# Splitting of the quantum Hall transition in disordered graphenes

Mikito Koshino and Tsuneya Ando
*Department of Physics, Tokyo Institute of Technology 2-12-1 Ookayama, Meguro-ku, Tokyo 152-8551, Japan*
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Integer quantum Hall effect is studied for a noninteracting electron in a monolayer graphene. We calculate the Hall conductivity within a single Landau level in the presence of randomness in the bond couplings and in the on-site potential, and estimate the critical energies for the quantum Hall transition. We show that valley-degenerated ($K$ and $K'$ points) Landau levels contain two displaced critical energies indicating that an extra Hall plateau appears inside, while the localization is found to be much stronger in the Landau level $N=0$ than in $N=1$.

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The recent progress of the fabrication of atomically thin graphene sheets makes it possible to access their unusual electronic properties.[1–5] The monolayer graphene has a semimetallic electronic structure where the conduction and valence bands touch at the Brillouin zone corners, $K$ and $K'$ points. The low energy spectrum has a linear dispersion analogous to the massless Dirac fermion, and has attracted theoretical interests as relativistic problems in the condensed matter. We study in this paper the integer quantum Hall effect for a noninteracting electron in graphene.

In a magnetic field, the spectrum splits into Landau levels which are fourfold due to the spin and valley degeneracies.[6] It has been observed that high-mobility samples exhibit the quantum Hall effect (QHE),[3,4] where the Hall plateaus emerge at $\sigma_{xy}=(n+1/2)4e^2/h$ with integers $n$, as expected from theories.[7–9] Moreover, the recent experiment in high magnetic fields reports the lifting of the valley ($K$ and $K'$) and spin degeneracies.[5] The effects of disorder in the graphene in magnetic fields was theoretically studied in the self-consistent Born approximation,[7,9,10] while the localization effect, which is essential in observing a quantized Hall conductivity, is not considered in those references.

The valley degeneracy in Landau levels poses a basic problem in the localization theory. In the usual QHE it is known that the extended states are left at only a single energy in each Landau level, at which the Hall conductivity jumps by $-e^2/h$.[11] In the degenerated levels like those in graphene, it is nontrivial how many critical energies appear, and such a problem needs to be addressed when we consider a system with a relatively strong disorder. A similar problem has been investigated in some specific models of the spin degenerate Landau levels in ordinary 2D metals. They assumed a random Zeeman field which couples different spin states and observe the splitting of the extended levels.[15–20] In graphene we have the degeneracy in valleys besides spins, and expect that the splitting is caused by the scalar disorder potential which is diagonal in the spin space. The localization in graphene in quantum Hall regime was recently studied in a tight-binding honeycomb lattice.[21]

Here we theoretically study the QHE in graphene to consider the lifting of the valley degeneracy induced by the disorder. We numerically calculate the Hall conductivity and the localization length in finite systems within the effective mass and a single Landau level approximation. We estimate the critical energies for the extended states in the thermodynamic limit from the scaling behavior of the Hall conductivity and the localization length. We follow the similar analysis applied to the usual QHE in semiconductors.[22,23]

We start with the effective mass Hamiltonian in an ideal graphene in a magnetic field given by[10,24]

$$\mathcal{H}_0=\frac{\gamma}{\hbar}\begin{pmatrix}0 & \pi_x-i\pi_y & 0 & 0\\ \pi_x+i\pi_y & 0 & 0 & 0\\ 0 & 0 & 0 & \pi_x+i\pi_y\\ 0 & 0 & \pi_x-i\pi_y & 0\end{pmatrix}, \quad (1)$$

where $\boldsymbol{\pi}=\mathbf{p}+e\mathbf{A}$ with the electron momentum operator $\mathbf{p}$ and the vector potential $\mathbf{A}=(0,Bx)$ in the Landau gauge, and $\gamma=\sqrt{3}a\gamma_0/2$ with $a$ being the lattice constant and $\gamma_0$ the hopping integral between nearest-neighbor carbon atoms. A graphene is composed of a honeycomb network of carbon atoms, where a unit cell contains a pair of sublattices, denoted by $A$ and $B$. The Hamiltonian (1) operates on a four-components wave vector $(F_A^K,F_B^K,F_A^{K'},F_B^{K'})$, where $F_A^K$ and $F_B^K$ represent the envelope functions at $A$ and $B$ sites for $K$ point, respectively, and $F_A^{K'}$ and $F_B^{K'}$ for $K'$.

