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Theory of unconventional quantum Hall effect in strained graphene

Bitan Roy¹, Zi-Xiang Hu^{2,3}, Kun Yang¹

¹*National High Magnetic Field Laboratory, Florida State University, FL 32306, USA*

²*Department of Physics, Chongqing University, Chongqing 400044, China*

³*Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544, USA*

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We show through both theoretical arguments and numerical calculations that graphene discerns an unconventional sequence of quantized Hall conductivity, when subject to both magnetic fields (B) and strain. The latter produces time-reversal symmetric pseudo/axial magnetic fields (b). The single electron spectrum is composed of two inter-penetrating sets of Landau levels (LLs), located at $\pm\sqrt{2n|b \pm B|}$, $n = 0, 1, 2, \dots$. For $b > B$, these two sets of LLs have opposite *chiralities*, resulting in *oscillating* Hall conductivity between 0 and $\mp 2e^2/h$ in electron and hole doped system, respectively, as the chemical potential is tuned in the vicinity of neutrality point. The electron-electron interactions stabilizes various correlated ground states, e.g., spin-polarized, quantum spin-Hall insulators at and near the neutrality point, and possibly the anomalous Hall insulating phase at incommensurate filling $\sim B$. Such broken symmetry ground states have similarities as well as significant differences from their counterparts in the absence of strain. For realistic strength of magnetic fields and interactions, we present scaling of interaction induced gap for various Hall states within the zeroth Landau level.

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Successful fabrication of two-dimensional electron gas, e.g, Gallium-Arsenide (GaAs) heterostructure, provided unique opportunity to observe a novel aspect of low-dimensional electronic systems, quantization of Hall conductivity (σ_{xy}). At weaker magnetic fields (~ 1 T), even the low-mobility samples discern quantized plateaus of σ_{xy} at various integers of e^2/h . This phenomena is referred to as *integer quantum Hall effect* (IQHE)¹. Rather more striking observation is the plateaus of that quantity at various, for example $1/3$, fractions of e^2/h , in improved samples, however at stronger fields (~ 10 T)². Whereas the IQHE arises from free motion of fermions in magnetic fields³, its fractional version necessarily requires strong electron-electron interactions to develop mobility gap within a partially filled Landau level⁴.

Integer quantization of σ_{xy} occurs when the chemical potential (μ) lies within a mobility gap, filled by localized states, separated by two extended conducting edge modes carrying the quantized Hall current⁵. As the magnetic field (B) is reduced, more and more extended states, at well separated energies, get occupied. Total Hall current, the *algebraic* sum of it carried by each of the edge modes, then encounters quantized increment, due to identical *chirality* of all the edge states⁶.

Besides the GaAs heterostructure, the new generation two-dimensional electronic system, *graphene*, discerns a sequence of Hall plateaus at fillings $\nu = \pm 4(n + \frac{1}{2})$, subject to relatively low fields⁷, while additional plateaus, for example at $\nu = 0, \pm 1, \pm 4$, show up as the field is enhanced^{8,9}. Otherwise, all the LLs support the current carrying states with identical chirality, as in GaAs¹⁰. Moreover, due to its mechanical flexibility under strain, graphene may experience yet another *effective* magnetic field, resulting from deliberate bulging¹¹. Such strain induced pseudo/axial magnetic field (b) preserves the time reversal symmetry (TRS), and points in opposite direc-

tions at two inequivalent Dirac points, suitably chosen here at $\vec{K} = (1, 1/\sqrt{3})(2\pi/a\sqrt{3})$ and $-\vec{K}$ ¹². Therefore, subject to strain as well as an external magnetic field, one can expose the gapless Dirac quasi-particles, near two Dirac points with different effective fields, $|B \pm b|$, possibly pointing in *opposite* directions, respectively. Hence, an interplay of these two gauge fields, concomitantly an unconventional quantization of the Hall conductivity can be realized in graphene.

It is perhaps worth considering the Hall response of this system when $B > b (\neq 0)$ first¹³. The spectrum of non-interacting Dirac quasi-particles is then comprised of two inter-penetrating sets of LLs at well separated energies $\pm\sqrt{2n(B \pm b)}$, with degeneracies $(B \pm b)/2\pi$ per unit area, and all the LLs experience the effective orbital magnetic fields in the same direction. Hence, every current carrying states have identical chirality. Consequently, as the chemical potential sweeps through various LLs, the total Hall current adds up, and the quantization of σ_{xy} is expected to occur at all integers of e^2/h . However, the plateaus appear at incommensurate fillings, due to distinct degeneracies of the LLs¹⁴.

