Spin polarization of the $\nu=5/2$ quantum Hall state

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We numerically study the spin polarization of the fractional quantum Hall state at filling factor $\nu=5/2$. By using both exact diagonalization and the density matrix renormalization group methods on the sphere, we are able to analyze more values of partial spin polarization (in addition to fully polarized and unpolarized) than any previous studies. We find that for the Coulomb interaction the exact finite-system ground state is fully polarized, for shifts corresponding to both the Moore-Read Pfaffian state and its particle-hole conjugate (anti-Pfaffian). This result is found to be robust against small variations in the interaction and change of shift. The low-energy excitation spectrum is consistent with spin-wave excitations of a fully magnetized ferromagnet.

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I. INTRODUCTION

The most striking feature of the Laughlin state describing the fractional quantum Hall (FQH) effect at filling fraction $\nu=1/3$ (Ref. 1) is the appearance of quasiparticle excitations with fractional charge and fractional statistics. The idea of particles that do not behave as fermions or bosons, something that can occur in two spatial dimensions, is still a reason for wonder, and a motivation for seeking phases of matter with exotic excitations in low dimensions. The Laughlin wave function served as a foundation to explain all the odd-denominator incompressible FQH states.[2–6] However, it does not include the possibility of an even-denominator state. Therefore, the quantum Hall plateau observed at $\nu=5/2$ (Refs. 7–12) poses a special challenge.

While various theories have been proposed for this state,[13–21] much of the excitement has been generated by the possibility that it is a non-Abelian topological state. In ground-breaking work, Moore and Read[13] proposed the Pfaffian wave function as a description of electrons in an incompressible half-filled Landau level (LL). Greiter *et al.*[14] conjectured that this ground state may be realized at $\nu=5/2$. Recently, it was noted that there is another possible state, the so-called anti-Pfaffian,[15,16] which would be degenerate in energy with the Pfaffian state in the absence of Landau-level mixing. Since excitations above both the Pfaffian[22–25] and anti-Pfaffian[15,16,26] ground states are non-Abelian anyons, it has been suggested[27] that the $\nu=5/2$ plateau can be a platform for topological quantum computation. Therefore, determining the nature of the $\nu=5/2$ state has gained additional urgency, beyond FQH physics.[28]

In order to set a context for the importance of our theoretical numerical study of the 5/2 spin-polarization question, we first briefly describe the highly confusing experimental status of the subject. Immediately following the original discovery of the 5/2 FQHE, Eisenstein *et al.*[29] found that the application of a modest in-plane magnetic field destroys the FQHE. This was interpreted quite naturally as direct evidence for the 5/2 FQH state being spin unpolarized, leading to proposed spin-singlet wave functions[19] describing the 5/2 FQH state which, however, turned out to have very poor overlap with the exact numerical wave function. All subsequent measurements[30,31] of the 5/2 FQHE in the presence of an in-plane magnetic field have verified its suppression in the presence of even a weak in-plane magnetic field. The most direct interpretation of such an in-plane field induced destruction of the 5/2 FQHE as arising from the Zeeman splitting induced spin-polarization effect (i.e., the original unpolarized FQH state becoming spin-polarized under the in-plane field) becomes questionable, however, when one realizes that experimentally the 5/2 FQHE is observed over a very large range of perpendicular magnetic fields, ranging from 2 (Ref. 32) to 12 T,[33] and therefore, the 5/2 FQHE can obviously survive very large spin-polarizations. A more plausible scenario is that the in-plane magnetic field induced destruction of the 5/2 spin polarization arises[19,34] from the orbital coupling[35] of the in-plane field and not at all from the Zeeman coupling which depends on the total magnetic field. Efforts[36] to directly measure the 5/2 spin polarization through the resistive NMR technique have so far been unsuccessful although similar measurements[37,38] at $\nu=1/2$ in the lowest Landau level have unambiguously established the spin-unpolarized (or partially polarized) nature of the (non-FQH) 1/2 state in weak magnetic fields (up to 5–8 T, much higher than magnetic fields where the 5/2 FQHE is routinely observed). Taken together, all of this experimental evidence provides a highly conflicting picture for the spin-polarization of the 5/2 FQH state, with both spin-polarized and spin-unpolarized (certainly partially polarized) states being plausible, particularly at low magnetic fields.

