

Spin and valley ordering of fractional quantum Hall states in monolayer graphene

Ngoc Duc Le  and Thierry Jolicoeur 

Université Paris-Saclay, CNRS, CEA, Institut de Physique Théorique, Paris, France



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We study spin and valley ordering in the quantum Hall fractions in monolayer graphene at Landau level filling factors $\nu_G = -2 + n/3$ ($n = 2, 4, 5$). We use exact diagonalizations on the spherical as well as toroidal geometry by taking into account the effect of realistic anisotropies that break the spin/valley symmetry of the pure Coulomb interaction. We also use a variational method based on eigenstates of the fully SU(4) symmetric limit. For all the fractions we study, there are two-component states for which the competing phases are generalizations of those occurring at neutrality $\nu_G = 0$. They are ferromagnetic, antiferromagnetic, charge-density wave, and Kékulé phases, depending on the values of Ising or XY anisotropies in valley space. The varying spin-valley content of the states leads to ground-state quantum numbers that are different from the $\nu_G = 0$ case. For filling factor $\nu_G = -2 + 5/3$, there is a parent state in the SU(4) limit that has a flavor content (1, 1/3, 1/3, 0) where the two components that are one-third filled form a two-component singlet. The addition of anisotropies leads to the formation of new states that have no counterpart at $\nu_G = 0$. While some of them are predicted by the variational approach, we find notably that negative Ising-like valley anisotropy leads to the formation of a state that is a singlet in both spin and valley space and lies beyond the reach of the variational method. Also fully spin polarized two-component states at $\nu = -2 + 4/3$ and $-2 + 5/3$ display an emergent SU(2) valley symmetry because they do not feel point-contact anisotropies. We discuss implications for current experiments concerning possible spin transitions.

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I. INTRODUCTION

The fractional quantum Hall effect [1] (FQHE) occurs in two-dimensional electron systems in a strong perpendicular field, and it is characterized notably by a gap for all charged excitations at some fractional filling ν of the Landau levels. Such gaps are due to electron-electron Coulomb interactions. In this regime, there are excitations with fractional charges and also statistics, Abelian or even non-Abelian in some cases. There are possible opportunities for fabrication of new electronic devices using the non-Abelian statistics for quantum computation [2] or the interlayer phase coherence that occurs in bilayer systems for dissipationless devices [3].

For many years after its discovery, the FQHE was studied almost only in the special two-dimensional electron gases formed in GaAs/GaAlAs heterojunctions. In this setup, the electron Landé g -factor and the dielectric constant of the host material conspire to reduce the Zeeman energy with respect to the Coulomb energy scale. As a consequence, the spin degree of freedom in the lowest Landau level cannot be considered as frozen by the external magnetic field, and FQHE ground states as well as their excited states are not always fully spin-polarized. This leads notably to quasiparticles that have nontrivial spin textures called skyrmions [4,5]. The study of electron gases in materials such as AlAs [6] added an extra degeneracy due to the relevance of several valleys for the electronic states.

The discovery of monolayer graphene has opened an even richer arena [7–23] for the FQHE since there is also an additional twofold valley degeneracy that comes into play.

The central $N = 0$ Landau level of monolayer graphene is approximately fourfold-degenerate because of spin and valley degrees of freedom, and it is partially filled for a range of filling factor $-2 \leq \nu_G \leq +2$. Integer quantum Hall states [24] also appear at fillings $\nu_G = 0, \pm 1$, and this is an instance of quantum Hall ferromagnetism: Coulomb interactions lead to gap opening also at these integer filling factors.

At neutrality $\nu_G = 0$ theory predicts [25,26] competing phases with various patterns of spin and valley ordering. One can have ferromagnetic, antiferromagnetic, Kékulé, or charge-density-wave states. While these states are degenerate if one makes the approximation of full SU(4) symmetry in spin/valley space, anisotropies will select one of these states in real samples. Changing parameters like the ratio of Zeeman energy to Coulomb energy can induce transitions between such ground states. An appealing scenario has been presented to explain a transition from an insulator to a quantum spin Hall state as the transition between the canted antiferromagnetic state and the ferromagnetic state. When the central Landau level is partially filled, we expect the formation of FQHE states, and they will also have some pattern of spin and valley ordering. The fully SU(4) symmetric case has been explored in many works [27–36]. Inclusion of anisotropies has been studied by Abanin *et al.* [37] at the level of wave functions, and an extension of Hartree-Fock theory has also been proposed by Sodemann and MacDonald [38]. While the results of mean-field theory have been confirmed by exact diagonalizations [39] for $\nu_G = 0$, this has not been checked for the fractional quantum Hall states.

In this paper, we introduce a set of variational wave functions constructed out of exact eigenstates of the SU(4) symmetric limit. The wave functions are dressed by a spin and flavor configuration that is determined by minimizing the energy. The anisotropy energy can be expressed solely in terms of the pair correlation function of the parent symmetric state. This approach generalizes the mean-field treatment of quantum Hall ferromagnetism. Within this framework, we obtain the phase diagrams for the fractions $\nu_G = -2 + n/3$ ($n = 2, 4, 5$). We also perform extensive exact diagonalizations in the spherical [40,41] and torus geometry to check the validity of the variational approach. For fractions $\nu_G = -2 + n/3$ ($n = 2, 4, 5$) there are two competing ground states in the SU(4) limit. At $\nu_G = -2 + 2/3$, we have the fully polarized particle-hole partner of the $\nu_G = -2 + 1/3$ as well as a singlet state with two-component structure, well known from previous studies [42]. At $\nu_G = -2 + 4/3$, the competing states are the two-component particle-hole partner of the singlet with spin-valley content $(2/3, 2/3, 0, 0)$ and a state with a filled shell by addition to the $\nu = 1/3$ Coulomb ground state with spin-valley content $(1, 1/3, 0, 0)$. At $\nu_G = -2 + 5/3$, we have a two-component state $(1, 2/3, 0, 0)$ where the $2/3$ state is the fully polarized state and there is also a three-component state $(1, 1/3, 1/3)$ that is built from a filled Landau level plus a spin-singlet $2/3$ state as pointed out by Sodemann and MacDonald [38]. The phase diagrams from the variational method are in agreement with the diagonalization results except for the fraction $\nu_G = -2 + 5/3$, where a large portion of the phase space is occupied by a correlated singlet state that cannot be reproduced by our set of wave functions. To clarify its structure, we compute the pair correlation function for all combinations of spin/valley indices, and we find that there is an enhanced probability for pair formation of opposite spin. We discuss possible ways of favoring this new phase in real samples of graphene. While the regions of stability of the different patterns in spin and valley configurations are correctly predicted variationally, the quantum numbers are different in several important cases involving antiferromagnetism. Also we observe that fully polarized phases for the states $(1, 1/3, 0, 0)$ and $(1, 2/3, 0, 0)$ still form SU(2) valley multiplets even though the Hamiltonian does not have such a symmetry. This is due to the special point-contact form of the anisotropies. For all the fractions we have studied there are in general spin transitions when one varies the magnetic field. Multicomponent states are preferred at small Zeeman energies.

In Sec. II we introduce the Coulomb interactions and anisotropies that govern the spin/valley ordering of quantum Hall states. Section III give results for fractions $\nu_G < -1$. In Sec. IV we give evidence for similar physics at $\nu_G = -2 + 4/3$ and $\nu_G = 0$. The phases for the three-component state at $\nu_G = -2 + 5/3$ are discussed in Sec. V. We give a simplified treatment of spin transitions in Sec. VI and Sec. VII contains our conclusions.

