DMRG study of fractional quantum Hall effect and valley skyrmions in graphene

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Abstract. The ground state and low-energy excitations of graphene and its bilayer are investigated by the density matrix renormalization group (DMRG) method. We analyze the effect of Coulomb interaction between the electrons including valley degrees of freedoms. The obtained results show finite charge excitation gap at various fractional fillings $\nu_{n} = 1/3, 2/5, 2/3$ in the $n = 0$ and 1 Landau levels of single-layer graphene (SLG) and $n = 2$ Landau level of bilayer graphene (BLG). The lowest charge excitations at $\nu = 1/3$, and 1 in SLG are valley skyrmions.

1. Introduction
Graphene is an atomic scale two-dimensional electron system with low-energy electrons in two valleys, K and K’ in the Brillouin zone. The K and K’ are inequivalent Brillouin zone corners defined by triangular sublattices of hexagonal structure of carbon atoms. In contrast to conventional two-dimensional systems, the single-electron wavefunction has two sublattice components reflecting two triangular sublattices of graphene, which are connected by nearest-neighbor hopping element $t$. Such two components wavefunction and the valley degrees of freedom are unique properties of graphene [1, 2, 3, 4]. In the present paper, we investigate how these characteristics affect fractional quantum Hall states, which is expected to be realized in high magnetic field [5, 6].

In magnetic field, the presence of two valleys is observed in half-integer Hall conductivity[7, 8]

$$\sigma_{xy} = (n + \frac{1}{2}) \frac{4e^2}{\hbar},$$

at $\nu = \pm 2, \pm 6, \pm 10, \cdots$ with factor 4 for single-layer graphene (SLG), which reflects 4-fold Landau level (LL) degeneracy, resulting from spin and valley symmetry in graphene.

The two components single-particle Hamiltonian for the K-valley of SLG[4] is written as

$$\mathcal{H}^{(SLG)}_{K} = \frac{\sqrt{2}h v_F}{\ell_B} \begin{pmatrix} 0 & a \\ a^\dagger & 0 \end{pmatrix},$$

where $a \equiv (\pi_x - i\pi_y)eB/\sqrt{2}\hbar$ is the magnetic ladder operator and $\pi = p - eA$ is the kinetic momentum. $v_F$ is the Fermi velocity of SLG, $\ell_B = \sqrt{\hbar/eB}$ is the magnetic length, and $2 \times 2$...
matrices represent sublattice degrees of freedom in graphene. $H_{K'}^{(SLG)}$ is the transpose of $H_{K}^{(SLG)}$. The eigenenergy is given by

$$\epsilon_n = \pm \hbar v_F \sqrt{2n/\ell_B}.$$  \hspace{1cm} (3)$$

and the eigenvectors are $|0\rangle_{K}^{(SLG)} = (0, 0)^t$ for $n = 0$ and $|n, \pm\rangle_{K}^{(SLG)} = (|n-1\rangle, \pm |n\rangle)^t/\sqrt{2}$ for $n \geq 1$. Here, $|n\rangle$ is the eigenvector of the number operator $N \equiv a^\dagger a$ with an eigenvalue $n$.

The bilayer graphene (BLG) has an ordinary parabolic spectrum in the vicinity of the neutrality point. In a magnetic field, the effective Hamiltonian for BLG is written in the form

$$H_{K}^{(BLG)} = \hbar \omega_c (0 a^2 (a^\dagger)^2 0),$$  \hspace{1cm} (4)$$

and its eigenenergy is

$$\epsilon_n = \pm \hbar \omega_c \sqrt{n(n-1)}.$$  \hspace{1cm} (5)$$

Here, $\omega_c = eB/m$ with $m$ being the effective mass of BLG. The eigenvectors in eq. (4) are $|0, 0\rangle_{K}^{(BLG)} = (0, 0)^t$, $|0, 1\rangle_{K}^{(BLG)} = (0, 1)^t$ for the zero energy level and $|n, \pm\rangle_{K}^{(BLG)} = (|n-2\rangle, \pm |n\rangle)^t/\sqrt{2}$ for $n \geq 2$.

The relevant energy scales in graphene in a magnetic field are as follows: (i) LL separation around the neutrality point, $\sqrt{2}\hbar v_F/\ell_B \approx 400 \sqrt{B}[T]\Omega$ for SLG, while $\sqrt{2}\hbar \omega_c \approx 30 \times (B[T])[K]$ for BLG, (ii) Zeeman coupling, $\Delta_z \equiv g\mu_B |B| \approx 1.5 \times (B[T])[K]$, and (iii) the Coulomb energy $e^2/\epsilon \ell_B \approx 100 \sqrt{B}[T]\Omega$.