The existence of non-Abelian quasiparticles at $\nu=5/2$ depends on (at least) the following premises: (i) Coulomb repulsion in the second LL (SLL) has a form conducive to pairing and (ii) the electrons are fully spin polarized. There is strong evidence from numerics that (i) is satisfied[20,26,34,39–42] (especially when finite layer thickness is taken into account[35]). Recent experiments which are consistent with a quasiparticle charge $e/4$ (Refs. 43 and 44) give further support to this hypothesis, but cannot rule out Abelian paired states which also could have $e/4$ quasiparticle charge. However, there is less evidence that (ii) holds. In GaAs, the Zeeman energy is approximately 50 times smaller than the cyclotron energy as a result of effective mass and g factor renormalizations, so the magnetic field need not fully polarize the electron spins. Electron-electron interactions, which are roughly comparable to the cyclotron energy in current experiments at $\nu=5/2$, (or even larger, see Ref. 32) can, therefore, determine the spin physics of the ground state (which is what happens at $\nu=1,1/3$, where the ground state would be spontaneously polarized even if the Zeeman energy was precisely zero). While the Pfaffian and anti-Pfaffian states are fully spin polarized, there are also paired states which are not fully polarized,[17,21,45,46] such as the so-called (3,3,1) state. Therefore, the experiments observing charge $e/4$ quasiparticles do not rule them out. Experiments which seek to directly probe the spin polarization at $\nu=5/2$ are inconclusive.[36] Since the proposed non-Abelian states, whether the Pfaffian or the anti-Pfaffian, are all fully spin polarized whereas the competing spin-unpolarized states [e.g., the hollow-core state or the (331) state] are all Abelian, it becomes imperative that the issue of 5/2 spin polarization is resolved by a serious numerical calculation, which is what we achieve in this work.

For the last 25 years numerical methods have had strong predictive power in the study of FQH systems, and have become a fundamental validation tool for theories. In a seminal paper,[34] Morf showed that in a half-filled SLL, the fully polarized state has lower energy than the spin-singlet state in systems of up to 12 electrons. Based on this result, he argued that the electrons in the SLL are fully polarized at $\nu=5/2$, which ran counter to the prevalent view at the time (based on tilted-field experiments[29]). Later, Park *et al.*[18] compared the energies of different ground-state candidates, and concluded that a polarized Pfaffian is favored against a polarized composite fermion (CF) sea, and unpolarized composite fermion sea. Recently, Dimov *et al.*[45] reached the same conclusion by comparing the Pfaffian and Halperin's (3,3,1) state[17,46] using variational Monte Carlo. In all these works, all trial states have energies that are substantially higher than the unpolarized ground-state energy at $\nu=5/2$ obtained by Morf.

II. METHOD

The existing numerical evidence suggests that the half-filled SLL is either fully polarized, or partially polarized. However, the latter possibility has not been explored, probably due to numerical limitations. In this work we overcome these limitations by combining exact diagonalization with the recently introduced density matrix renormalization group (DMRG) method for studying FQH states on the spherical geometry.[42,47] This DMRG approach relies on concepts of exact diagonalization and numerical renormalization group, and yields variational results in a reduced basis, in the form of a matrix-product state. Contrary to other variational methods, it does not rely on an ansatz or prior knowledge of a trial wave function. The obtained energies are quasiexact, in the sense that the accuracy is under control, and improves as the number of states in the basis is increased.[48,49] We have typically used 4000 DMRG states, which exploits the limits of our computational capability.