II. INTERACTIONS AND ANISOTROPIES IN MONOLAYER GRAPHENE

We now discuss the effective electron-electron interactions within the $N = 0$ Landau level of monolayer graphene. The

Coulomb interaction is SU(4) symmetric to an excellent approximation. It leads to an energy scale that is constructed out of the magnetic length $E_C = e^2/(\epsilon\ell)$, where $\ell = \sqrt{\hbar/(eB)}$, and ϵ is the dielectric permittivity of the system. The unitary SU(4) symmetry mixing spin and valley degrees of freedom is, however, reduced by several phenomena. It has been proposed to encapsulate these splittings into the following Hamiltonian [26,43] acting only on the valley degrees of freedom:

$$\mathcal{H}_{\text{aniso}} = \sum_{i<j} [g_{\perp}(\tau_i^x \tau_j^x + \tau_i^y \tau_j^y) + g_z \tau_i^z \tau_j^z] \delta^{(2)}(\mathbf{r}_i - \mathbf{r}_j), \quad (1)$$

where the τ_i^{α} Pauli matrices operate only in valley space. It is convenient to parametrize the two coefficients $g_{\perp,z}$ with an angular variable θ :

$$g_{\perp} = g \cos \theta, \quad g_z = g \sin \theta, \quad (2)$$

in addition to an overall strength g , which we take as positive. It is convenient to convert the parameters $g_{\perp,z}$ into two separate energy scales:

$$u_{\perp} = \frac{g_{\perp}}{2\pi\ell_B^2}, \quad u_z = \frac{g_z}{2\pi\ell_B^2}. \quad (3)$$

One can define dimensionless strengths of anisotropies by factoring out the Coulomb energy scale:

$$\tilde{g} = (g/\ell_B^2)/[e^2/(\epsilon\ell_B)]. \quad (4)$$

One-body energy level splitting occurs through the Zeeman effect that acts on the spins and sublattice splitting onto the valley indices:

$$\mathcal{H}_{\text{1body}} = -\epsilon_Z \sum_i S_i^z + \Delta_{AB} \sum_i T_i^z. \quad (5)$$

The Zeeman energy ϵ_Z is $g\mu_B B_T$, where B_T is the total field, and the Landé factor $g = 2$ since spin-orbit coupling is negligible in graphene. The spin S^z is $\sigma^z/2$ and the valley isospin T^z is $\tau^z/2$. We note that the direction of the field is arbitrary due to spin rotation invariance. On the contrary, the sublattice symmetry breaking takes place between the two valleys. In the case of the commonly used hBN substrate, typical values of the splitting Δ_{AB} are of the order of 10 meV and are magnetic-field-independent. The special Hamiltonian Eq. (1) has some symmetry properties that are independent of the filling factor [44].

We note that the magnitude of the couplings $g_z, g_{\perp}$ is still uncertain. Constraints on their values come from the metal-insulator transition in a tilted field observed at neutrality [11].

If we consider the integer quantum Hall state at $\nu = 1$, then there is a set of exact eigenstates of the Coulomb problem with a closed form given by a single Slater determinant $|\Psi_{\nu=1}\rangle = \prod_m c_{m\alpha}^{\dagger} |0\rangle$, where $|\alpha\rangle$ is an arbitrary four-component vector in spin-valley space [45,46]. The integer m is the index of the orbital Landau level, and the product runs over all values of m , corresponding to complete filling of the level. This state is an exact eigenstate provided one neglects Landau level mixing. This fact is aptly called quantum Hall ferromagnetism [24]. The arbitrariness in the direction of $|\alpha\rangle$ is fixed presumably by lattice effects beyond the simple continuum models we consider [43]. Notably, such a wave function vanishes when electrons coincide in real space, and so it is insensitive to

perturbations like the anisotropies of Eq. (1). We now discuss the special case of graphene neutrality $\nu = 2$. At this filling factor, there are exactly two filled Landau levels. In the fully symmetric SU(4) limit, one notes that a Slater determinant is an exact eigenstate:

$$|\Psi_{\nu=0}\rangle = \prod_m c_{m\alpha}^\dagger c_{m\beta}^\dagger |0\rangle, \quad (6)$$

where the orbital index m (whose precise definition is geometry-dependent) takes all allowed values corresponding to complete integer filling, and α, β are two orthogonal vectors. Due to the SU(4) symmetry, these two vectors are arbitrary. The anisotropies will induce energy differences among all possibilities and determine the ground-state spin-valley ordering. The mean-field treatment is performed by taking the expectation value of the anisotropy Hamiltonian Eq. (1) in the Slater determinant of Eq. (6). The result is given by a functional of the two vectors α and β :

$$\begin{aligned} \epsilon_a &= \frac{1}{N_\phi} \langle \Psi_{\nu=0} | \mathcal{H}_{\text{aniso}} | \Psi_{\nu=0} \rangle \\ &= \sum_{i=x,y,z} u_i [\text{tr}(P_\alpha \tau_i) \text{tr}(P_\beta \tau_i) - \text{tr}(P_\alpha \tau_i P_\beta \tau_i)], \end{aligned} \quad (7)$$

where we have defined the anisotropy energy per flux quantum ϵ_a , the projectors onto the trial vectors:

$$P_\alpha = |\alpha\rangle\langle\alpha|, \quad P_\beta = |\beta\rangle\langle\beta|, \quad (8)$$

and the couplings are $u_x = u_y = u_\perp, u_z$. By minimization of this functional, one finds four phases in the absence of Zeeman energy: ferromagnetic (F), antiferromagnetic (AF), charge density wave (CDW), and Kékulé (KD).

All transitions between these various states are first-order within mean-field theory, and this is confirmed by exact diagonalizations [39]. With nonzero Zeeman energy, the most notable change is that the AF phase becomes canted (CAF). The tilted-field experiments of Ref. [11] enable the variation of the ratio of Zeeman versus Coulomb energy scales. Since there is a metal-insulator transition in this setup, a natural explanation is that they observe the CAF-F transition. To be consistent with this scenario, one deduces bounds on anisotropies $u_\perp \simeq -10\epsilon_z$, $u_z + u_\perp > 0$.

We now discuss trial wave functions that can be used to describe the fractional quantum Hall states with spin and valley degrees of freedom. We first make several remarks that apply to the SU(4) symmetric limit. Note that any SU(2) Coulomb eigenstate is also an SU(4) eigenstate. Only the degeneracy will change. If we have some SU(2) Coulomb eigenstate constructed with two spin-valley vectors α and β and filling factor $\nu_{\alpha\beta}$, then we can glue a filled $\nu = 1$ complete Landau level for any vector γ , and obtain another exact eigenstate of the Coulomb interaction with now filling factor $\nu = 1 + \nu_{\alpha\beta}$. The energy of this new state is now given by $E_{1+\nu_{\alpha\beta}} = E_1 + E_{\nu_{\alpha\beta}}$, where $E_1 = -\sqrt{\pi}/8E_C$ is the energy of the completely filled level. In first-quantized language, this gluing operation is the multiplication by the Vandermonde determinant of the $\nu = 1$ state. Note that this gluing operation also works if we use a single-component state $\hat{\Psi}_\alpha$ instead of $\hat{\Psi}_{\alpha\beta}$.

In addition to the full particle-hole symmetry mapping ν to $4 - \nu$, one can also perform a particle-hole symmetry on

only two flavors mapping (ν_1, ν_2) to $(1 - \nu_1, 1 - \nu_2)$, and the total filling is then transformed from ν to $2 - \nu$. Under this operation, the energy becomes $E_{2-\nu} = E_\nu + 2(1 - \nu)E_1$. These mappings allow us to identify at least some of the eigenstates found by exact diagonalization. Of course there are also multicomponent states that cannot be generated from the two-component case. Some of them have been found at filling factor $\nu = 2/3$ in a previous study [44]. It is possible also to use these mappings to construct trial wave functions once we have a one- or two-component state as obtained, for example, by the composite fermion construction [47,48]. For the fractions we study, which are most prominent in experiments, we cannot use known multicomponent generalizations [49,50] of the Laughlin wave function because they lead to more complicated fractional fillings.