We focus mainly on many-body states in nonzero LLs of SLG and BLG. We introduce the effective filling factors of the topmost partially filled $n$th LL,

$$\nu_{n}^{(SLG)} = \nu - 4(n - 1/2)$$  \hspace{1cm} (6)$$

for SLG and

$$\nu_{n}^{(BLG)} = \nu - 4(n - 1)$$  \hspace{1cm} (7)$$

for BLG. Here, $\nu_n \leq 4$ and $n \geq 2$ for BLG.

2. Model and Method

Since the LL separation is larger than typical Coulomb energy $e^2/\epsilon \ell_B$ in high magnetic fields, we first project Coulomb interaction Hamiltonian onto a certain LL. The projected Hamiltonian onto the $n$th LL is written as

$$H = \frac{1}{L^2} \sum_{i<j} \sum_{q} V(q) e^{-q^2/2[F_n(q)]^2} e^{i\mathbf{q} \cdot (\mathbf{R}_i - \mathbf{R}_j)},$$  \hspace{1cm} (8)$$

where $\mathbf{R}_i$ is the guiding center coordinate of the $i$th particle. The relativistic form factor in the $n$th LL of SLG is written as

$$F_{0}^{(SLG)}(q) = L_0 \left(q^2/2\right)$$  \hspace{1cm} (9)$$

and

$$F_{n \geq 1}^{(SLG)}(q) = (1/2) \left[L_{|n|} \left(q^2/2\right) + L_{|n|-1} \left(q^2/2\right)\right].$$  \hspace{1cm} (10)$$
For the \( n(\geq 2) \)th LL in BLG,
\[
F_{n \geq 2}^{(\text{BLG})}(q) = (1/2) \left[ L_{[n]} \left( \frac{q^2}{2} \right) + L_{[n]-2} \left( \frac{q^2}{2} \right) \right].
\] (11)

Here, \( L_n(x) \) are the Laguerre polynomials. In the spherical geometry, it is convenient to write the Hamiltonian as
\[
H^{(n)} = \sum_{i<j} \sum_m V^{(n)}_{m} P_{ij}[m],
\] (12)
where \( P_{i,j}[m] \) projects onto states in which particles \( i \) and \( j \) have the relative angular momentum \( \hbar m \), and \( V^{(n)}_{m} \) is their interaction energy in the \( n \)th LL.[11] Using the above form factors, the pseudopotentials[13, 11] are given by
\[
V^{(n)}_{m} = \int_0^\infty dq 2\pi q V(q)e^{-q^2}[F_n(q)]^2 L_m(q^2).
\] (13)

The corresponding integrals for electrons on the surface of a sphere that are used in the present work are described in refs. [11, 14, 15]. Note that our Hamiltonian eqs. (8) and (12) have SU(2) symmetry in the valley degrees of freedom.

In the following, we treat the valley degrees of freedom \( K \) and \( K' \) in the language of the pseudospin, while real spin degrees of freedom are supposed to be frozen by Zeeman splitting. LL mixing is also neglected.

We calculate the exact wave functions of the ground and low-energy excited states in SLG and BLG, using the density matrix renormalization group (DMRG) method[16, 17, 18], which is applied to torus[17, 18] and spherical geometries[11, 13, 14, 15, 19, 21, 22]. The accuracy of the results is systematically controlled by the truncation error, which is smaller than \( 10^{-4} \) in the present calculation. We investigate systems of various sizes with up to 40 electrons in the unit cell keeping 1400 basis states in each block[17, 18].

3. Results
3.1. \( \nu_n = 1 \) and \( 1/3 \) states
At \( \nu_n = 1 \) integer fillings, the pseudospins of valley degrees of freedom are completely polarized through the exchange Coulomb interaction. Since fully pseudospin-polarized quasiparticle excitations require energy to the next higher LL, we calculate the unpolarized and partially polarized excitations within the same LL by the DMRG method.

The pseudospin polarization and the energy of the lowest charge excitation are shown in Fig. 1 for systems in spherical geometry. This figure shows that the pseudospin-unpolarized state is the lowest excited state when the system size is sufficiently large in SLG (\( n = 0, 1, \) and 2) and BLG (\( n = 2 \)). The extrapolated values of the pseudospin-unpolarized excitation gaps \( \Delta_e \) in units of \( e^2/(\epsilon f_B) \) are 0.63, 0.28, and 0.42 in the \( n = 0, 1, \) and 2 LLs of SLG, and 0.48 in the \( n = 2 \) LL of BLG[22].

In the \( n = 2 \) LL, the lowest quasiparticle excitation in small systems (\( N_e \leq 20 \)) has a large pseudospin polarization \( P = 1 - 2/N_e \) both for SLG and BLG, where \( P \equiv (N_K - N_{K'})/(N_K + N_{K'}) \) with \( N_K \) (\( N_{K'} \)) being the number of electrons in the \( K \) (\( K' \)) valley. These results show the instability of the unpolarized \( P = 0 \) excitations in small systems. This is consistent with the fact that the unpolarized excitations are unstable in higher LLs because of the long-range nature of the effective exchange interaction, which increases the energy of the skyrmion-like pseudospin-unpolarized state.