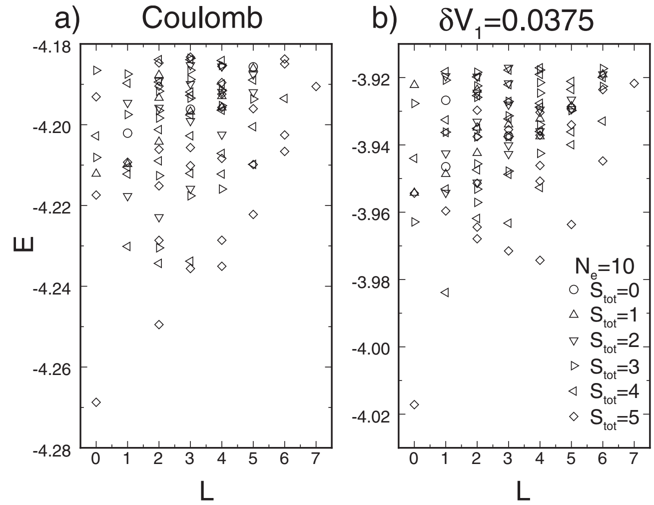

FIG. 1. Low-energy spectrum of system with $N_e=10$ electrons and shift $S=3$ on the sphere obtained with exact diagonalization for: (a) Coulomb interactions and (b) Coulomb interactions with the V_1 pseudopotential varied to maximize the overlap between the numerical ground state and the Moore-Read state for the case of fully spin-polarized electrons.

The Hamiltonian that describes a Landau level is dictated by the Coulomb interaction between electrons, making this the quintessential strongly correlated problem. In the spherical geometry, it is written in an angular momentum representation, which is parametrized by Haldane's pseudopotentials V_L (Refs. 2 and 50) that describe the interaction between two electrons with relative angular momentum L.[51] In the lowest LL, V_1 dominates, explaining why the Laughlin state yields such a good description at $\nu=1/3$, since it is the exact ground state of a hard-core Hamiltonian with $V_L=0$ for $L \neq 1$. However, in the second LL, the relative magnitude of the pseudopotentials is such that V_3 becomes comparable to V_1, therefore introducing a competition between pairing and Coulomb repulsion, crucial to stabilize the Pfaffian. (Notice that even-L pseudopotentials only become relevant for partially polarized or unpolarized states).

III. RESULTS

Incompressible states at filling fractions ν are characterized on the sphere by the number of electrons N_e and flux quanta N_Φ obeying the relation $N_\Phi=N_e/\nu-S(\nu)$, where $S(\nu)$ is the so-called shift function. The shift for the Pfaffian $\nu=5/2$ state is $S=3$, and its particle-hole conjugate, the anti-Pfaffian, is at $S=-1$. In the absence of Landau-level mixing, these states become energetically degenerate in the thermodynamic limit.

In Fig. 1 we present the low-energy spectrum of a system with $N_e=10$ electrons obtained using exact diagonalization on the sphere at half-filling, with the shift $S=3$ corresponding to the Moore-Read (MR) Pfaffian state. All values are in units of e^2/ℓ_0, where $\ell_0=\sqrt{\hbar c/eB}$ is the magnetic length. The ground state is fully magnetized ($S_{tot}=N_e/2=5$), and also has the same orbital angular momentum ($L=0$) as the MR state;

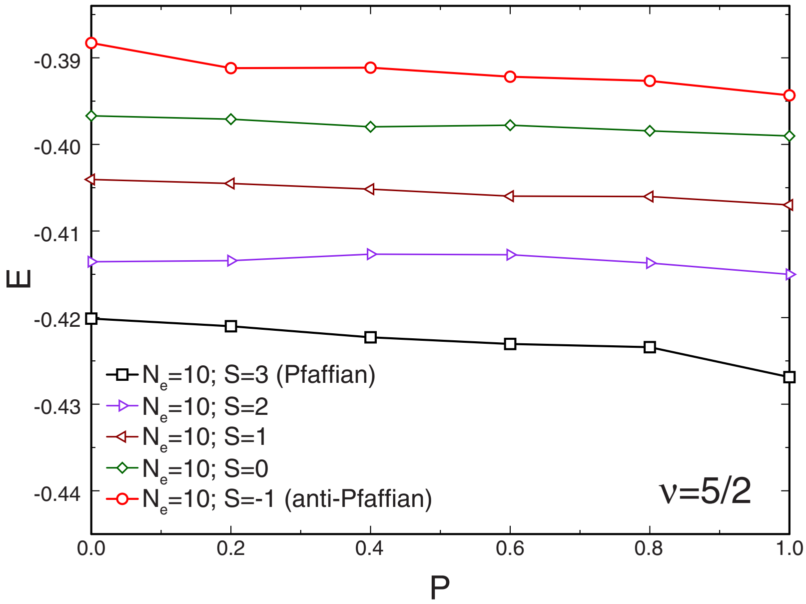

FIG. 2. (Color online) Ground-state energies obtained with DMRG, as a function of polarization $P=2S_{\text{tot}}/N_e$, for $N_e=10$, for the second LL at filling fraction $\nu=5/2$. We show results for a shift $S=3$, corresponding to the Pfaffian, and $S=-1$, corresponding to the anti-Pfaffian. We also show results for intermediate shifts. Lines are a guide to the eyes.