We adhere to the view that anisotropies are not strong enough to destroy the Coulomb correlations in a given trial state. This means that the small symmetry-breaking perturbations Eq. (1) will choose the orientation of the free vectors α, β, γ in a trial state $\Psi = \{\prod_m c_{m\gamma}^\dagger\} \hat{\Psi}_{\alpha\beta}^\dagger |0\rangle$, where the operator $\hat{\Psi}_{\alpha\beta}^\dagger$ creates a state with two components α, β . Sodemann and MacDonald [38] have proposed an approximate scheme based on an extension of Hartree-Fock theory to estimate the anisotropy energy as a function of the arbitrary trial vectors. We note that it is in fact feasible to compute directly the expectation value of the Hamiltonian for anisotropies in the trial states, bypassing any Hartree-Fock-like approximation. Since the anisotropic interactions are purely pointlike, the expectation value of the Hamiltonian Eq. (1) can be expressed in terms of the pair correlation function at the origin $g_{\alpha\beta}(0)$ generalizing the formula for $\nu = 2$:

$$\epsilon_a = \sum_{i=x,y,z} u_i \sum_{\alpha\beta} g_{\alpha\beta}(0) [\text{tr}(P_\alpha \tau_i) \text{tr}(P_\beta \tau_i) - \text{tr}(P_\alpha \tau_i P_\beta \tau_i)], \quad (9)$$

where the pair correlation function is that of the trial wave function. We define a more compact notation:

$$\epsilon_a = \sum_{\alpha\beta} g_{\alpha\beta}(0) \mathcal{F}_{\alpha\beta}, \quad (10)$$

where now the sum over α, β runs over all values involved in the trial wave function. The sum runs only over distinct values due to the Pauli principle [$g_{\alpha\alpha}(0) = 0$]. If we consider trial states obtained by gluing a filled shell, then there are no nontrivial correlations between the completely filled shell and the other electrons: $g_{1\alpha}(0) = \nu_\alpha$. The case with two filled Landau levels $\nu_\alpha = \nu_\beta = 1$ gives the previous formula for the anisotropy energy Eq. (7). If we take a single-component state with filling ν_2 and glue a $\nu = 1$ shell, then we obtain an energy that is simply the $\nu = 2$ formula multiplied by a ν_2 factor. Hence without any further calculation, we can be sure that the phase diagram is identical to that of the $\nu = 2$ case with the same set of spin-valley vectors. However, since the number of electrons is different in the two components, the quantum numbers of the ground state are different from those of the $\nu = 2$ case.

We now discuss the case with three occupied flavors with content $(1, \nu, \nu)$. The trial state is now a two-component state with flavor content (ν, ν) with a filled shell $\nu = 1$ glued onto

it. The anisotropy energy is now given by

$$\epsilon_a^{(1,\nu,\nu)} = \nu[\mathcal{F}_{\alpha\beta} + \mathcal{F}_{\alpha\gamma}] + g_{\beta\gamma}(0)\mathcal{F}_{\beta\gamma}. \quad (11)$$

For the trial states we consider, the partially filled states will involve the two-component $\nu = 2/3$ and $2/5$ spin-singlet states that have a very small pair correlation between different spin values $g_{\alpha\beta}(0) \approx 10^{-3}$. This very small number only slightly changes the phase boundaries and can be safely discarded.

When discussing trial states, we omit the unoccupied spin-valley states when displaying the component structure of the wave function, i.e., $(1, 1/3, 0, 0)$ is written simply $(1, 1/3)$. However, when describing an irrep we use all four components, i.e., $(7, 4, 0, 0)$ stands for an $SU(4)$ irrep defined by its highest weight.

III. FRACTIONS FOR $\nu < 1$

A. The $\nu = 1/3$ state

At filling factor $\nu = 1/3$ the one-component Coulomb ground state is an exact (in the limit of no Landau level mixing) eigenstate of the $SU(4)$ symmetric case, and it is a member of the irrep with highest weight $(N_e, 0, 0, 0)$. This means that the spatial part of the wave function is multiplied by a fully symmetrized wave function with all electrons in the same spin/valley state. The Zeeman field will orient the spin component, and there will be a residual $SU(2)$ valley symmetry. Introduction of anisotropies Eq. (1) will have no effect on this eigenstate since the wave function exactly vanishes when two electrons coincide because of the Pauli principle, and the model anisotropies involve only contact interactions. In the real world, there will also be further anisotropies involving relative angular momentum 1 and more that will act upon the eigenstate. However, it is worth mentioning that theoretical estimates of anisotropies are much smaller than the values required to explain the tilted-field transition between the F and CAF states at $\nu_G = 0$. So this means that presumably also the anisotropies involving relative angular momentum 1 and higher are not well known and may be larger than naive estimates, so they could possibly be relevant even in the range of filling factor $\nu < 1$.

B. The $\nu = 2/3$ state

The situation is richer for $\nu = 2/3$. Several competing states are known to be present at this filling factor. First of all, there is the one-component particle-hole symmetric of the $\nu = 1/3$ state, which is again a one-component state. In the composite fermion description, this fully polarized state has negative effective flux, and composite fermions occupy two effective Λ levels [48]. With two components, one can also construct a singlet state where now only one CF Λ level is occupied by singlet pairs. For pure Coulomb interactions, the singlet state has lower energy than the polarized state by approximately $0.009E_C$ in the thermodynamic limit. These two states compete directly on the torus geometry, while on the spherical geometry they have a different shift: the polarized state is realized for $N_\phi = (3/2)N_e$ and the singlet state for $N_\phi = (3/2)N_e - 1$.

While these two states are well-established in two-component FQHE systems, we note that there is evidence [44] for the formation of three-component and four-component states that are slightly lower in energy by $\approx 0.002E_C$. These enigmatic states are not easily explained by composite-fermion theory, and finite-size limitations lead to a large uncertainty in energy difference estimation. Such states are formed for $N_\phi = (3/2)N_e - 2$ on the sphere, and they also appear on the torus geometry.

All these pure Coulomb eigenstates can be embedded in the four-component case giving rise to degenerate $SU(4)$ multiplets. Of course the $SU(4)$ singlet [44] observed for $N_e = 8$ is unaffected by anisotropies apart from a change in energy. The polarized $2/3$ state does not feel the δ -function interactions of Eq. (1), but the singlet state has a nonvanishing probability of having two electrons at the same location provided they have different flavors: $g_{\alpha\neq\beta}(0) \neq 0$. This probability is small and is known to be of the order of 10^{-3} from exact diagonalization or CF wave functions. As a consequence, the splitting induced by anisotropies is of order $g \times g_{\alpha\neq\beta}(0)$. If we use the variational approach, we obtain an energy functional that has exactly the same expression as in the $\nu = 2$ case apart from the overall scale. This means that the phase diagram is that of $\nu = 2$. We have checked by exact diagonalization that this phase diagram is correct beyond perturbation theory. Notably all characteristics of the phase transitions are unchanged between $\nu = 0$ and $2/3$. The ground-state quantum numbers of the finite system with $N = 6$ and $N_\phi = 8$ are consistent with the pattern of spin and valley ordering for $\nu = 2$.

IV. THE FRACTION $\nu = 4/3$

We now turn to the richer situation with fractions appearing for filling factors greater than 1 (and also less than 2 because of particle-hole symmetry). At the fraction $4/3$, we know that there are exact eigenstates in the $SU(4)$ symmetric limit obtained by adding a $\nu = 1$ shell to the $\nu = 1/3$ polarized eigenstate of the Coulomb problem. The flavor content of such a state is thus $(1, 1/3)$. There is also an eigenstate obtained by taking a $\nu = 2/3$ singlet involving only two flavors and making a particle-hole transformation on both flavors so that its final flavor content is $(2/3, 2/3)$. With the known properties of the particle-hole transformation in fact we already know that the $(2/3, 2/3)$ state has lower Coulomb energy than $(1, 1/3)$ from the energies of the parent states in the thermodynamic limit. This remark was made in Ref. [38]. Beyond these two exact eigenstates, it is not guaranteed that there are not intruders implying more components.