Rather more interesting situation arises when $b > B$. For $B = 0$, the pseudo Dirac LLs, placed at $\pm\sqrt{2nb}$ ¹⁵⁻¹⁸, near two valleys have opposite chirality, henceforth the TRS is preserved. As long as $b > B > 0$, two inequivalent sets of LLs, now located at $\sqrt{2n(b \pm B)}$ (Fig. 1, left column), with respective degeneracies $(b \pm B)/2\pi$ per unit area, continue to enjoy opposite chirality (Fig. 1, lower right column). Consequently, as the chemical potential starts to deviate from the charge neutrality point (CNP), the Hall conductivity is restricted within $\pm 2e^2/h$ (when more LLs near one valley is filled) and 0 (when both valleys are equally populated); see Fig. 1(upper right column). The \pm sign corresponds to hole and electron doped systems, respectively, and note it is *opposite* to

what one has in the absence of the strain-induced field, b .

Even though the Hall conductivity stays bounded, as the chemical potential is enhanced, more and more current carrying edge states with opposite chirality get filled. In the absence of back scattering that equilibrates these counter-propagating edge modes, the two terminal conductance G_{xx} is expected to increase monotonically. However, the lack of equilibration ruins the quantization of Hall conductance in a four-terminal measurement¹⁹. But in reality, there is always back scattering between counter-propagating edge modes that live along the same edge; this not only equilibrates these modes but also localize them, except for the two additional modes associated with the occupied extra LLs. As a result both σ_{xy} and G_{xx} are quantized at the same value.

The oscillatory sequence of σ_{xy} is strictly true only in the vicinity of the CNP. The spacing of the Dirac LL decreases with the LL index (n), and the effective magnetic field for two sets of LLs are different. Hence, far away from the CNP, LL crossing is unavoidable, and one may see quantized plateaus of σ_{xy} at $3e^2/h$ or higher. If $B \ll b$, the LL crossing occurs for $n \gg 1$. Assuming that the chemical potential is not too far from the Dirac points, one can then safely neglect the LL crossing.

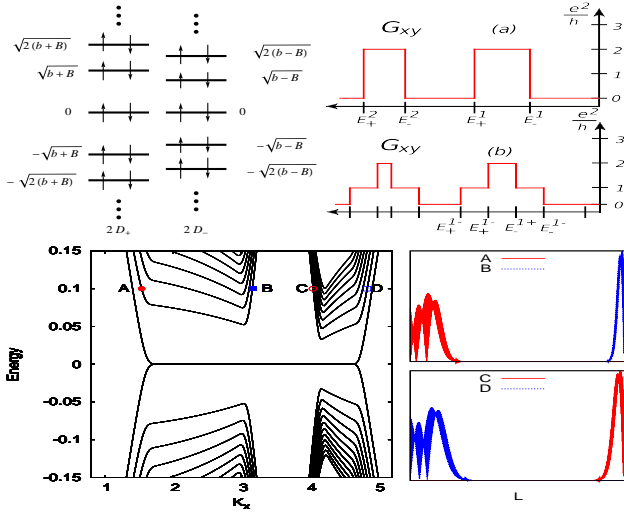


FIG. 1: (Color online) Upper row:: Left: Spin degenerate interpenetrating LLs of $H_D[A, a]$. Here we have shown the LLs for $n = 0, \pm 1, \pm 2$ only. Two LLs have the degeneracies $2D_{\pm} = (b \pm B)$ per unit area. Right: Schematic variation of Hall conductances G_{xy} in a hole doped graphene, without (a) and with (b) Zeeman splitting (Δ_z). Here, $E_{\sigma}^n = \sqrt{2n(b + \sigma B)}$, $E_{\sigma}^{n\alpha} = E_{\sigma}^n + \alpha\Delta_z$ with $\sigma, \alpha = \pm$. In electron doped system, G_{xy} changes sign. We only show the spin splitting of $n = 1$ LL. Splitting of $n = 2$ LL is identical. Lower Row:: The energy spectrum (left) and wave-functions (WFs) (right) for a strained graphene in magnetic field when $B < b$. WFs localized on one edge, live on opposite side at two valleys, explicitly, A(B) and D (C) are localized on left (right) edge, therefore carrying opposite chirality.

