Hall conductivity, having opposite signs between the K and K' valleys, has been calculated in monolayer graphene with a gap in the presence of short-range scatterers within a single-site approximation. In the case of sufficiently weak disorder, the gap is not destroyed and the Hall conductivity there is quantized into $\pm e^2/2h$, being not affected by higher order scattering. In the band continuum, it is considerably enhanced over the result in the ideal graphenes free from scatterers. With the increase of disorder, the quantized value remains the same as long as the gap is present, but the enhancement in the band continuum near the gap becomes smaller. In the case of large disorder where the gap collapses, the Hall conductivity becomes smaller than the quantized value and monotonically decreases as the energy moves away from zero energy.

For strong scatterers, asymmetry between the conduction and valence band appears and becomes larger with the increase of the impurity strength. For scatterers with attractive potential, the disorder parameter $W$ is effectively enhanced in the conduction band and reduced in the valence band. The behavior is opposite for repulsive scatterers. Effects of skew scattering modifying the cyclotron motion remain small and do not play significant role.

Similar calculations have been performed also in bilayer graphene. The qualitative features of the results are essentially the same as in the monolayer graphene, except that the Hall conductivity is quantized into $\pm e^2/h$ in the gap region and the energy dependence in the band continuum becomes more complicated because of the sign change at energies away from the gap.

Acknowledgments

This work has been supported in part by MEXT Grants-in-Aid for Scientific Research on Innovative Areas “Science of Atomic Layers” (Project No. 2506, 26107534)
and Scientific Research (Project No. 24540339) in Japan.

Appendix A: Broad Resonance

The quantity \( g_{jj}^{(0)}(\varepsilon + i0) \), defined in Eqs. (12) and (13), is written as

\[
g_{jj}^{(0)}(\varepsilon + i0) = (\varepsilon \pm \Delta)g(\varepsilon + i0),
\]

(A1)

where + for \( j = 1 \) and − for \( j = 2 \), and \( g(\varepsilon) \) varies weakly as a function of energy except in the extreme vicinity of \( \varepsilon = \pm \Delta \). Then, the denominator of \( u_1(\varepsilon) \) becomes

\[
1 - uG_{11}^{(0)} = g \left[ \frac{|g^*|}{|g|^2} - u(\varepsilon + \Delta) \right].
\]

(A2)

Thus, a broad resonance for \( u_1(\varepsilon) \) occurs when the following is satisfied:

\[
g \left( \frac{\text{Re} g}{|g|^2} - u(\varepsilon + \Delta) \right) = \frac{g \text{Re} g}{|g|^2} \left[ 1 - uG_{11}^{(0)}(\varepsilon) \right] = 0, \quad (A3)
\]

with

\[
G_{11}(\varepsilon) = \frac{|u_{11}^{(0)}(\varepsilon + i0)|^2}{\text{Re} G_{11}(\varepsilon + i0)}. \quad (A4)
\]

Similar broad resonance occurs for \( u_2(\varepsilon) \) when the same condition, with \( G_{22}^{(0)}(\varepsilon) \) being replaced with \( G_{22}^{(0)}(\varepsilon) \), is satisfied. The appearance of this very broad resonance is similar to that in the case of lattice defects. For lattice defects, however, the potential range is smaller than the lattice constant and scattering between the K and K’ valleys play important roles.

Figure 7 shows some examples of (a) the effective scattering strength for large \( \tilde{u} \) and (b) \( \tilde{G}_{11}^{(0)}(\varepsilon) \) and \( \tilde{G}_{22}^{(0)}(\varepsilon) \). The resonance energies \( \varepsilon_1 \) and \( \varepsilon_2 \) corresponding to \( u_1(\varepsilon) \) and \( u_2(\varepsilon) \) are denoted by downward arrows \( (\varepsilon_1 < \varepsilon_2) \). According to Eq. (A3), they are obtained by the crossing points of \( \tilde{G}_{11}(\varepsilon) \) and \( \tilde{G}_{22}(\varepsilon) \) with the horizontal line given by \( |u_{12}/(4\pi\gamma^2)|^{-1} \) in Fig. 7(b).

In Fig. 7(a) broad resonance peaks appear in \( T_2^\perp \) and \( T_2 \) in the case of large \( |\tilde{u}| \). Their positions are approximately given by \( \varepsilon_1 \) and \( \varepsilon_2 \), which becomes more apparent for larger \( |\tilde{u}| \). A broad resonance appears also in \( T_2^\perp \), but its peak lies between those of \( u_1 \) and \( u_2 \). The reason is that the skew scattering appears due to the presence of the cross term \( \propto \text{Im}(u_1 u_2^*) \), as shown in Eq. (18).

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