A. The $(1, 1/3)$ state

In the torus geometry, there is no shift so these two states directly compete when we fix the flux and the number of particles; they differ only by the flavor partitioning. In this geometry, the state $(1, 1/3)$ is an excited state and it is thus computationally demanding to study it.

In the sphere geometry for the first candidate $(1, 1/3)$ the total number of electrons is partitioned into two flavors $N_e = N_1 + N_2$, and N_1 electrons fully fill a spherical shell with flux

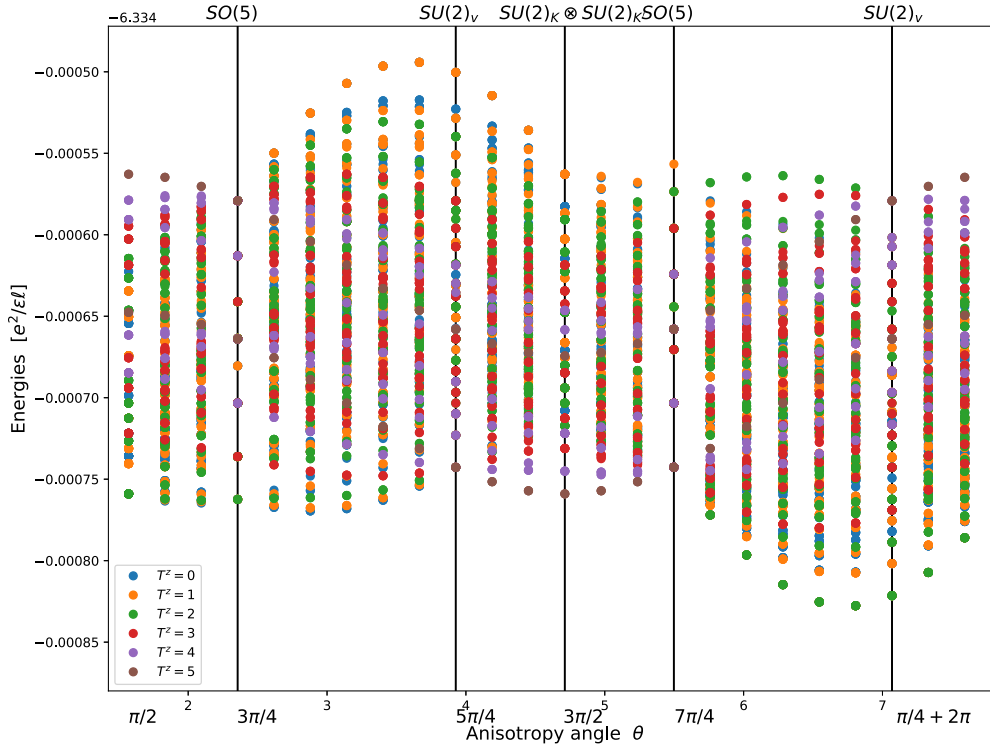


FIG. 1. Energy levels as a function of anisotropy for $\nu = 4/3$ on the sphere geometry with $N_e = 10$ and $N_\phi = 6$. The shift of the sphere geometry selects the two occupied components $(1, 1/3)$ of the highest-weight state. All these levels fan out from the parent unperturbed $SU(4)$ irrep, which is $(7, 3, 0, 0)$. In the $SU(4)$ symmetric limit, this irrep is not the ground state but it is the fourth excited state (fifth-lowest-lying eigenstate). However, it is the lowest-lying state with the expected quantum numbers for the $(1, 1/3)$ state. The vertical lines mark the special symmetry points of the anisotropic interaction model we use. We identify four different phases. They can be called F.A.F.KD and CDW as in the neutral case with the caveat that the quantum numbers do not match those predicted by simple trial wave functions. Notably, the AF phase is valley-unpolarized and spin-singlet. Also, the ground state of the F phase is fully spin-polarized as expected but forms $SU(2)$ valley multiplets with $S = 5$ and $T = 2$. Unlike the $\nu = 2$ case, phases AF and KD no longer have the same quantum numbers, and the phase transitions between them now involve a true level crossings at the $SO(5)$ point.

N_ϕ while N_2 electrons form the usual $\nu = 1/3$ state:

$$N_\phi = N_1 - 1, \quad N_\phi = 3(N_2 - 1), \quad (12)$$

so that the flux-number of particles relationship is given by

$$N_e = \frac{4}{3}N_\phi + 2. \quad (13)$$

Hence we can use the sphere geometry to study separately the two states $(1, 1/3)$ and $(2/3, 2/3)$. We have performed exact diagonalizations of the system with $N_e = 10$ and $N_\phi = 6$. While there is definitely a low-lying state with zero angular momentum $L = 0$ and irrep $(7, 3, 0, 0)$ as expected, it is not the ground state. Indeed, the true ground state spans the irrep $(4, 4, 1, 1)$ with $L = 0$, and the irrep $(7, 3, 0, 0)$ is only the fourth excited state at this system size. At these rather small system sizes, we consider that these states that lie below $(7, 3, 0, 0)$ are likely quasiparticle states with flavor changing excitations. The irrep $(7, 3, 0, 0)$ is split by the anisotropies as shown in Fig. 1. We have used a small value $\tilde{g} = 10^{-4}$ so that the states are not mixed with the nearby irreps. The low-lying states centered onto the parent symmetric state $(7, 3, 0, 0)$ are displayed in Fig. 1. There are four distinct phases separated by first-order transitions. The range of existence of these four phases is similar to the case for $\nu = 2$. However, the quantum

numbers we find are not always those predicted by the variational approach:

(i) For $-\pi/4 < \theta < +\pi/2$, there is a phase with $S = 5$ and $T^z = 2$ as expected for a ferromagnetic state. Since the two valleys should be populated by, respectively, seven and three electrons, one can have indeed the maximum possible spin $S = 5$ while T^z is given by the difference in valley occupation. However, this is not the whole story since we observe that states with $T^z = 0, 1, 2$ are exactly degenerate while the full Hamiltonian does not have $SU(2)$ symmetry in the whole phase but only at the special point $\theta = \pi/4$. This is not predicted by the wave function in Eq. (6).

(ii) For $+\pi/2 < \theta < +3\pi/4$, we find a phase with $S = 0$ and $T^z = 0$, which is natural to call antiferromagnetic. However, it is definitely not in agreement with the variational quantum numbers ($S = 2$ and $T^z = 2$).

(iii) For $+3\pi/4 < \theta < +5\pi/4$, the ground state has $S = 2$ and $T^z = 0$. The value of T^z points to XY valley order, and these values are those predicted variationally. So we call this phase a Kékulé phase.