To compute the LL spectrum, we here construct an 8-component Dirac spinor $\Psi = (\Psi_{\uparrow}, \Psi_{\downarrow})^T$, where $\Psi_{\sigma}^T = [u_{\sigma}^{\dagger}(\vec{K} + \vec{q}), v_{\sigma}^{\dagger}(\vec{K} + \vec{q}), u_{\sigma}^{\dagger}(-\vec{K} + \vec{q}), v_{\sigma}^{\dagger}(-\vec{K} + \vec{q})]$, with $\sigma = \uparrow, \downarrow$ as electrons spin projection along the z -direction. The orbital effects of the real (B) and pseudo (b) magnetic fields can be captured by the Hamiltonian¹⁴⁻¹⁶

$$H_D[A, a] = I_2 \otimes i\gamma_0\gamma_i(\hat{q}_i - A_i - i\gamma_3\gamma_5 a_i), \quad (1)$$

where $B(b) = \epsilon_{3ij}\partial_i A(a)_j$. The gamma matrices are $\gamma_0 = I_2 \otimes \sigma_3$, $\gamma_1 = \sigma_3 \otimes \sigma_2$, $\gamma_2 = I_2 \otimes \sigma_1$, $\gamma_3 = \sigma_1 \otimes \sigma_2$, $\gamma_5 = \sigma_2 \otimes \sigma_2$ ²⁰. The spectrum of $H_D[A, a]$ is comprised of two sets of *interpenetrating* LLs at energies $\pm\sqrt{2n(b + \alpha B)}$, with respective degeneracies $\Omega(b + \alpha B)/2\pi$ for $\alpha = \pm$, shown in Fig. 1²¹. Here $n = 0, 1, 2, \dots$ and Ω is the area of the strained graphene sample. With $b > B$ states within the zeroth LL (ZLL) are localized on only one sub-lattice, say A for example, while they reside on complementary sub-lattices near two Dirac points if $B > b$ ¹⁴. For each spin flavor, there exists $(b \pm B)\Omega$ states at precise zero energy per unit area, guaranteed by an ‘‘index theorem’’^{23,24}, respectively near the Dirac points at $\pm\vec{K}$. However, the valley degeneracy for all the LLs at finite energies is removed, as they are exposed to different *effective* magnetic fields.

Let us first register the Hall response of the non-interacting system, see Fig. 1(a). For $\mu = 0$, the ZLL, containing $4\Omega b$ states, is half-filled. Then a particle-hole symmetry of the spectrum, generated by $I_2 \otimes \gamma_0$ for example²⁵, guarantees that $\sigma_{xy} = 0$. Even when $0 < \mu < \sqrt{b - B}$, σ_{xy} remains pinned at zero, which can be confirmed upon subscribing the Středa formula²⁶ for the Hall conductivity, reads as $\sigma_{xy} = \left(\frac{\partial N}{\partial B}\right)_{\mu}$, in the natural units $e = c = 1$. N is the electronic density in the bulk below the chemical potential. Derivative with respect to B is taken at fixed μ , measured from the half-filled band. In order to place the chemical potential such that $0 < \mu < \sqrt{b - B}$, one needs to fill $N = 2\Omega b$ (independent of B) states from the CNP, yielding a *zero* Hall conductivity. On the other hand, if $\sqrt{b - B} < \mu < \sqrt{b + B}$, $\delta N = -2\delta B$ and hence $\sigma_{xy} = -2$. The factor 2 counts the spin degeneracy of the LL. Upon further doping when $\sqrt{b + B} < \mu < \sqrt{2(b - B)}$, the Hall conductivity returns to *zero*. Hence, with odd (even) number (modulo 2 due to spin) of LLs below the chemical potential, one gets $\sigma_{xy} = -2(0)$, as long as there is no LL crossing. Origin of such oscillating Hall conductivity is the following. Two sets of LLs near $\pm K$ experience effective magnetic fields $(b \pm B) > 0$, but point in opposite directions. So, the current carrying states of these two LLs have opposite *chirality*. When odd number (modulo 2) of LLs above the CNP are filled, $\sigma_{xy} = -2$, since there is imbalance in the occupation of the LLs near two Dirac points. With an even number (modulo 2) of filled LL, the Hall currents from the LLs near $\pm\vec{K}$ exactly cancels each other, giving $\sigma_{xy} = 0$. Hall conductivity oscillates between 0 and $+2e^2/h$, when $\mu < 0$ (hole doping).