The eigenstates are labeled by $(j,n,k)$ with the valley index $j=K,K'$, the Landau level index $n=0,\pm1,\ldots$, and the wave vector $k$ along $y$ direction.[6,10] The eigenenergy depends only on $n$ as $\varepsilon_n=\hbar\omega\,\mathrm{sgn}(n)\sqrt{|n|}$ with $\hbar\omega=\sqrt{2}\gamma/l$ and the magnetic length $l=\sqrt{\hbar/eB}$, which are not at even intervals unlike the usual metal. The wave functions are written as

$$\mathbf{F}_{nk}^K=\frac{C_n}{\sqrt{L}}\exp(-iky)\begin{pmatrix}\mathrm{sgn}(n)(-i)\phi_{|n|-1,k}\\ \phi_{|n|,k}\\ 0\\ 0\end{pmatrix},$$

$$\mathbf{F}_{nk}^{K'}=\frac{C_n}{\sqrt{L}}\exp(-iky)\begin{pmatrix}0\\ 0\\ \phi_{|n|,k}\\ \mathrm{sgn}(n)(-i)\phi_{|n|-1,k}\end{pmatrix}. \quad (2)$$

where $\phi_{n,k}(x)=(2^n n!\sqrt{\pi}l)^{-1/2}e^{-z^2/2}H_n(z)$, with $z=(x-kl^2)/l$ and $H_n$ being the Hermite polynomial, and

 

$$C_n = \begin{cases} 1 & (n=0), \\ 1/\sqrt{2} & (n \neq 0), \end{cases}$$

$$\mathrm{sgn}(n) = \begin{cases} 0 & (n=0), \\ n/|n| & (n \neq 0). \end{cases} \tag{3}$$

While we do not know the detail of the disorder potential in graphene, we here consider two possible model scatterers: random on-site potential and random hopping. The first one is a scatterer localized at a particular $A$ or $B$ sites with a random amplitude. A scatterer on $A$ site at $\mathbf{R}_A$ is represented as[10]

$$U(\mathbf{r}) = \begin{pmatrix} 1 & 0 & z_A^* z_A' & 0 \\ 0 & 0 & 0 & 0 \\ z_A'^* z_A & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} u_s \delta(\mathbf{r} - \mathbf{R}_A), \tag{4}$$

and that for $B$ site at $\mathbf{R}_B$ as

$$U(\mathbf{r}) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & z_B^* z_B' \\ 0 & 0 & 0 & 0 \\ 0 & z_B'^* z_B & 0 & 1 \end{pmatrix} u_s \delta(\mathbf{r} - \mathbf{R}_B), \tag{5}$$

where $z_X = e^{i\mathbf{K}\cdot\mathbf{R}_X}, z_X' = e^{i\mathbf{K}'\cdot\mathbf{R}_X}$ with $X=A,B$, and $u_s = (\sqrt{3}a^2/2)U_s$ with $U_s$ being the amplitude of the on-site potential.

As the other one we consider the randomness in the hopping integral in a bond connecting neighboring $A$ and $B$ sites. This should be possible in the presence of the local lattice distortion, or a scatterer localized at a point between neighboring sites. The effect of the lattice deformation on the electronic states was discussed in carbon nanotubes, in terms of electron-phonon interactions for acoustic[12] and optical phonons.[13] The valley mixing due to the lattice distortion was discussed in Ref. 14. We here treat just simply the short range bond randomness which is uncorrelated among different bonds. If the hopping integral between neighboring atoms at $\mathbf{R}_A$ and $\mathbf{R}_B$ shifts from $\gamma_0$ to $\gamma_0 + \delta\gamma$, we have

$$U(\mathbf{r}) = \begin{pmatrix} 0 & z_A^* z_B & 0 & z_A^* z_B' \\ z_B^* z_A & 0 & z_B^* z_A' & 0 \\ 0 & z_A'^* z_B & 0 & z_A'^* z_B' \\ z_B'^* z_A & 0 & z_B'^* z_A' & 0 \end{pmatrix} u_h \delta(\mathbf{r} - \mathbf{r}_i) \tag{6}$$

with $u_h = (\sqrt{3}a^2/2)\delta\gamma$. When the real space origin is suitably chosen, the phase factors such as $(z_A^* z_B')$ take values of $1, \omega, \omega^{-1}$ with $\omega = \exp(2\pi i/3)$, depending on the position of the bond. As stated, we limit our discussion on a short-ranged potential and rule out a long-ranged one with a length scale much larger than the lattice constant, since it does not cause intervalley mixing and thus never splits Landau levels.