the overlap between the numerical ground state and the MR state in this case is 70%. We also find that the full magnetization is a robust property of the ground state when some interaction parameters are varied. In the same figure we present results of the same system with a slightly modified Hamiltonian, in which the V_1 pseudopotential is tuned to maximize the overlap between the numerical ground state and the Moore-Read state for fully spin-polarized electrons; the overlap is 98% in this case. (Notice that the overlaps on the sphere are larger than on the torus[40] and disk.[41,52]) Just as in the Coulomb case, the ground state is fully polarized. What is noteworthy about this spectrum is that the first excited state has $L=1$ and $S_{\text{tot}}=4=N_e/2-1$; this is what we expect for the lowest-energy spin-wave excitation on top of a fully magnetized ferromagnetic ground state. While the spectrum of the Coulomb case does not quite show such behavior at this particular system size, we believe it is a finite-size artifact; we expect for larger system sizes the lowest-energy excitation should be a spin wave, just as we see for $\delta V_1 =0.0375$.

In Fig. 2 we plot the ground-state energies of a system with $N_e=10$ electrons at half-filling, as a function of the polarization $P=2S_{\text{tot}}/N_e$ obtained with the DMRG method. We present results at shift values $S=3$ and $S=-1$, corresponding to the Pfaffian and anti-Pfaffian, respectively, and also, for completeness, at intermediate values. We have found excellent agreement with exact diagonalization results, with errors in the sixth digit, establishing the accuracy of the technique. In all cases, the evidence clearly shows that the fully polarized state has lower energy, and that the energy increases monotonically with decreasing polarization. For shifts $S=0,1,2$, the energy differences only appear in the fourth digit. One possible interpretation is that these values of the shift correspond to excitations above the Pfaffian and anti-Pfaffian ground states. If these excitations were skyrmionlike (i.e., with many reversed spins), we would expect the ground-state at these values of the shift to be a spin-singlets. The addition of a Zeeman energy to the Hamiltonian will even more strongly rule out the possibility of an unpolarized or even partially polarized ground state, even for the lowest magnetic field (≈ 3 T) observation[32] of the 5/2 FQH state.

In Fig. 3 we show the ground-state energy as a function of the number of electrons N_e for different values of the polarization P, shift $S=3$, and zero Zeeman splitting. We have rescaled the energies by a factor $\sqrt{(N_\Phi-2)/2N_e}$ to take into account finite-size effects on the sphere,[34,53] where we are assuming an underlying inert filled ($\nu=2$) lowest Landau level.[54] Our data reproduce the results obtained by Morf[34] in smaller systems, and we extend the study to $N_e=14$ for the unpolarized systems, and $N_e=26$ for the fully polarized

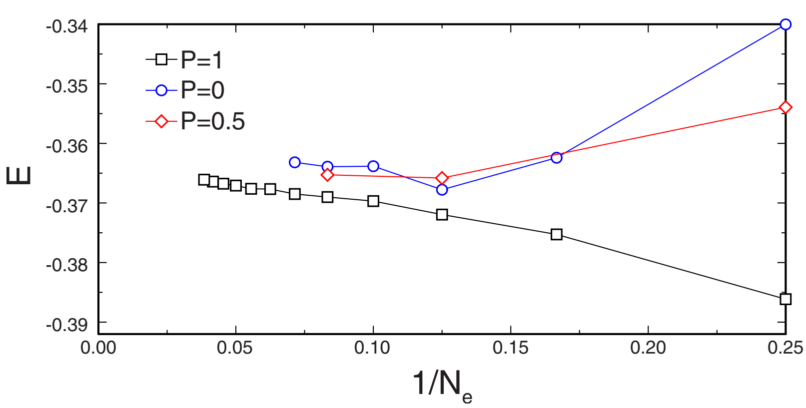

FIG. 3. (Color online) Ground-state energies obtained with DMRG, as a function of $1/N_e$, for different values of polarization P, and shift $S=3$. Energies are in units of the magnetic length and have been rescaled following Ref. 34 (see text). Lines are a guide to the eyes.