(iv) Finally, for $+5\pi/4 < \theta < +7\pi/4$, we find $S = 2$ and $T^z = 5$. The maximal value of T^z means that all electrons reside in a single valley, i.e., a given sublattice as in a

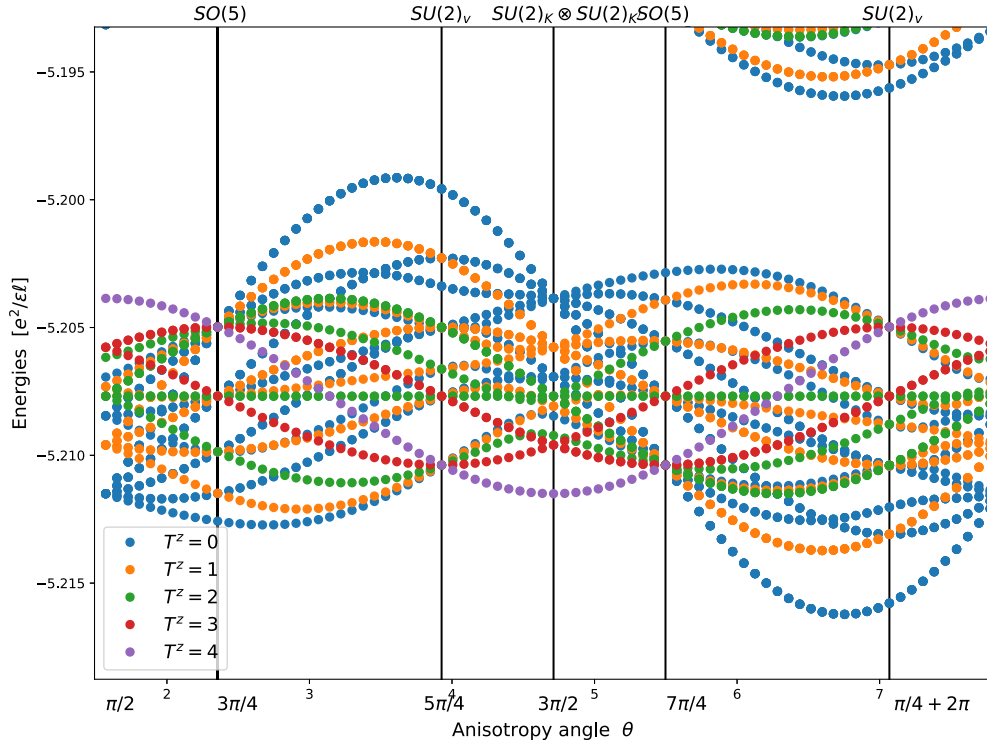


FIG. 2. Energy levels as a function of anisotropy for $\nu = 4/3$ on the sphere geometry with $N_e = 8$ and $N_\phi = 5$. The shift of the sphere geometry selects the $SU(2)$ two-component singlet $(2/3, 2/3)$ of the two occupied components of the highest-weight state. The parent unperturbed $SU(4)$ irrep is $(4,4,0,0)$, which is the ground state in the symmetric limit. The vertical lines mark the special symmetry points of the anisotropic interaction model we use. We identify four different phases. The quantum numbers are exactly the same as in the neutrality case $\nu = 2$. We thus observe that the transition between AF and KD phases does not involve a ground-state level crossing but presumably happens through the collapse of a tower of states.

charge-density-wave state, and the total spin is correctly predicted by the variational wave function.

The most intriguing result is the appearance of exact valley multiplets when the state is completely polarized. This can be explained by the following line of reasoning: when we have full spin polarization, the electrons occupy the two valleys, and in the case of the $(1, 1/3)$ state one of these valleys is completely filled. If we perform a two-component particle-hole transformation on the populated valleys, we obtain a state $(0, 2/3)$ that is fully polarized since only one valley is occupied by holes. As a consequence, there is no effect of anisotropies since they involve only a contact interaction, requiring space coincidence of electrons (as is the case of the $\nu = 1/3$ state discussed in Sec. III A). This does not imply that such states have energies independent of $g_z, g_\perp$ parameters because they appear in the one-body terms in the particle-hole transformation. So there is a subset of states that do not feel degeneracy-lifting anisotropies when they are simply given by contact interactions. Note that this argument is also valid for excited states as long as they are also fully spin-polarized.

The total spin and valley polarizations certainly led us to name these phases F, AF, KD, and CDW as in the $\nu = 2$ case. So the symmetry-breaking pattern is the same as the neutrality case. However, one of these four phases (AF) cannot be described by trial product wave functions if we use for the spinors α and β the spinors that describe the $\nu = 2$ phase diagram. Another difference with respect to the

neutrality case is that AF and KD phases do not have the same quantum numbers, so the first-order transition between them involves a ground-state level crossing unlike the $\nu = 2$ case [39].

B. The $(2/3, 2/3)$ state

The well-known $SU(2)$ singlet state for $\nu = 2/3$ is obtained with a unit shift on the sphere geometry $N_\phi = (3/2)N_e - 1$ with $N_e = N_\uparrow + N_\downarrow$. If we make the particle-hole transformation $N_{\uparrow,\downarrow} \rightarrow N_\phi + 1 - N_{\uparrow,\downarrow}$, we obtain the relation $N_\phi = (3/4)N_e - 1$. When embedded in the four-component space, we expect to find an irrep with highest weight $(N_e/2, N_e/2, 0, 0)$ as the ground state. The degeneracy is then lifted by the anisotropy: in Fig. 2 we present results of exact diagonalizations in the sphere geometry for $N_e = 8$ electrons and $N_\phi = 5$. The important conclusion from this calculation is that the ground-state quantum numbers are now exactly the same as in the $\nu = 2$ case. So the phase diagram is the same as in the $\nu = 2$ case with the same behavior at the phase transition points. Notably, the AF/KD phase transition has no ground-state level crossing.

This is exactly what we find with the variational approach. Indeed with the particle-hole symmetry of the singlet state, we have now $g_{\alpha\beta}(0)$ of order unity and an energy functional Eq. (9) equal to that of $\nu = 2$ except from an overall factor.