With respect to the ideal wave function (2), we note that the Landau level $N=0$ is special in that its amplitude is nonzero only on either of sublattices, $B$ sites for $K$ and $A$ sites for $K'$. Consequently the random on-site potential purely gives the intravalley matrix elements within $K$ or $K'$, while the random hopping gives the intervalley mixing. The wave functions in other levels $N \neq 0$ always have nonzero amplitudes both on $A$ and $B$ sites, so that either type of the disorder causes the intervalley mixing.

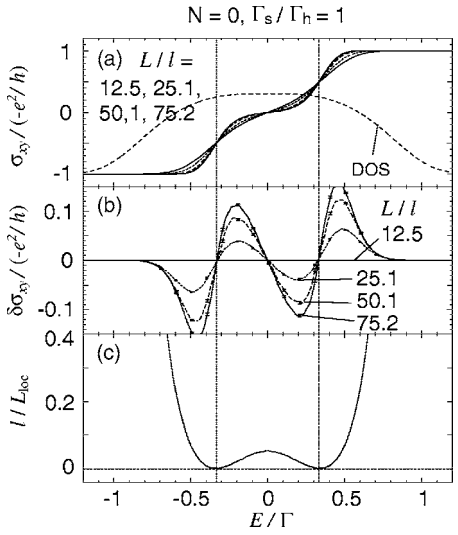


FIG. 1. (a) Hall conductivity per spin, (b) its difference measured from the smallest sample, and (c) the inverse of the localization length in the Landau level $N=0$ in graphenes with $\Gamma_s = \Gamma_h = \Gamma/\sqrt{2}$ and several sizes $L$. Vertical dashed lines represent energies for $\sigma_{xy}/(-e^2/h) = \pm 1/2$.

We consider a square sample of graphene with a side length $L = \sqrt{2\pi}Ml$ with an integer $M$. We assume that two kinds of model scatterers are distributed independently with the integrated amplitudes $\pm u_s, \pm u_h$ and number densities $n_s, n_h$, for random on-site and hopping terms, respectively. The width of each broadened Landau level can be estimated within the self-consistent Born approximation in a similar way to Refs. 7, 10, and 25 as $\Gamma = (\Gamma_s^2 + \Gamma_h^2)^{1/2}$ with $\Gamma_s^2 = n_s u_s^2/(\pi l^2)$ and $\Gamma_h^2 = 2n_h u_h^2/(\pi l^2)$, independently of the Landau level index. We assume that the disorder is moderate so that the inter-Landau level mixing can be neglected.

The Hall conductivity is calculated by the Kubo formula at zero temperature with the numerically obtained eigenstates in a single Landau level, where we take into account the mixing of the states between different Landau levels up to the first order of $U/\hbar\omega$. We apply the Thouless number method to estimate the localization length. Every quantity is averaged over a number of samples with various configuration of the disorder potential and boundary phase factors. The typical sample number is of the order of $10^4$ for $L/l = 25.1$ and $10^3$ for $L/l = 75.2$.

Figure 1 shows the results obtained for the Landau level $N=0$ with $\Gamma_s = \Gamma_h = \Gamma/\sqrt{2}$, where (a) the Hall conductivity $\sigma_{xy}$ and the density of states per spin, (b) the difference of $\sigma_{xy}$ measured from the smallest sample, and (c) the inverse of the localization length $L_{\mathrm{loc}}$ are plotted against the Fermi energy. We see that the Hall conductivity becomes size-independent at $\sigma_{xy}/(-e^2/h) = \pm 1/2$, and in other region it approaches the nearest integer as the system size increases. This is compatible to two-parameter scaling theory.[11] We expect in an infinite system that the states are extended only at those size-

