Coupled charge and valley excitations in graphene quantum Hall ferromagnets

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Graphene is a two-dimensional carbon material with a honeycomb lattice and Dirac-type low-energy spectrum. In a strong magnetic field, where Coulomb interactions dominate against disorder broadening, quantum Hall ferromagnetic states realize at integer fillings. Extending the quantum Hall ferromagnetism to the fractional filling case of massless Dirac fermions, we study the elementally charge excitations which couple with the valley degrees of freedom (so-called valley skyrmions). With the use of the density matrix renormalization group (DMRG) method, the excitation gaps are calculated and extrapolated to the thermodynamic limit. These results exhibit numerical evidences and criterions of the skyrmion excitations in graphene.

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I. INTRODUCTION

A recent experimental realization of single-layer graphene sheets\textsuperscript{1} has made it possible to confirm a number of theoretical predictions of intriguing electric properties of massless Dirac fermion systems\textsuperscript{2} including unconventional quantum Hall effects (QHE)\textsuperscript{3,4} with the half-integer Hall conductivity\textsuperscript{2} as

\[ \sigma_{xy} = \frac{4e^2}{h}(n + \frac{1}{2}) \]  

at \( \nu = \pm 2, \pm 6, \pm 10, \cdots \), where a factor 4 is the Landau level (LL) degeneracy, accounting for spin and valley symmetry in graphene. \( \nu = 2\pi \ell_B^2 \rho \) is the filling factor, \( \ell_B = \sqrt{\hbar/eB} \) is the magnetic length, \( \rho \) is the carrier density measured from charge neutral Dirac point.

In addition to these unconventional quantized values, which can be solely understood on the basis of the massless Dirac fermion spectrum in a magnetic field:

\[ E_n = \text{sgn}(n)\hbar v_F \sqrt{2n}/\ell_B, \]  

recent experimental studies in a sufficiently strong magnetic field revealed new quantum Hall states at \( \nu = 0, \pm 1, \pm 4, \pm 8 \) where the electron-electron interaction may play a crucial role. Here relevant energy scales in graphene in a magnetic field are (i) Landau level (LL) separation between \( n = 0 \) and \( n = \pm 1 \), \( \hbar \omega_0 \equiv \sqrt{2}\hbar v_F/\ell_B \simeq 400\sqrt{B/T}|K| \), (ii) Zeeman coupling, \( \Delta_z \equiv g\mu_B|B| \simeq 1.5\times(B/T)|K| \), and (iii) the Coulomb energy, \( e^2/\ell_B \simeq 100\sqrt{B/T}|K| \). The activation energy measurements\textsuperscript{5} have shown that at \( \nu = \pm 4 \) the gap has linear \( B \) dependence and reasonably corresponds to \( \Delta_z \), indicating Zeeman spin splitting. At \( \nu = \pm 1 \), however, the gap is approximately scaled by \( \sqrt{B} \), which indicates that the gap originates from the Coulomb interaction. There have been a number of theoretical investigations of these states, and there are two leading theoretical scenarios for the origin of the gap. One is the quantum Hall ferromagnetism (QHF)\textsuperscript{6} in which valley degrees of freedom, referred to as pseudospins, spontaneously split via the exchange energy at \textit{all} integer fillings\textsuperscript{8,9,10,11,12,13}. Second is the spontaneous mass generation\textsuperscript{14,15,16} which predicts a gap \textit{only} in the \( n = 0 \) LL. Although they are not entirely orthogonal to each other and the order parameters in the two theories can coexist\textsuperscript{18} excitation properties, including the existence of gaps in \( n \neq 0 \) LLs, are different.

In the QHF theory, the ground state at \( \nu_n = 1 \), where \( \nu_n \) is the filling factor for \( n \)th Landau level defined by

\[ \nu_n = \nu - 4(n - 1/2), \]  

is fully spin and valley polarized, and the wave function can be represented by

\[ |\Psi\rangle = \prod_m c_m^\dagger |0\rangle, \]  

where we assign the valley \( K \) and \( K' \) in graphene as \( z \)-component of pseudospin \( \tau = K \) or \( K' \). Excitations from the symmetry broken states are described by (pseudo)spin wave and (pseudo)spin textures called skyrmions\textsuperscript{18,19,20,21,22} or other types, depending on the LL index \( n \). Yang et al\textsuperscript{19} estimated skyrmion excitation energy within the framework of Hartree-Fock (HF) approximation.