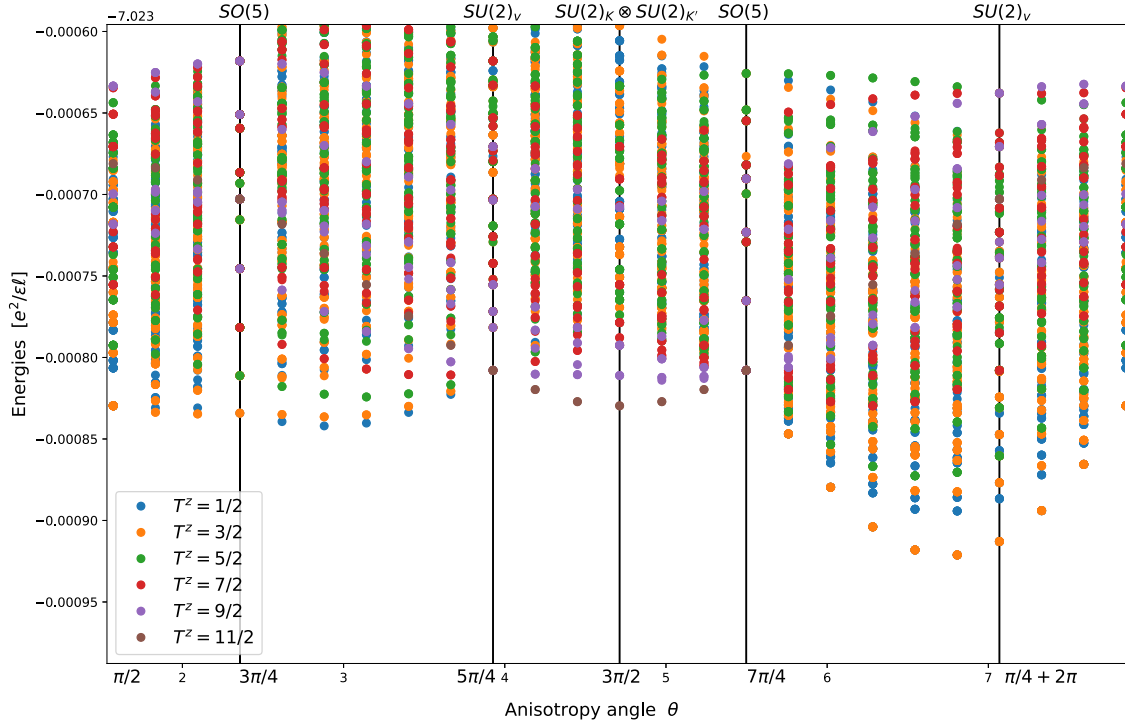


FIG. 3. Energy levels vs anisotropy angle θ for filling factor $\nu = 5/3$ on the sphere geometry with $N_e = 11$ and $N_\phi = 6$ selecting the $(1, 2/3)$ state. The parent $SU(4)$ irrep is $(7, 4, 0, 0)$. This state is not the absolute ground state in the $SU(4)$ limit: it is the sixth excited state. One finds four phases consistent with the $\nu = 2$ phase diagram but with distinct quantum numbers. There is a ferromagnetic phase for $-\pi/4 < \theta < +\pi/2$ with $S = 11/2$ and $T^z = 1/2, 3/2$, so there is an emergent $SU(2)$ valley symmetry, an antiferromagnetic phase for $+\pi/2 < \theta < +3\pi/4$ with $S = T^z = 3/2$, a Kékulé phase for $+3\pi/4 < \theta < +5\pi/4$ with $S = 3/2$ and $T^z = 1/2$, and a charge-density-wave phase for $+5\pi/4 < \theta < +7\pi/4$ with $S = 3/2$ and $T^z = 11/2$. All transitions are first-order with level crossings.

While the $(2/3, 2/3)$ state is below the $(1, 1/3)$ state at zero Zeeman energy, there may be a transition between these states that will be sensitive to the precise phase that is realized. This is discussed in Sec. VI.

V. THE FRACTION $\nu = 5/3$

Two possible candidates at this fraction are now $(1, 2/3)$, which is a two-component state, and $(1, 1/3, 1/3)$, which is a genuine three-component state.

A. The two-component state $(1, 2/3)$

The first state is obtained by adding the polarized, i.e., one-flavor, $\nu = 2/3$ state to a filled level. This polarized state with $\nu = 2/3$ is the one-component particle-hole transform of the polarized Coulomb eigenstate at $\nu = 1/3$. The flux-number of particles is thus given by

$$N_\phi = N_1 - 1, \quad N_\phi = 3/2 \times N_2, \quad N_e = N_1 + N_2, \\ N_\phi = \frac{3}{5}(N_e - 1).$$

We have performed sphere exact diagonalizations for $N_e = 11$ and $N_\phi = 6$. In the $SU(4)$ limit there is a lowest-lying state with $(7, 4, 0, 0)$ irrep and $L = 0$ as expected for the state obtained from gluing a complete shell to the $2/3$ state, but it is not the ground state. This is the same phenomenon that we observe at $\nu = 4/3$. We posit that these extra states are

flavor-changing quasiparticle excitations, and we focus only on the fate of the $(7, 4, 0, 0)$ multiplet. By using a small value of the anisotropy $\tilde{g} = 10^{-4}$, the irrep is split in many levels, but they do not mix with other multiplets. The result of this calculation is displayed in Fig. 3.

As in the case of the $(1, 1/3)$ state, the quantum numbers are exactly those expected from using the spinors α and β describing the various orderings of $\nu = 2$ F, AF, KD, CDW. Also since AF and KD do not have the same quantum numbers, there is a level-crossing phase transition at the $SO(5)$ point between the AF and KD phases.

In the fully polarized sector, we observe also the appearance of degeneracies due to the $SU(2)$ valley symmetry not only at the special point $\theta = \pi/4$ but in the whole F phase. The manifold of $S = 11/2$ states involves indeed $T^z = 1/2$ and $3/2$, while the variational prediction is that we should observe only $T^z = 3/2$. This is due to the same phenomenon we found for the ferromagnetic phase in the case of the $(1, 1/3)$ state. The two-component particle-hole symmetric state of the fully polarized states has valley content $(0, 1/3)$, so the holes being polarized do not feel the point-contact anisotropies.

B. The three-component state

For the three-component state, one now replaces the $\nu = 2/3$ polarized state by the two-component singlet state at the same filling factor leading to a flavor content $(1, 1/3, 1/3)$.

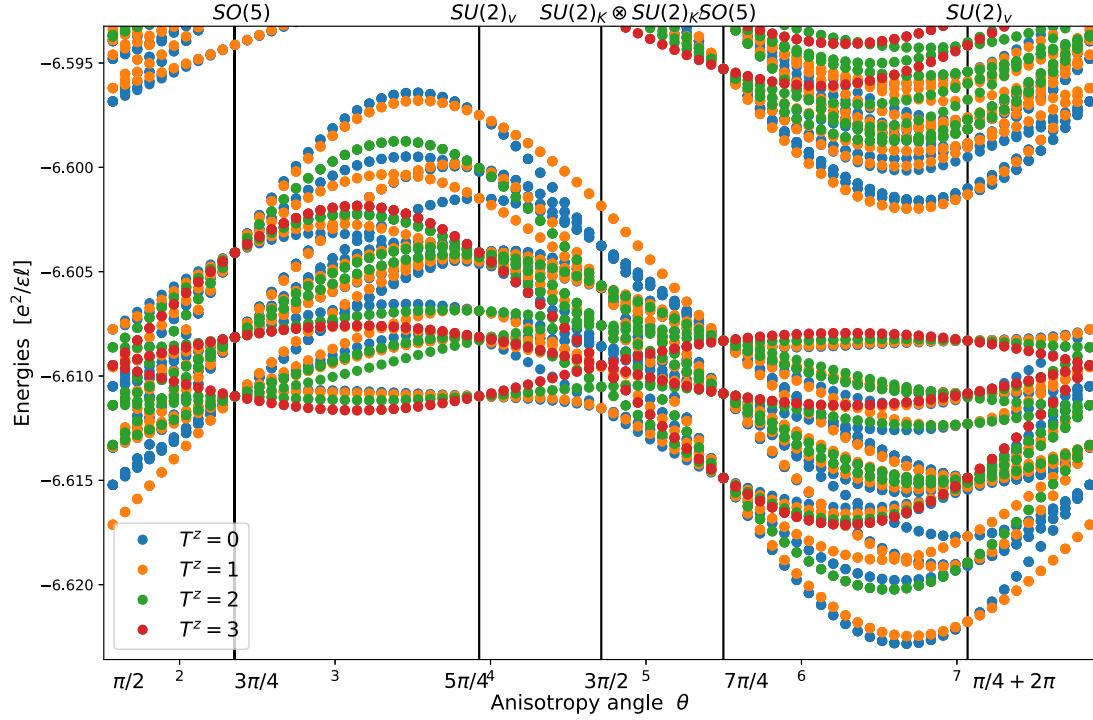


FIG. 4. Energy levels vs anisotropy angle θ for filling factor $\nu = 5/3$ on the sphere geometry with $N_e = 10$ and $N_\phi = 5$. This special shift favors the singlet state for the two partially occupied Landau levels so that the flavor content is $(1, 1/3, 1/3)$. The parent $SU(4)$ irrep is $(6, 2, 2, 0)$ and it is the ground state. The magnitude of the anisotropy is $\tilde{g} = 10^{-2}$. We observe five phases whose quantum numbers are displayed in Fig. 5. The five quantum phase transitions are first-order with true level crossings.

We call N_1 the number of electrons in the fully filled LL, and N_2, N_3 are the electron numbers in the two flavors forming the singlet state. We obtain thus a shift on the sphere that is different from that of the previous state:

$$N_\phi = N_1 - 1, \quad N_\phi = 3/2 \times (N_2 + N_3) - 1, \\ N_e = N_1 + N_2 + N_3, \quad N_\phi = \frac{3}{5}N_e - 1.$$

We have studied in detail the case $N_e = 10, N_\phi = 5$. In the $SU(4)$ limit we are already certain that this state is lower in energy than $(1, 2/3)$ since the $\nu = 2/3$ singlet is lower in energy than the polarized state at the same filling factor. We are also certain that there is such an eigenstate of the $SU(4)$ symmetric Coulomb problem.