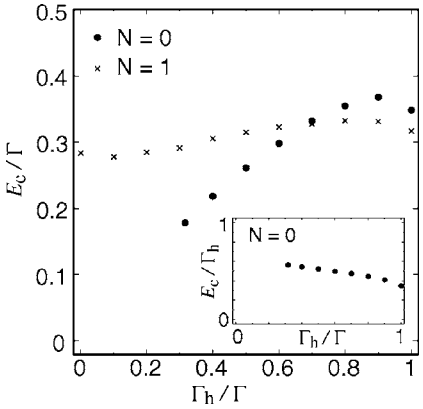


FIG. 2. Critical energy $E_c$ plotted as a function of $\Gamma_h$ for $N=0$ and $N=1$. (inset) Ratio of $E_c$ to $\Gamma_h$ against $\Gamma_h$ for $N=0$.

independent points, at which the Hall conductivity jumps by $-e^2/h$. The localization length, calculated independently from the Thouless number, confirms that this conjecture, as $L_{\rm loc}$ diverges at two distinct critical energies which perfectly agree with the fixed points of $\sigma_{xy}$.

As discussed, splitting of the extended levels in $N=0$ vanishes at $\Gamma_h=0$ since the valley mixing is caused only by the random hopping. In a real system the effect of the random hopping may be relatively smaller than that of the random on-site potential, so it is of interest to see the limit of $\Gamma_h \ll \Gamma_s$. We perform here a similar analysis on changing $\Gamma_h$ relative to $\Gamma=(\Gamma_s^2+\Gamma_h^2)^{1/2}$. Figure 2 shows a plot of the critical energy $E_c$ as a function of $\Gamma_h$, where the splitting actually decreases as $\Gamma_h$ goes to 0. The inset shows $E_c/\Gamma_h$ plotted against $\Gamma_h$, where we can see that $E_c/\Gamma_h$ is likely to approach a constant in the limit of $\Gamma_h \to 0$. This suggests that the splitting width is always of the order of $\Gamma_h$ however large $\Gamma_s$ is.

We estimate the critical exponent of the localization length $L_{\rm loc}$ in the quantum Hall transition by fitting data to $L_{\rm loc} \propto |E-E_c|^{\nu}$. In Fig. 3(a), we show the log-log plot of $L_{\rm loc}$ against $E-E_c$, where the critical energy $E_c$ is assumed to be the energy of $\sigma_{xy}/(-e^2/h)=\pm 1/2$. We have plotted only the

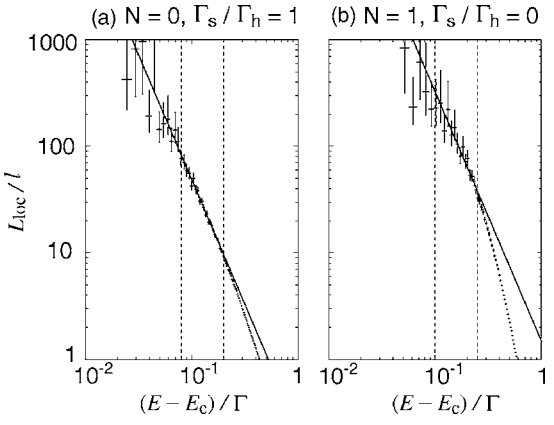


FIG. 3. Log-Log plots of the localization length against the Fermi energy measured from the critical energy, for (a) $N=0$ with $\Gamma_s/\Gamma_h=1$ (Fig. 1) and (b) $N=0$ with $\Gamma_s/\Gamma_h=0$ (Fig. 4). Fitting with $\nu=2.34$ is shown as straight lines. Vertical dashed lines show the energy region used to estimate the critical exponent.