The chiral nature of the edge modes in the presence

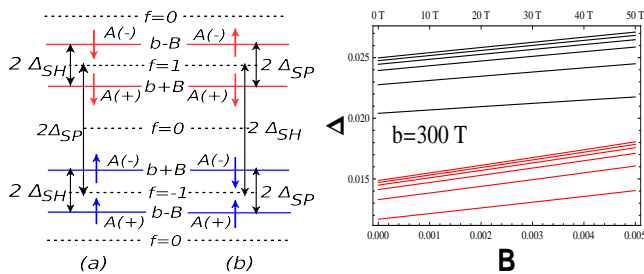


FIG. 2: (Color online) Left: Two possible (a,b) interaction driven splitting of the ZLL. Dotted lines correspond to requisite location of the chemical potential for $\sigma_{xy} = fe^2/h$. \pm corresponds to the ZLL states localized near the valley at $\pm\vec{K}$. Right: Dimensionless activation gap (Δ/Λ) for $\sigma_{xy} = 0, \pm e^2/h$ (black, red) Hall states when $b = 300$ T and $0 \text{ T} < B < 50 \text{ T}$, for $\delta = 0, 0.03, 0.07, 0.14, 0.3, 0.7$ (from top to bottom), assuming $\Lambda \sim 1/2.5\text{\AA}$, the ultra-violet cutoff over which the dispersion is approximately linear. g_c is the zero field criticality. Lower x-axis denotes B/Λ^2 (dimensionless).

of strain and magnetic field can also be seen in a finite honeycomb lattice, with the zigzag edge. The orbital effect of the real and axial magnetic field can respectively be captured by, attaching a Peierls phase, $t_{ij} \rightarrow t_{ij} \exp(2\pi i \frac{e}{hc} \int_i^j \vec{A} \cdot d\vec{l})$, and introducing local modification, to the nearest-neighbor (NN) hopping amplitudes. We here modify the hopping only along one of the three bonds, oriented orthogonal to the zigzag edge^{21,22}. Such simple deformation yields slightly inhomogeneous Fermi velocities and thus LL energies. Nevertheless, one can still observe the peculiarities of the edge modes arising from the time-reversal invariance. It is evident from Fig. 1(lower row) that the chiralities of two states localized near one zigzag edge are opposite if $b > B$, similar to when $B = 0$, but $b \neq 0$.²¹ LLs near two Dirac points appear at different energies. Therefore, as one changes the chemical potential the Hall conductivity keeps oscillating between $\pm e^2/h$ and 0 (we consider spinless fermions). If on the other hand, the real magnetic gets stronger, the edge modes near two Dirac points share identical chiralities, and σ_{xy} changes monotonically.^{14,21} An interesting possibility is $B = b$. Only one of the Dirac points is then exposed to finite magnetic field, yielding plateaus of σ_{xy} at $\nu = 2(n + \frac{1}{2})$, while the other one remains semi-metallic, contributing to σ_{xx} simultaneously.^{21,27}

The Zeeman splitting (Δ_z) lifts the spin degeneracy from all the LLs, $\sqrt{n(b \pm B)} \rightarrow \sqrt{n(b \pm B)} \pm \Delta_z$. The Zeeman gap scales as $\Delta_z \sim B(\text{Tesla}) \text{ K}$. Hence, it cannot cause LL crossing near the CNP. The Hall conductivity remains pinned to zero, when $\mu = 0$ due to the particle-hole symmetry, generated by $\sigma_1 \otimes \gamma_0$.²⁵ It remains so even when the chemical potential lies in between the Zeeman shifted ZLL at Δ_z , and $\sqrt{b-B} - \Delta_z$, since then $\delta N = 2b\Omega$ in the Středa formula. Otherwise, for $\sqrt{b+\sigma B} + \sigma\Delta_z < \mu < \sqrt{b+\sigma B} - \sigma\Delta_z$, $\sigma_{xy} = -(\frac{3+\sigma}{2})e^2/h$, where $\sigma = \pm 1$. Therefore, the Zeeman splitting introduces additional Hall plateau at

$\mp e^2/h$, in electron and hole doped systems, respectively; see Fig. 1(b).