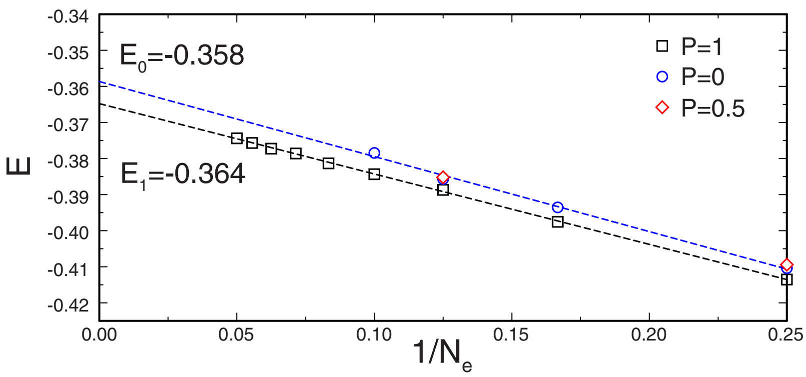

FIG. 4. (Color online) Ground-state energies obtained with DMRG, as a function of $1/N_e$, for different values of polarization P and shift $S=-1$, corresponding to the anti-Pfaffian. Dashed lines indicate a linear extrapolation in $1/N_e$. Energies are in units of the renormalized magnetic length, same as in Fig. 3 (see text).

states. For polarization $P=0.5$, we study system sizes up to $N_e=14$. Notice that the calculations at finite polarization involve a much larger Hilbert space. Moreover, the Hamiltonian now includes terms mixing spin, making these calculations computationally expensive, and preventing us from reaching larger system sizes. Based on extrapolations with the number of DMRG states, we estimate our errors to be 10^{-3} for the largest systems considered, which is of the order of the symbol size. As previously noticed in Ref. 34, the results at finite polarizations exhibit very strong finite-size effects. This makes any attempt to extrapolate energies to the thermodynamic limit unreliable, even using the larger system sizes studied here.

In Fig. 4 we show the ground-state energy as a function of $1/N_e$ for a shift $S=-1$, corresponding to the anti-Pfaffian. Notice that this calculation involves four more orbitals than the previous case, making it computationally more demanding. An extrapolation to the thermodynamic limit yields a value of $E(P=1)=-0.364$, identical to the best available estimate for the Pfaffian,[42] as expected for the particle-hole conjugate state. Interestingly, the partially polarized states show a smoother behavior here than the one observed for $S=3$, indicating that finite-size effects may play a less important role. This allows one to estimate the ground-state energy of the unpolarized state in the thermodynamic limit, $E(P=0)=-0.358$. This result is substantially lower than the variational energy for the (3,3,1) state, $E_{331}=-0.331$, obtained by Dimov *et al.*,[45] indicating that the competing unpolarized state may not be a known paired state.

IV. DISCUSSION

In interpreting this data, it is worth remembering that our Hamiltonian is fully spin-rotation invariant since we do not keep the Zeeman term. Therefore, any polarization which develops is a result of spontaneous symmetry breaking and will be accompanied by gapless Goldstone bosons (i.e., spin waves). If the ground state is fully polarized, then the $S_{tot}=N/2$ multiplet will have the lowest energy. The other multiplets will have energies which are higher by $\sim 1/N$ since the spectrum of a ferromagnet is $\omega \propto k^2$ as a consequence of the conservation of the order parameter. If the ground state is partially polarized, then some $0<S_{tot}<N/2$ multiplet will have the lowest energy. The other multiplets will have energies which are higher by $\sim 1/N$ since, again, there is a ferromagnetic order parameter which is conserved. If the ground state spontaneously breaks spin-rotational symmetry but does not have a ferromagnetic moment, such as the (3,3,1) state, then the ground state in a finite system will be a spin singlet, but the gap to other multiplets will be $\sim 1/\sqrt{N}$ since the order parameter is not conserved. Finally, if the ground state is a spin singlet in the thermodynamic limit, then the lowest-energy state will have $S_{tot}=0$ and there will be a finite gap to the other multiplets, even in the $N\rightarrow\infty$ limit. Our data are most consistent with a ferromagnetic ground state. Extrapolating to larger system sizes, we expect that the $S_{tot}=N/2$ multiplet will continue to have the lowest energy, but the gap to other multiplets will shrink as $\sim 1/N$.