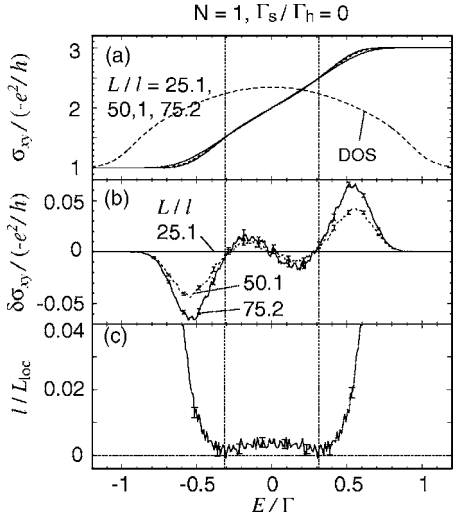


FIG. 4. Plots similar to Fig. 1 for the Landau level $N=1$ with $\Gamma_s/\Gamma_h=0$.

points in $|E|>|E_c|$, where the statistical error is relatively small. In the plot the slope seems to converge to a certain value on going to $E=E_c$. The critical exponent is estimated at $\nu=2.3\pm0.2$ from the points from $0.08<(E-E_c)/\Gamma<0.2$, which is consistent with $\nu=2.34$ known for the usual QHE, and also agree with theories in the spin degenerate Landau levels with random Zeeman field.[16–18]

We go on to consider the next lowest Landau level $N=1$. In this level, as discussed above, the intervalley mixing is caused by both of the random hopping and on-site potentials as well. Figure 4 shows similar plots to Fig. 1, obtained for $N=1$ with the random hopping only, or $\Gamma_s=0$ and $\Gamma_h=\Gamma$. We observe that $\sigma_{xy}$ is still fixed at half integers, while the size dependence is much slower than in $N=0$. In plot (c) we barely observe two dips around those two energies, at which we expect $L_{\rm loc}$ to diverge. The localization length between $\pm E_c$ is obviously much longer than in $N=0$. Figure 3(b) shows the log-log plot of $L_{\rm loc}$ against $E-E_c$. While the numerical error is larger than in $N=0$, we roughly obtain $1.5<\nu<2.5$ from the points $0.08<(E-E_c)/\Gamma<0.25$, which does not contradict $\nu=2.34$.

If we switch on and increase $\Gamma_s$, we can show that the localization length between $\pm E_c$ becomes even longer, and we fail to resolve two distinct minima in $1/L_{\rm loc}$ even in $\Gamma_s \sim \Gamma_h$. However, the size dependence in $\sigma_{xy}$ as observed above persists in all the region of $\Gamma_s/\Gamma_h$, and we can obtain $E_c$ from the fixes points in $\sigma_{xy}$. The result in Fig. 2 shows that $E_c$ is always of the order of $\Gamma$, or the total width of the Landau level. We do not observe any changes in the critical exponent in finite $\Gamma_s$.

To summarize, we have studied the quantum Hall effect in valley degenerated Landau levels in graphene. We have observed the splitting of the quantum Hall transition in $N=0$, given the bond randomness between carbon atoms, while in $N=1$ the splitting occurs also in the on-site potential as well.

We emphasized that the splitting is always due to the intervalley mixing, for which the disorder must be short-ranged, or of the order of the lattice constant. We do not know the typical disorder length scale in a realistic situation,

while in theory the transport property is insensitive to the potential range within the self-consistent Born approximation.[7,10] It is also unclear how much the system contains the bond randomness, which is essential for the intervalley mixing particularly in $N=0$. Nevertheless, we expect a splitting with a finite width to be observed in a sufficiently low temperature, unless the intervalley mixing is absolutely absent.

Our numerical results quantitatively show that the localization length in the intermediate plateau is much shorter in $N=0$ than in $N=1$, at least when $\Gamma_h \sim \Gamma_s$. This suggests that the system size (or the phase coherent length) required to observe the splitting is particularly small at $N=0$, and that is consistent with the experiment[5] where the valley splitting was found only at $N=0$. Of course we cannot exclude other scenarios based on the electron-electron interaction, which interprets the phenomena in terms of the quantum Hall ferromagnet.[26]

Finally we comment on a possibility of the Landau level splitting in bilayer graphene. Recently the Landau level sequence of bilayer graphene was investigated experimentally[3,28] and theoretically.[27] It was shown that each Landau level is degenerated in valleys and spins similarly to a monolayer, while only at $E=0$ the degeneracy is doubled, i.e., a pair of levels overlaps *in the same valley and spin*. The wave functions of this special pair have an amplitude at the same sublattice depending on the valley. Thus we do not need intervalley or intersublattice matrix elements to couple those levels, so that we expect that the level splitting at $E=0$ occurs even in a long-range and scalar potential, which may be dominant in realistic samples. We leave the calculation and further discussions for future works.

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