The fractional quantum Hall effects (FQHE) in graphene have been studied by Apalkov and Chakraborty\textsuperscript{23}. As a consequence of the relativistic nature of electrons in graphene, the effective electron-electron interactions in \( n \neq 0 \) LLs differ from that of conventional two-dimensional systems\textsuperscript{24,25} with the use of the exact diagonalizations they have calculated the magnetoroton energy at \( \nu_n = 1/3 \) when spin and valley are fully polarized. Their results show that the magnetoroton energy in the \( n = 1 \) LL is larger than that in the \( n = 0 \) LL in finite systems\textsuperscript{26}. Nevertheless, the magnetoroton excitation is charge neutral and it is not connected to the charged gap which is necessary to realize the FQHE. Moreover, the valley degrees of freedom which couple with charge excitations must be taken into account since there is no external symmetry breaking effect for valley degrees of freedom. The
excitation structures and the size of the activation gaps in the thermodynamic limit have not yet been clarified systematically.\(^\text{24}\)

In this paper we extend the quantum Hall ferromagnetism to the fractional filling case of graphene and show analogous properties of pseudospin ferromagnetism and topological excitations in the fractional quantum Hall effect (FQHE) states in graphene. We start with the projected Coulomb interaction Hamiltonian onto a certain LL, and study charge and valley excitations, where 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 the Zeeman splitting. We calculate the exact wave functions of QHF ground states and low-energy excited states basing on the density matrix renormalization group (DMRG) method, and confirm the existence of the skyrmion excitations of valley degrees of freedom not only at integer filling \(\nu = 1\) but also at fractional filling \(\nu = 1/3\) for the LL index \(n = 0, 1\) and 2. The skyrmion energies at these fractions are calculated and extrapolated to the thermodynamic limit. The existence of the finite gaps at \(\nu_n = 1\) in the \(n \neq 0\) LLs strongly supports the QHF but not the mass generation scenarios. We note that the DMRG method is suitable for the present study, since we need to treat a large number of basis of the many-body Hilbert space including the pseudospin degrees of freedom. To the best of our knowledge, there is no numerical work so far to estimate reliable extrapolated energies of the skyrmion excitation in the thermodynamic limit even in the conventional FQHE systems.\(^\text{24}\)

II. MODEL AND METHOD

We assume that the total magnetic field is strong enough to cause complete spin splitting, and neglect spin flip excitations. We also neglect LL mixing for simplicity, although the ratio \((e^2/\ell_B)/(\hbar \omega_0)\) is not so small. The effect of LL mixing is discussed later. Taking account of valley degrees of freedom, we apply the DMRG method\(^\text{26,27,28}\) on the spherical geometry\(^\text{29,30,31,32,33}\).

The projected Hamiltonian onto the \(n\)th Landau level is written\(^\text{30}\)

\[
H^{(n)} = \sum_{i<j} \sum_m V^{(n)}_{m} P_{ij}[m],
\]

where \(P_{ij}[m]\) projects onto states in which particles \(i\) and \(j\) have relative angular momentum \(hm\), and \(V^{(n)}_{m}\) is their interaction energy in the \(n\)th Landau level.\(^\text{30}\) Using the relativistic form factor in the \(n\)th Landau level\(^\text{22}\)

\[
F_0^R(q) = L_0 \left( q^2/2 \right)
\]

and

\[
F_{n \neq 0}^R(q) = (1/2) \left[ L_{|n|} \left( q^2/2 \right) + L_{|n|+1} \left( q^2/2 \right) \right],
\]

the pseudopotentials\(^\text{29,30}\) are given by

\[
V^{(n)}_{m} = \int_0^{\infty} \frac{dq}{2\pi} q V(q) e^{-q^2} \left[ F_{n}^R(q) \right]^2 L_m(q^2).
\]

Here \(L_m(x)\) are the Laguerre polynomials. The corresponding integrals for electrons on the surface of a sphere which are used in the present work are described in Refs.\(^\text{30,31,32}\). Note that our Hamiltonian Eq. (5) has SU(2) symmetry in the valley degrees of freedom. A symmetry breaking correction to Eq. (5) which stems from the honeycomb lattice structure of graphene\(^\text{33}\) is of order of \(a/\ell_B\) (\(a\) being a lattice spacing) in units of \(e^2/\ell_B\) and neglected in the following.