A strain induced charge density wave order (not spontaneously generated) always persists within the ZLL, since all these states are localized on one sub-lattice. This configuration is a natural ground state for the residual NN Coulomb repulsion. Two valleys at $\pm\vec{K}$ hosts $\Omega(b \pm B)$ states, hence a ‘valley polarized’ *anomalous Hall insulator* cannot develop at the CNP. It may however be realized at incommensurate filling, $\nu \propto B$ about the neutrality point. A spin Hall (SH) order, $\Delta_{SH} = \langle \Psi_\sigma^\dagger \vec{\sigma} \otimes i\gamma_1\gamma_2 \Psi_\sigma \rangle$ ^{28,29}, corresponding to a spin-triplet, intra-sublattice circulating currents, can however develop upon occupying two valleys with opposite spin. It also carries a finite *ferromagnetic* moment $\propto B$, the difference of LL degeneracies. Since the entire ZLL is localized on one sub-lattice, a ferromagnet (FM) order is tied with an anti-ferromagnet (AF) order. Yet another, namely a spin polarized (SP) state can also be realized at the CNP. It carries FM ($\Delta_{FM} = \langle \Psi_\sigma^\dagger \vec{\sigma} \otimes I_4 \Psi_\sigma \rangle$) and AF ($\Delta_{AF} = \langle \Psi_\sigma^\dagger \vec{\sigma} \otimes \gamma_0 \Psi_\sigma \rangle$) orders, simultaneously¹⁶. The Zeeman coupling locks the spin of the SP state along the direction of the real field (B), and gives $\Delta_{FM} \neq 0$. However, the onsite-Hubbard interaction (U), possibly the strongest interaction in graphene³⁰, favors an AF order in the vicinity of the CNP. The second-neighbor repulsion (V_2) favors the SH state³¹. The spin polarized state can also be realized even when $B = 0$ ¹⁷, which has been identified as pure ferromagnetic state in Ref.¹⁷. The AF/SH order parameter anti-commutes with $H_D[A, a]$. Hence, apart from splitting the ZLL, they optimally lower the energy of the filled Dirac sea by shifting all the LLs at finite energies, $\pm\sqrt{2n(b \pm B)} \rightarrow \pm\sqrt{2n(b \pm B) + \Delta_{AF/SH}^2}$. The spin-polarized gap within the ZLL is $\Delta_{SP} = \Delta_{AF} + \Delta_{FM} \sim U$, whereas $\Delta_{SH} \sim V_2$, to the leading order.³² Though such insulations in pristine graphene can only take place for sufficiently strong repulsive interactions,²⁰ existence of macroscopically degenerate LLs permits such ordering even when the interactions are infinitesimal, in the presence of magnetic fields.^{14,15,33,34} Next we study the interplay of these orders.

For small Zeeman coupling the ground state energy per unit area at half filling with AF (\vec{N}) and SH (\vec{C}) orders is

$$E[\vec{N}, \vec{C}] = \frac{\vec{N}^2}{4g_a} + \frac{\vec{C}^2}{4g_c} + E_0[\vec{N}, \vec{C}], \quad (2)$$

where $g_{a(c)} \sim U(V_2)$. $E_0[\vec{N}, \vec{C}]$ is the ground state energy per unit area of the effective single particle Hamiltonian

$$H_{HF} = H_D[A, a] - (\vec{N} \cdot \vec{\sigma}) \otimes \gamma_0 - (\vec{C} \cdot \vec{\sigma}) \otimes i\gamma_1\gamma_2. \quad (3)$$

With negligible Zeeman coupling a spin-anisotropy can be neglected and one can take $\vec{N}(\vec{C}) = (N(C), 0, 0)$, for simplicity. The spectrum of H_{HF} is composed of LLs at energies $\pm e_{n,\alpha}$, with degeneracies $\Omega(b + \alpha B)/4\pi$, where

$e_{n,\alpha} = [2n(b + \alpha B) + (N + \alpha C)^2]^{1/2}$, and $\alpha = \pm$. The ground state of H_{HF} at half filling, has all the states with negative energies filled, while the rests are empty. Minimization of $E[N, C]$, with respect to N and C , yields *two* coupled gap equations, which for $N > C$ read as

$$\frac{\pi^{3/2}}{2g_i} = \frac{\xi_i}{X_i} + \sum_{n \geq 1, \alpha = \pm}^{i \neq j} \left(\frac{b + \alpha B}{2e_{n,\alpha}} + \frac{X_j}{X_i} \alpha \frac{b + \alpha B}{2e_{n,\alpha}} \right) \quad (4)$$