The only remaining question is if there are some states that are lower in energy. Indeed, it may very well be that by spreading the electrons into more flavors, one can reduce the energy cost of Coulomb repulsion. If we consider the possible existence of an $SU(3)$ singlet state at filling $2/3$ with shift 2 on the sphere [44], then it implies the existence of a state with flavor content $(1, 2/9, 2/9, 2/9)$ and a flux given by $N_\phi = (3/5)N_e - (7/3)$. We observe on the sphere geometry that the ground state for $N_e = 14$ and $N_\phi = 7$ is spanned by the irrep $(8, 2, 2, 2)$. Since we already know [44] that there is a $SU(3)$ singlet $(2, 2, 2)$ for $N_e = 6$ and $N_\phi = 8$, this is in fact only a consistency check. Due to the severe size limitations of exact diagonalizations, we cannot shed further light on this issue, and we limit ourselves to the states $(1, 2/3)$ and $(1, 1/3, 1/3)$. If there are states like $(1, 2/9, 2/9, 2/9)$, they are relevant only at small Zeeman energy.

Our exact diagonalization results on the sphere geometry are presented in Fig. 4. We find now a phase diagram *different* from the neutrality case. There are five phase transitions, and all of them involve level crossings in the finite systems. The five phases we observe have quantum numbers displayed in Fig. 5. Some of them may be captured by the variational approach, but not all.

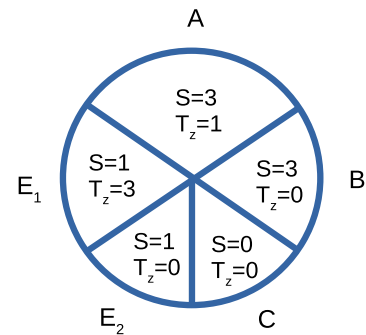


FIG. 5. Phase diagram for the $\nu = 5/3$ with $N_e = 10$ and $N_\phi = 5$. The parent $SU(4)$ irrep is $(6, 2, 2, 0)$. This is valid on the sphere geometry. On the torus geometry, the quantum numbers are slightly different since the number of states per Landau level differs by one unit. While A, B can be captured plausibly by the variational method, this is not the case of the singlet phase C . The $E_{1,2}$ phases are found to be degenerate variationally, while our results show that they differ by the type of valley ordering. The Zeeman energy has been set to zero.

Since we are dealing with a three-component state, it is no longer possible to have full spin or valley polarization. The maximal value of the spin is observed in the range $-\pi/4 < \theta < +3\pi/4$. In this regime, we observe two phases *A* and *B* that differ by the valley T^z value.

(i) The *A* phase has no valley *XY* order, and it can be described by $\{\alpha, \beta, \gamma\} = \{|K \uparrow\rangle, |K' \uparrow\rangle, |K' \downarrow\rangle\}$ with $T^z = 1$ and $S = 3$.

(ii) The *B* phase or $-\pi/4 < \theta < +\pi/4$ has $T^z = 0$, and it is plausibly described by a state with $\{\alpha, \beta, \gamma\} = \{|\mathbf{t}_\perp \uparrow\rangle, |-\mathbf{t}_\perp \uparrow\rangle, |-\mathbf{t}_\perp \downarrow\rangle\}$. Due to the three-component nature of the state, it is not possible to obtain $T^z = 0$ by using states with definite projections onto $|K\rangle, |K'\rangle$, but one has to use *XY* valley ordered states.

The transition between *A* and *B* phases is thus associated with the change of the valley order from Ising-type in *A* to *XY*-type in *B*.

The region $3\pi/4 < \theta < 3\pi/2$ has now only partial spin polarization and is divided into two phases that differ by a change in the value of the valley polarization.

(i) We find a phase E_1 for $3\pi/4 < \theta < 5\pi/4$ with the maximal value of T^z . $\{\alpha, \beta, \gamma\} = \{|K \uparrow\rangle, |K \downarrow\rangle, |K' \downarrow\rangle\}$.

(ii) In the lower quadrant $5\pi/4 < \theta < 3\pi/2$, we have a phase E_2 with $T^z = 0$ indicative of *XY* valley ordering whose candidate ordering pattern is given by $\{\alpha, \beta, \gamma\} = \{|\mathbf{t}_\perp \uparrow\rangle, |-\mathbf{t}_\perp \downarrow\rangle, |\mathbf{t}_\perp \downarrow\rangle\}$. The transition between E_1 and E_2 corresponds to changing the valley order from the Ising-like *z*-axis to the valley *XY* plane. A variational treatment does not distinguish between Ising or *XY* character in this range of anisotropies. Indeed, all states are degenerate with trial energy in Eq. (9).

(iii) Finally there is a fifth phase that we call *C* for $3\pi/2 < \theta < 7\pi/4$, which is a spin singlet $S = 0$ as well as valley unpolarized $T^z = 0$. It is not possible to capture such a phase with the class of variational states discussed above. If we look at the full set of degenerate states in the $SU(4)$ limit, one notes that the irrep (6,2,2,0) that we study contains notably symmetric states like (3,2,2,3) from which one can construct states with zero spin and zero isospin values. It is an open question to obtain explicitly a wave function with the correct quantum numbers for the *C* phase.

To shed some more light on the nature of the *C* phase, we have computed the pair correlation function $g_{\alpha\beta}(r)$ of the exact ground state in the sphere geometry. With a ground state having zero spin and $T^z = 0$, there are only four independent combinations of spin-valley that are plotted in Fig. 6. At short distance, the leading correlation is $g_{K\uparrow K\downarrow}(0) = g_{K'\uparrow K'\downarrow}(0)$. This function has a maximum at the origin while all other cases have a deep minimum as expected from Coulomb repulsion. This may point to the formation of spin $S = 0$ singlet pairs in each valley. On the contrary, the antiferromagnetic-like repulsion between $K \uparrow$ and $K' \downarrow$ is maximal at a finite distance $\approx 2.5\ell$.

VI. SPIN TRANSITIONS

In the case of filling factor $\nu = 2/3$, it is well known [42] that one can induce a spin transition between the singlet state and the fully polarized state. Indeed, while the polarized

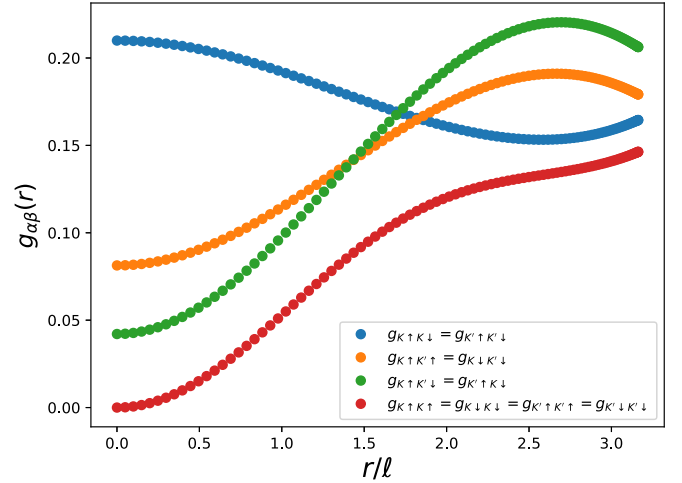


FIG. 6. The various pair correlation functions $g_{\alpha\beta}(r)$ calculated in the middle of the singlet *C* phase for $\theta = 3\pi/2 + \pi/8$. The sphere geometry is used with $N_e = 10$, $N_\phi = 5$. The chord distance r varies from zero up to $\sqrt{10}\ell$. Since we have $S^z = 0$ and $T^z = 0$ in this phase, there are only four distinct correlations.