Finally, and for completeness, we calculated the ground-state energies as a function of polarization for a system of $N_e=10$ electrons, at filling fraction $\nu=1/2$, i.e., in the lowest LL. Results for different shifts are displayed in Fig. 5. The most striking observation is that the ground state is partially polarized for all the values of shift considered. Thus, the situation at $\nu=1/2$ is very different from filling fraction $\nu=5/2$, as a result of the difference between the effective interaction (i.e., the pseudopotentials) in the lowest and second Landau levels. These results are in qualitative agreement with calculations of the Coulomb energies of polarized and unpolarized trial wave functions at half-filling of both the lowest[18] and second[45] Landau levels. Notice that we have set the Zeeman energy to zero in this calculation. Since the energy splitting between the partially polarized states and the full-polarized state is small for shift $S=2$ (corresponding to the compressible ground state[55,56]), we expect to be able to tune the system between partially and fully polarized compressible ground-states at $\nu=1/2$ by increasing the Zeeman energy via a tilted field. On the other hand, our results lead us to expect that the plateau at $\nu=5/2$ is fully spin polarized even for vanishing Zeeman energy.

Our numerical results for the $\nu=1/2$ state, as shown in Fig. 5, are completely in agreement with the experimental findings of Refs. 37 and 38. Resistive NMR measurements find that the $\nu=1/2$ plateau is fully polarized at high magnetic fields but is not at low magnetic fields, where it is partially polarized. Since the Zeeman energy (relative to the Coulomb energy) increases with increasing magnetic field, this is consistent with our numerical findings above. We emphasize that our prediction for the $\nu=5/2$ state is the oppo-

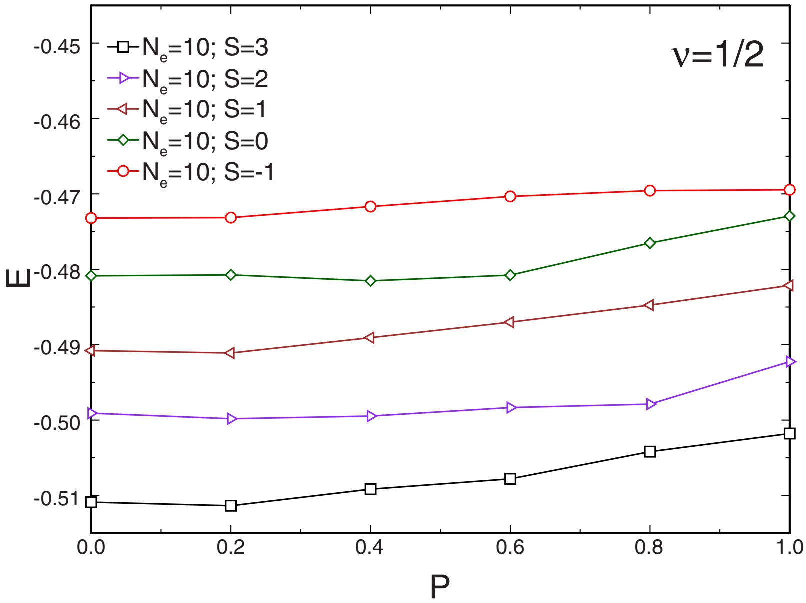

FIG. 5. (Color online) Ground-state energies obtained with DMRG, as a function of polarization $P=2S_{\text{tot}}/N_e$, for $N_e=10$, and different values of the shift. Results are for the first LL, corresponding to a filling fraction $\nu=1/2$. Lines are a guide to the eyes.