for $i, j = 1, 2$, where $g = (g_a, g_c)$, $X = (N, C)$, $\xi = (b, B)$. The ultra-violet divergent in the first term of the gap equations is independent of AF or SH orders. The cut-off (Λ) independence of the physical observable gap, then demands $g_a \equiv g_c$ for both AF and SH order to be finite simultaneously. Since in graphene $U > V_2$, possibly a spin polarized state ($N \equiv \Delta_{AF} \neq 0, C \equiv \Delta_{QSH} = 0$) is formed at the CNP. Even though, with $b > B$, there exists a series of $\sigma_{xy} = 0$ plateau, only the one near $\mu = 0$ bears an AF order, while the rest arises from lack of ‘valley reflection symmetry’. Placing the chemical potential close to the first excited state at $\pm \Delta_{SP}$, a spin Hall order develops additional incompressible Hall state, leading to $\sigma_{xy} = \pm e^2/h$, see Fig. 2(a). If on the other hand, $V_2 > U$, yielding $C > N$, the splitting of the ZLL gets reversed, see Fig. 2(b).

Minimizing the ground state energy, one can find the gap equation for $\sigma_{xy} = 0$ Hall state near the CNP. For fixed axial magnetic field ($b = 300T$), the interaction induced gap at the neutrality point increases linearly with the real magnetic field, when $0 \text{ T} < B < 50 \text{ T}$, (Fig. 2, right column). Scaling of the gap is insensitive to exact nature of the order parameter. The activation gap for $\sigma_{xy} = \pm e^2/h$ state within the ZLL is smaller than, but similar to that for $\sigma_{xy} = 0$. Such hierarchy comes solely from the ZLL. Exactly half of the ZLL contributes to the gap for $\sigma_{xy} = 0$ state, whereas fewer states from the ZLL contribute to the gap for $\sigma_{xy} = \pm 1$ Hall state.²¹ Otherwise, activation gaps for both the Hall states scale sub-linearly with the interaction, $\delta = (g\Lambda)^{-1} - (g_*\Lambda)^{-1}$, where g_* is zero field criticality for insulation. If the magnetic fields become *inhomogeneous*, the LLs at finite energies disappears, giving rise to a continuous spectrum, though the ZLL, protected by the ‘index theorem’, stays unaffected. Therefore, interaction induced gap formation occurs even when the fields are non-uniform. However, the gaps then closely follow the profile of the magnetic fields.²⁴ With *weak* inhomogeneous fields, the quantization of σ_{xy} is expected to survive.

In the absence of the axial field or even when $B > b$, the states within the ZLL, localized near two valleys live on complimentary sub-lattices^{14,34}. Therefore, a conventional AF order develops by filling up states on two sublattices with opposite spin projections. However, the

staggered spin moments on two sub-lattices are of different magnitudes. Therefore, one may argue such a correlated phase as *ferrimagnetic* as well¹⁴.

In experiment¹¹, the *uniform* axial field is localized only in certain region of the sample. Particles circling that region pick up an axial Aharonov-Bohm phase (ABP), only if they travel through the strained region, since the axial gauge potential is proportional to strain. It is identical for the trajectories in opposite directions, whereas the ABP due to the real magnetic field are of opposite sign for these trajectories.³⁵ Consequently, the trajectories with opposite circulation, acquires different effective ABP, namely, sum and difference of it due to two fields. In Hall conductivity measurement, the terminals need to be attached to the regions with at least finite strain, though b can be zero. In *molecular graphene*³⁶, and strained graphene on Ru substrate³⁷, the axial field can possibly be realized in the entire sample. Hence the peculiar Hall conductivity, we propose here, may become easily observable in those systems.

To summarize, we here demonstrate the possible quantization of Hall conductivity (σ_{xy}) in strained graphene, subject to magnetic fields. We show that when strain induced pseudo magnetic field is stronger than the real one, Hall conductivity remains bounded between 0 and $\mp 2e^2/h$, in electron and hole doped graphene respectively. The Zeeman coupling introduces additional Hall plateaus at $\mp e^2/h$. Such quantization relies on sufficient backscattering among the counter propagating edge modes, and only true in the vicinity of the CNP, where LL crossing can safely be neglected. Depending on the relative strength of the finite ranged components of the Coulomb interaction, various broken symmetry phases can be realized within the ZLL. For example, on-site and next neighbor repulsion respectively favors anti-ferromagnet and spin Hall ground state. In contrast to conventional situation, the anti-ferromagnet order, in the strain dominated regime ($B \ll b$), is always tied with a ferromagnet order. For fixed b , the many-body gaps inside the ZLL, scales linearly with real magnetic field (B) and sublinearly with interaction (δ), as long as $B \ll b$.

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