state has a higher Coulomb energy, increasing the Zeeman energy will lower it eventually below the singlet state. The crossing happens when the Zeeman energy equals the energy difference between the two states:

$$\Delta E = \epsilon_z B_{\text{crit}}. \quad (14)$$

This prototypical transition is simple because of the well-defined magnetization of the two competing states. Here in monolayer graphene, the situation is richer since the competing states that we have studied above can have various magnetizations according to the value of the anisotropy parameters. The Coulomb energy scales as $\propto \sqrt{B}$, while anisotropy energies and the Zeeman energy scale linearly with B . The energy per particle of a state i has thus three contributions:

$$\epsilon_i = E_{Ci} + a_i B + \epsilon_z m, \quad (15)$$

where we have defined the magnetization per particle m and the Coulomb energy E_{Ci} . A spin transition between two states 0 and 1 arises when the Coulomb energy difference is equal to the contribution from anisotropies and Zeeman energy:

$$\Delta \epsilon_{01}(B_{\text{crit}}) = (a_0 - a_1 + z) B_{\text{crit}}. \quad (16)$$

The Zeeman factor z depends upon the magnetization of the two competing states, and in the case of monolayer graphene it takes different values in different parts of the anisotropy phase diagram.

We now give a simplified description of spin transitions for the fractions we have studied. We limit ourselves to situations with only a perpendicular field, and also we ignore the possibility of spin canting. Indeed, the effect of the canting is restricted to low enough fields. At large enough values of the field, one obtains a fully polarized state or a collinear antiferromagnet depending on the filling fraction. Certainly spin canting may drive interesting transitions, but detailed

predictions are hampered by our lack of knowledge about the values of anisotropies.

A. $\nu = 2/3$

At filling factor $2/3$, the polarized state is insensitive to anisotropies while the singlet state can be in any of four phases F, AF, CDW, and KD as shown in Sec. III B. In KD or CDW, the state is a spin singlet so it is insensitive to the Zeeman coupling. We thus expect a spin transition toward the fully polarized state at some field value Eq. (16). The AF state turns into a canted antiferromagnetic state that becomes fully polarized beyond some field value. Once in this fully polarized state, as is the case of the F phase, the state lowers its energy at the same rate as the polarized $\nu = 2/3$ state so that there will be no crossing, hence there will be no spin transition in the AF or F phases.

B. $\nu = 4/3$

The phase diagrams for the states $(1, 1/3)$ and $(2/3, 2/3)$ are similar: there is the same number of phases with their domain of stability having the same range of anisotropy angle θ , but the difference is now in their total magnetization. In the F phase, the two states have the same total spin value, so they never cross under Zeeman coupling. In the KD and CDW phases, the situation is different. In the state $(2/3, 2/3)$ there is zero net magnetization in both cases KD and CDW, while in the state $(1, 1/3)$ the KD phase has now a net magnetization equal to $1/3$ of the saturation value, and the CDW phase has an even smaller magnetization (but nonzero). So we deduce that there can be a spin transition in both phases KD and CDW.

C. $\nu = 5/3$

The situation is more complex since now the phase diagrams of the two competing states $(1, 2/3)$ and $(1, 1/3, 1/3)$ do not overlap exactly as a function of anisotropy. We describe the situation by using as a reference the phases of the $(1, 2/3)$ state. In the F phase, the state $(1, 2/3)$ is fully polarized with magnetization $M = M_{\text{sat}}$, while A and B phases of $(1, 1/3, 1/3)$ have only $M = M_{\text{sat}}/\nu$ so we expect a spin transition. In KD and CDW phases, the higher-lying state $(1, 2/3)$ has $M = M_{\text{sat}}/3$ while the competing phases in $(1, 1/3, 1/3)$ are the C and E_2 phases (see Fig. 5). In the singlet C phase we have $M = 0$, and in the E_1 and E_2 phases $M = M_{\text{sat}}/5$, so there will be a spin transition. Its location B_{crit} will be phase-dependent because there are (still unknown) contributions from anisotropies in the value of the critical field in Eq. (16).

The general picture is that states with maximal spread-out of electrons in various spin-valley components will be favored only at small Zeeman energies. Notably graphene experiments with large Zeeman splittings and large sublattice effects like measurements in Ref. [20] will involve only states like $(1, 1/3)$ and $(1, 2/3)$ as well as their generalizations to other fractions. Genuine multicomponent states will require a minimal effect of the one-body fields.

VII. CONCLUSION

We have studied the impact of anisotropies relevant to the description of monolayer graphene in the regime of the fractional quantum Hall effect. At neutrality, the phase diagram involves four phases F, AF, KD, and CDW. Simple generalizations of this diagram apply for $\nu = (1/3, 1/3)$, $(2/3, 2/3)$, and $(1, 2/3)$ states. This is found from exact diagonalizations on the sphere geometry, and it is also confirmed by a variational approach involving parent Coulomb eigenstates. The two spin-valley vectors α, β that characterize the spin-valley order in the variational approach are identical to the neutral case. Since the occupations of the two filled states are in general not equal, it means that the quantum numbers of the ground state are now different from the neutral case. As a consequence, all first-order transitions involve level crossings. Indeed, there is no evidence for exotic phase transitions [51].

In the case of $\nu = (1, 1/3)$, there are also four phases whose range of stability is the same as the neutral case, but the quantum numbers are not all predicted by the variational method. While CDW and KD-like phases have spin and valley quantum numbers correctly predicted, we find that the antiferromagnetic phase is a spin singlet with no net valley polarization. Interestingly, we find that the fully polarized states partly escape effects of anisotropy and still form SU(2) valley multiplets even though this is not a symmetry of the Hamiltonian (their energies still depend upon g_z and $g_{\perp}$). This emergent symmetry also appears in the polarized eigenstates of the $(1, 2/3)$ state.

The case $\nu = (1, 1/3, 1/3)$ is different. We observe five phases. Two of them can be described variationally. There are two distinct phases in our diagonalizations that differ by Ising valley order versus XY valley order while they are degenerate variationally. There is also a phase in which a spin singlet with presumably XY valley order occurs for negative Ising-like anisotropy. It is an open question how to write a wave function to describe this phase. The pair correlation function $g_{\alpha\beta}(0)$ shows an enhanced probability for electrons for opposite spins but in the same valley to be at the same location. This interesting situation requires, however, low Zeeman energy to be realized experimentally.

In present experiments, it is likely that one observes the two-component states $(1, 1/3)$ and $(1, 2/3)$. If they are fully polarized (the F phase), then we predict that they should escape degeneracy-lifting anisotropies of the form given in Eq. (1) and thus feature an emergent valley SU(2) symmetry. Invalidating this valley symmetry would invalidate the simplified model of Eq. (1), which is a crucial piece of our present understanding of IQHE and FQHE in graphene systems.

Recent experiments using scanning tunneling microscopy [52,53] have given evidence for a more complex picture at neutrality $\nu = 0$ than previously thought. Notably, there is evidence for phases beyond the four states F, AF, KD, and CDW.

There are at least two possible explanations. It may very well be that the anisotropies are not small in comparison to Coulomb and that the simple model Eq. (1) is not adequate. It may also mean that the Landau level mixing is

strong enough to change the phase structure. Such a possibility would invalidate standard theoretical treatments that focus on a fixed Landau level from the start. Also some of the experiments [52] favor a Kékulé state, which is at odds with the explanation of the metal-insulator transition [11]. This may mean that the anisotropy parameters are not in the range estimated in Ref. [11], in which case the explanation for the tilted-field transition becomes more elusive. It may be that the edge of the sample lies in a

different phase from the bulk, as observed in Hartree-Fock studies [54].

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