We calculate the ground state wave function using the DMRG method\(^\text{26}\), which is a real space renormalization group method combined with the exact diagonalization method. The DMRG method provides the low-energy eigenvalues and corresponding eigenvectors of the Hamiltonian within a restricted number of basis states. 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 in each block.\(^\text{27,28}\)

In the sphere geometry, the pseudospin (valley) polarized ground state at \(\nu = 1/q\) (\(q\) being an odd integer), the Laughlin state\(^\text{20}\) realizes when the total flux \(N_\phi\) is given by\(^\text{30}\)

\[
N_\phi(\nu, N_e) = \nu^{-1}(N_e - 1),
\]

where \(N_e\) is the number of electrons in the system. Elementary charged excitations from this pseudospin polarized ground state correspond to the ground state configurations of the system with additional/missing flux \(\pm 1\). In the following, we study two types of excitations: Laughlin’s quasiholes (quasiparticles)\(^\text{31}\) and skyrmion quasiholes (quasiparticles)\(^\text{28,19,20,21,22}\). Laughlin’s quasiholes

![FIG. 1: The pseudospin (valley) polarized excitation gap \(\Delta_e\) and the pseudospin (valley) unpolarized (skyrmion) excitation gap \(\Delta_s\) at \(\nu_n = 1/3\) in the \(n = 0\) and 1 LLs.](image-url)
(quasiparticles) correspond to the (pseudo)spin polarized excitations with ±1 flux, whose creation energy is given by

\[ \Delta^\pm = E(N_\phi \pm 1, P = 1) - E(N_\phi, P = 1), \]

where ± represents quasiholes and quasiparticles, respectively, and P is the polarization ratio of the pseudospin, i.e., \( P \equiv (N_K - N_{K'})/(N_K + N_{K'}) \) with \( N_K \) \( N_{K'} \) being the number of electrons in \( K \) \( K' \) valley.

Skyrmion quasiholes (quasiparticles) correspond to the (pseudo)spin singlet excitations, and their creation energy is given by

\[ \Delta^\pm_s = E(N_\phi \pm 1, P = 0) - E(N_\phi, P = 1), \]

which could be smaller than \( \Delta^\pm \).

The activation energy, referred to as the gap in the following, is given as a sum of these quasihole and quasiparticle energies, \( \Delta_c = \Delta^+_c + \Delta^-_c \) for pseudospin polarized excitations, and \( \Delta_s = \Delta^+_s + \Delta^-_s \) for pseudospin unpolarized excitations.

### III. Results

Figure 1 shows \( \Delta_c \) and \( \Delta_s \) at \( \nu_n = 1/3 \) as a function of \( 1/N_c \). In the \( n = 0 \) LL, the pseudospin (valley) polarized excitation gap \( \Delta_c \) is 0.101 \( e^2/(\ell_B) \) in the thermodynamic limit in good agreement with the previous work.\(^{24}\) In the \( n = 1 \) LL, \( \Delta_c = 0.115 \), which is larger than 0.101 in the \( n = 0 \) LL. This enhancement of \( \Delta_c \) stems from the unique properties of the pseudopotentials in \( n = 1 \) LL for relativistic particles; \( V^{(1)} = V^{(0)} \).\(^{22}\) The magneto-roton excitation energy in the \( n = 1 \) LL is also larger than that of the \( n = 0 \) LL.\(^{23}\)

The larger excitation gap in the higher LL has also been obtained for the pseudospin (valley) unpolarized excitations \( \Delta_s \); the unpolarized excitation gap \( \Delta_s \) in the \( n = 1 \) LL is 0.05 \( e^2/(\ell_B) \), which is larger than that in the \( n = 0 \) LL, \( \Delta_s = 0.03 \). We note that similar analysis has been done in Ref.\(^{23} \) with qualitatively different results.

The results for \( \nu_n = 1 \) are shown in Fig.2. The extrapolated value of the pseudospin unpolarized excitation gap \( \Delta_s \) for \( n = 0 \) LL is 0.63 \( e^2/(\ell_B) \), which is consistent with the previous HF studies and exact diagonalization studies.\(^{25}\) Even in the \( n = 1 \) and \( n = 2 \) LLs, \( \Delta_s \) are almost the same with the HF results obtained in the four-component model for graphene.\(^{26}\) These results show that the HF trial states for skyrmion excitation is essentially correct.