The elementally charge excitation gaps at the fractional fillings \( \nu_n = 1/3 \) are shown in Fig. 2. The pseudospin (valley)-polarized \( P = 1 \) excitation gap \( \Delta_e \) for \( n = 0 \) SLG is 0.101 in units of
Figure 1. Lowest charge excitation gaps in SLG and BLG at $\nu_n = 1$ in the $n = 0, 1$ and 2 LLs in the spherical geometry. $N_e$ is the number of electrons in the unit cell. Closed circles represent the pseudospin-unpolarized $P = 0$ (skyrmion) excitation gaps and open circles represent nearly pseudospin-polarized $P = 1 - 2/N_e$ excitation gaps. The crosses on the vertical axis represent results obtained by Hartree-Fock calculations[28].

Figure 2. Pseudospin (valley)-polarized excitation gap $\Delta_c$ and the pseudospin (valley)-unpolarized (skyrmion) excitation gap $\Delta_s$ at $\nu_n = 1/3$ in SLG ($n = 0$ and 1 LLs) and in BLG ($n = 2$ LL).

$e^2/(\ell B)$ in the thermodynamic limit, which is in good agreement with the previous work[15]. In the $n = 1$ LL of SLG, $\Delta_c$ is 0.115, which is larger than 0.101 in the $n = 0$ LL of SLG. Such enhancement of the excitation energy in $n = 1$ LL is obtained in the energy spectra of finite system[5].

In BLG, $\Delta_c = 0.103$ in the $n = 2$ LL, which is also slightly larger than that in the $n = 0$ LL of SLG. This increase in $\Delta_c$ in higher LLs is consistent with the increase in the difference in Haldane’s pseudopotential between $m = 1$ and 3; $V_1^n - V_3^n$ are 0.168 in units of $e^2/(\ell B)$ for BLG in the $n = 2$ LL, 0.198 for SLG in the $n = 1$ LL, and 0.166 for SLG in the $n = 0$ LL.

To study the pseudospin structure in the unpolarized excited states, we compare our numerical results with the Hartree-Fock (HF) trial states of skyrmions [23, 24, 25, 26, 27, 28].
ν are mapped onto the ν = 3.2. The HF trial state of quasihole skyrmions at ν = 1 is written in the form[10]

\[
|\Psi_{sk}\rangle = \prod_{m=-N_\phi/2}^{N_\phi/2} [\alpha_m c_{mK}^\dagger + \beta_m c_{m+1K}^\dagger]|0\rangle,
\]

Figure 3. Expectation values, \(\langle c_{m\tau}^\dagger c_{m\sigma}\rangle\), in pseudospin (valley) unpolarized excited states with one extra flux at \(\nu_n = 1\) and 1/3. \(N_\phi\) is the total flux.

where \(\langle c_{mK}^\dagger c_{mK}\rangle = |\alpha_m|^2\) and \(\langle c_{mK'}^\dagger c_{mK'}\rangle = |\beta_{m-1}|^2\). We have calculated the expectation values \(\langle c_{m\tau}^\dagger c_{m\sigma}\rangle\) from the wave function obtained in the present DMRG study. The results for \(\nu_1 = 1\) in SLG indicate that they are approximately given by \(\langle c_{m\tau}^\dagger c_{m\sigma}\rangle = 1/2 \mp m/N_\phi\) for \(\tau = K\) and \(\tau = K'\) as shown in Fig. 3(a). Similar results are also obtained for \(\nu_n = 1/3\) in the \(n = 0\) and 1 LLs of SLG as shown in Fig. 3(b), which shows that the pseudospin-unpolarized elementally charged excitations at these fillings are pseudospin (valley) skyrmions.

As seen in conventional 2DEGs, \(\nu = 1/3\) (valley or spin)-unpolarized excited states can be lower in energy than the polarized excited states. Indeed, as shown in Fig. 2, the unpolarized excitation gaps \(\Delta_s\) in SLG are 0.03 in the \(n = 0\) LL and 0.05 in the \(n = 1\) LL, which are much smaller than the polarized excitation gaps \(\Delta_e\) in the \(n = 0\) and 1 LLs, respectively. In the case of BLG, however, we find that valley unpolarized excited states have higher energies than polarized excited states. Consequently, the activation energy at \(\nu_2 = 1/3\) in BLG is 2-3 times larger than that in SLG.