site behavior: a fully spin-polarized ground state occurs even for zero Zeeman energy. Therefore, increasing the Zeeman energy will only make a spin-polarized state more stable at $\nu=5/2$ and there will not be a Zeeman-energy-induced transition, in contrast to $\nu=1/2$. The dichotomy between $\nu=5/2$ and $\nu=1/2$ states is understandable since the latter is a compressible state while the former is an incompressible quantized plateau and, therefore, there is no particular reason for them to have similar spin properties in the ground state. Figure 6 shows the spin S of the ground state at $\nu=1/2$ and flux $N_\phi=2N_e-2$, plotted vs system size, corresponding to a composite fermion sea. This pattern is easily seen to follow from Hunds first rule of maximizing S applied to the angular momentum shells of weakly interacting composite fermions at zero (effective) magnetic field. The data therefore is highly suggestive that in the absence of Zeeman gap the $\nu=1/2$ CF state is unpolarized. The only exception to this rule is at $N_e=4$ where the actual ground state S is 2 (solid symbol). However, the difference in energy between this and the Hunds rule state (open symbol) is 0.000 085 (0.004% of the ground-state energy). In all likelihood, it is caused by the aliasing of the CF state with the particle-hole conjugate of the Laughlin state for three electrons, which is fully polarized, and should be discounted. Setting aside this case, the second Hunds rule[56] on the angular momentum of the ground state (listed in Fig. 6 next to the symbols) appears to hold with one, possibly important, exception for $N_e=10$. Here the difference between the actual ground state at $L=1$ and Hund's rule state $L=3$ (indicated in parenthesis) is 0.014% of the ground-state energy and may be more significant. The pattern of L vs N_e should be 01101102332023320…, which matches that of Ref. 56 (if generalized to include spin). Without further studies, it is difficult to conclude whether this signifies a breakdown of Hund's second rule or is in fact an isolated exception. Whatever the case, it will not alter the spin polarization of the ground state.

In conclusion, we have numerically established that the ground state of the FQH Hamiltonian at filling fraction $\nu=5/2$, even in the zero Zeeman energy limit, is fully spin polarized. We also find, consistent with experimental findings, that the $\nu=1/2$ compressible composite fermion sea state in the lowest Landau level is partially spin polarized at low magnetic fields, but may become fully polarized at higher magnetic fields due to the Zeeman energy. Thus, $\nu=5/2$ and $\nu=1/2$ states have contrasting spin-polarization properties at low to intermediate magnetic fields. We believe that our results and the recent findings[35] of the expected topological degeneracy on the torus, when taken together with the observation of charge $e/4$ quasiparticles at $\nu=5/2$,[43,44] make a strong case for the 5/2 state to be non-Abelian. Our results should encourage efforts to observe non-Abelian anyons at this quantum Hall state and use them for topological quantum computation.

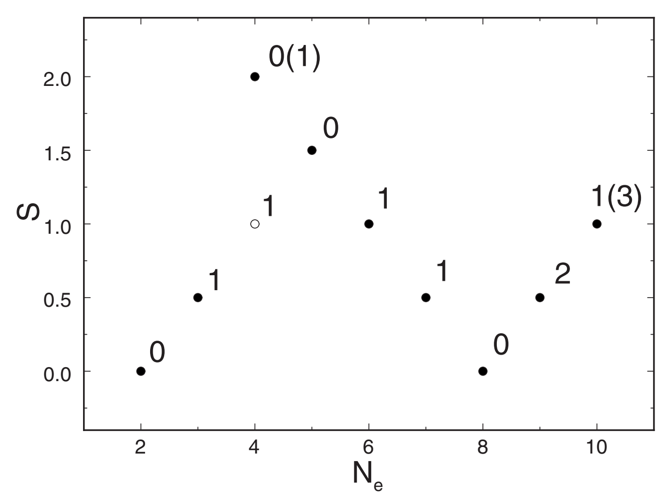

FIG. 6. Ground-state spin S for different system sizes, at $\nu=1/2$ and flux $N_\phi=2N_e-2$, corresponding to the composite fermion sea. The numbers next to symbols represent the total angular momentum. Empty symbols correspond to excited states. With the exception of $N_e=4$ and 10, all the values coincide with those expected from Hund's rule.

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