In the above analysis, we have neglected the effect of LL mixing. When we study higher LLs, we need to take account of LL mixing, because LL spacing of graphene decreases with the increase in its index \( n \). In conventional two-dimensional systems, it has been argued that LL mixing reduces the activation gap in the fractional QHE regimes.\(^{24}\)

To study the skyrmion-like structure in the pseudospin unpolarized excited states, we have calculated the two-particle correlation functions \( g_{rr'}(r) \).\(^{22,29-30} \) Figure 3 shows \( g_{rr'}(r) \) for the pseudospin unpolarized quasihole state at \( \nu_1 = 1/3 \). We find clear peak structure around the origin \( r = 0 \) for the electrons in the same valley, \( g_{KK}(r) \). On the other hand, the maximum appears at the opposite side on the sphere \( (r = \pi R) \) for the electrons in different valleys, \( g_{K'K}(r) \). These structures are consistent with the skyrmion-like pseudospin structure.

The HF trial state of quasihole skyrmions at \( \nu_n = 1 \) is written in the form:

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

FIG. 2: The pseudospin unpolarized (skyrmion) excitation gap \( \Delta_s \) at \( \nu_n = 1 \) in the \( n = 0 \), 1 and 2 LLs. The crosses on the vertical axis represent the results obtained by HF calculations.\(^{22}\) The pseudospin polarized excitation gaps in \( n = 2 \) LL are plotted by open circles.

FIG. 3: Two-particle correlation functions \( g_{rr'} \) of quasihole skyrmion state at \( \nu_1 = 1/3 \).
The skyrmion excitations at \( \nu_n = 1 \) are stable up to \( n = 2 \) LLs, as shown in Fig.5, in which the polarization energies of the quasi-hole skyrmions \( \Delta E(P) = E(N_\phi + 1, P) - E(N_\phi + 1, P = 0) \) are plotted. The clear \( P^2 \)-dependence shown in Fig.5 and its inset confirms that the pseudospin singlet state is the lowest excitation for \( n = 0, 1 \) and 2 LLs. In the \( n = 2 \) LL, the minimum at \( P = 0 \) appears only for systems whose number of electrons is larger than 16; that means the skyrmion excitations are stable only for large systems. This is also shown in Fig.2 as an upward cusp in \( \Delta_n \) at \( N_e \sim 18 \); the pseudospin singlet state becomes the lowest when the number of electrons exceeds 18, while the pseudospin polarized states marked by the open circles become the lowest for systems with \( N_e < 18 \).

In higher LLs (\( n \geq 3 \)), pseudospin singlet excitations have not been seen as the lowest excitation within our calculations up to 40 electrons. These results are qualitatively consistent with the HF analysis in Ref.\(^{10} \) which predicts the skyrmion excitation gap is smaller than the HF quasiparticle gap only for lower LLs below \( n = 3 \). The skyrmion excitation gap in \( n = 3 \) LL is close to the HF quasiparticle gap and it is difficult to stabilize skyrmions in \( n = 3 \) LL.

**IV. DISCUSSION**

Our DMRG calculation confirms the valley polarized ground state at \( \nu_n = 1 \) for \( n \leq 2 \) LLs and at \( \nu_n = 1/3 \) for \( n \leq 1 \) LLs. The (pseudo)spin polarized ground state at \( \nu_n = 1/q \) can be written simply as Laughlin’s Jastrow function\(^2 \) and elementally charge excitations are obtained by increasing or decreasing the flux quantum number \( N_\phi \) by 1. We have studied both (a) pseudospin polarized excitations (Laughlin’s quasiholes and quasiparticles) and (b) pseudospin unpolarized excitations (quasihole skyrmions and quasiparticle skyrmions). 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. In a high quality graphene sample, the \( \nu_n = 1 \) QH states have been observed in the \( n = 0 \) LL.\(^{22} \) Very recently, suspended graphene sheets with metallic contacts were succeeded.\(^{23} \) The reported mobility \( 2 \times 10^5 \) cm\(^2\)/Vs is close to the crudely obtained critical value where the FQHE realizes within available magnetic field \( \lesssim 50 \) T, estimated from the theory described in Ref.\(^8 \) and the skyrmion gap \( \Delta_s \approx 0.05(e^2/\epsilon d_B) \) obtained in the present work.

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