3.2. \(\nu_n = 2/5\) and 2/3 states

According to the composite fermion theory[29], \(\nu = m/(1 + 2m)\) fractional quantum Hall states are mapped onto the \(\nu_{\text{eff}} = m\) integer quantum Hall states. The \(\nu = 2/5\) fractional quantum Hall state is then mapped onto the \(n = 2\) integer quantum Hall state, where the lowest LL is doubly occupied by pseudospin-up and pseudospin-down electrons. We therefore expect a pseudospin-unpolarized ground state at \(\nu_{n} = 2/5\). In the \(n = 0\) LL of SLG, this is confirmed by the DMRG calculation as shown in Table 1. On the other hand, in the \(n = 1\) LL of SLG, the ground state is pseudospin-polarized state.

The pseudospin (valley)-unpolarized excitation gap \(\Delta_s\) at \(\nu_n = 2/5\) is also shown in Table 1. The \(\Delta_s\) from the unpolarized ground state in the \(n = 0\) LL of SLG is 0.04 \(e^2/(\epsilon\ell_B)\), and that from the polarized ground state in the \(n = 1\) LL of SLG is 0.035 \(e^2/(\epsilon\ell_B)\). In BLG, the polarized excitation gap is smaller than the unpolarized excitation gap, and \(\Delta_e = 0.052\).

We finally study the valley polarization in the ground state and the elementally charged excitations at \(\nu_n = 2/3\). The ground state at \(\nu_n = 2/3\) in the \(n = 0\) LL of SLG is pseudospin
Table 1. Pseudospin (valley) polarization in the ground state and the lowest charge excited state, and the unpolarized excitation gap $\Delta_s$ and the polarized excitation gap $\Delta_c$ extrapolated to the thermodynamic limit at the effective filling $\nu_n$ in the $n$th LL of single-layer graphene (SLG) and bilayer graphene (BLG).

| $\nu_n$ | LL | ground state | excited state  | $\Delta_s$ | $\Delta_c$ |
|---------|----|--------------|----------------|------------|------------|
| 1       | SLG 0 | polarized | skyrnion | 0.63       |            |
| 1       | SLG 1 | polarized | skyrnion | 0.28       |            |
| 1       | SLG 2 | polarized | skyrnion | 0.42       |            |
| 1       | BLG 2 | polarized | skyrnion | 0.48       |            |
| $1/3$   | SLG 0 | polarized | skyrnion | 0.03       | 0.101      |
| $1/3$   | SLG 1 | polarized | skyrnion | 0.05       | 0.115      |
| $1/3$   | BLG 2 | polarized | polarized | 0.103      |            |
| $2/5$   | SLG 0 | unpolarized | unpolarized | 0.04 (0.050)[30] |            |
| $2/5$   | SLG 1 | polarized | skyrnion | 0.035      | 0.058      |
| $2/5$   | BLG 2 | polarized | polarized | 0.052      |            |
| $2/3$   | SLG 0 | unpolarized | unpolarized | 0.08 (0.101)[30] |            |
| $2/3$   | SLG 1 | polarized | unpolarized | 0.10       | 0.115      |
| $2/3$   | BLG 2 | polarized | polarized | 0.103      |            |

unpolarized. However, in the $n = 1$ LL of SLG and the $n = 2$ LL of BLG, the size dependence of the polarization energy shows that the pseudospins are fully polarized in the ground state.

The valley unpolarized excitation gap $\Delta_s$ from the unpolarized ground state in the $n = 0$ LL of SLG is $0.08 \frac{e^2}{(\epsilon \ell_B)}$. In the $n = 1$ LL of SLG, we find that $\Delta_s$ is 0.10. The valley unpolarized elementally charge excitations at $\nu_n = 2/3$ in the $n = 1$ LL of SLG are not skyrnion-like pseudospin-textured states.

4. Summary
Our DMRG calculation confirms various types of quantum Hall states in graphene at $\nu_n = 1, 1/3, 2/5,$ and $2/3$ in the $n = 0$ and $1$ LLs of SLG and in the $n = 2$ LL of BLG. These results are summarized in Table 1, where the pseudospin polarizations for the ground state and the lowest charge excited state are listed with the elementally charge excitation energies $\Delta_c$ and $\Delta_s$. The elementally charge excitations are obtained by increasing or decreasing the flux quantum number $N_{\phi}$ by 1 for $\nu = 1, 1/3,$ and $2/5$, and by increasing or decreasing the flux quantum number by adding or removing a single electron in the system for $\nu = 2/3$. We have studied both (a) pseudospin-polarized excitations (Laughlin’s quasiholes and quasiparticles) and (b) pseudospin-unpolarized excitations (quasihole and quasiparticle skyrmions at $\nu_n = 1$ and $1/3$ in the $n = 0$ and $1$ LLs of SLG, and at $\nu_n = 1$ in the $n = 2$ LL of BLG). The activation energies obtained in finite systems are extrapolated to the thermodynamic limit, which give theoretical predictions for future experimental studies of the fractional quantum Hall states in graphene.

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