Half-Integral Spin-Singlet Quantum Hall Effect

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We provide numerical evidence that the ground state of a short range interaction model at \( \nu = 1/2 \) is incompressible and spin-singlet for a wide range of repulsive interactions. Furthermore it is accurately described by a trial wave function studied earlier. For the Coulomb interaction we find that this wave function provides a good description of the lowest lying spin-singlet state, and propose that fractional quantum Hall effect would occur at \( \nu = 1/2 \) if this state became the global ground state. Some conclusions in an earlier paper are invalidated by the present numerical study of a larger system; these will be indicated.
A large number of fractions have been observed in the fractional quantum Hall effect (FQHE) in a single two-dimensional layer of electrons [1, 2]. With the exception of 5/2 [3], all have odd-denominators [4]. An investigation of the 5/2 FQHE is the objective of this paper. Let us start by enumerating several relevant facts. (i) FQHE has not been observed at the related filling factor $\nu = 1/2$. At $\nu = 5/2$ the FQHE is seen in a relatively small range of parameters. (ii) Tilted field experiments have shown that the 5/2 FQHE is quickly destroyed by raising the Zeeman energy [5]. This suggests that the incompressible state is not fully polarized. We will assume, following Haldane and Rezayi (HR) [6], that it is spin-singlet. (iii) In numerical calculations investigating the nature of the states at $\nu = 1/2$ and 5/2, pure two-dimensional Coulomb interaction does not produce a spin-singlet ground state. In fact, there is good numerical evidence that the thermodynamic ground state at $\nu = 1/2$ is fully polarized even for vanishing Zeeman energy [7]. We wish here to point out here that our claim in an earlier paper [8], based on a study of systems of 4 and 6 electrons, that the Coulomb ground state is spin-singlet at $\nu = 1/2$ has been invalidated by the present 8 electron calculation [9].

Even though FQHE has not been observed (yet) at $\nu = 1/2$ in single-layer systems, in numerical calculations it is convenient to work at $\nu = 1/2$ rather than at $\nu = 5/2$. Following HR, we will assume that the physics of the FQHE at 5/2 can be investigated by replacing the Coulomb interaction at 1/2 by a model interaction which simulates the conditions at $\nu = 5/2$. Another advantage of working within the lowest LL is that one can use Haldane’s pseudopotentials $V_m$ [10], which completely specify the interaction. $V_m$ is the interaction energy of two electrons in a state with relative angular momentum $m$.

The FQHE at 5/2, and its potential observation at 1/2 in single layer, is still exciting a great deal of interest, and so far no consensus has emerged around a unique theoretical explanation. Haldane and Rezayi initially proposed a ‘pairing’ mechanism in the context of the hollow core model that gives rise to a spin-singlet incompressible state at $\nu = 5/2$, described by a hollow core state. However the hollow core state requires a considerably reduced repulsive interaction at short range between the electrons in order to be stablized. More recently, there has been interest in the nature of the compressible state at $\nu = 1/2$ as Halperin et al suggested [11], in the spirit of the composite fermion theory of the FQHE.
that the filling factor 1/2 corresponds to a Fermi liquid of spin polarized composite fermions (electrons that carry two flux quanta). The present work is, however, related to the possibility of an incompressible state at 1/2.

In this paper we propose the following scenario for the half integral FQHE. First we adopt an idealized short range interaction model characterized by the following choice of Haldane pseudopotentials $V_m = [\alpha, 1, 0, 0, ...]$. We find that the lowest energy spin-singlet (LESS) state of the 8 electron system shows all the properties of an incompressible state. This state remains the global ground state of the system up to $\alpha = 3.1$, beyond which a level crossing occurs, and the LESS state becomes an excited state. (The global ground state for $\alpha > 3.1$ is not incompressible). Furthermore we show that the LESS state is accurately described by a either the Haldane-Rezayi state ($\alpha \leq 1$) or a trial wave function proposed earlier by one of us [13] (for $\alpha \geq 1$). For the Coulomb interaction, the LESS state is still well described by the trial wave function, but the global ground state is not spin-singlet or incompressible. We expect that FQHE will occur at $\nu = 1/2$ if the LESS becomes the global ground state. What (if anything) will make the singlet state the overall ground state is not completely clear at the moment, but we argue that LL mixing can possibly lower the energy of this state sufficiently to make it the ground state.

Our trial wave function is given by

$$\chi_{1/2} = \left[ \prod_{j<k=1}^{N} (z_j - z_k) \right] \left[ \prod_{j<k=1}^{N/2} (z_j - z_k) \right] \left[ \prod_{j<k=\frac{N}{2}+1}^{N} (z_j - z_k) \right] \chi_2$$

(1)

where $z_j = x_j - iy_j$ denotes the position of the $j$th electron, $z_1, ..., z_{N/2}$ refer to spin-up electrons, $z_{N/2+1}, ..., z_N$ refer to spin-down electrons, and $\chi_2$ is the wave function of the state with two filled Landau levels, constructed as though the electrons were spinless. $\chi_{1/2}$ is a singlet state because it is given by a completely symmetric factor (symmetric with respect to the exchange of any two coordinates) times the spin-singlet state

$$\left[ \prod_{j<k=1}^{N/2} (z_j - z_k) \right] \left[ \prod_{j<k=\frac{N}{2}+1}^{N} (z_j - z_k) \right].$$

(This state clearly is singlet because it corresponds to fully occupied spin-up and spin-down states in the lowest LL.)
The appeal of this trial wave function becomes clear by noting the remarkable fact that all observed odd-denominator incompressible states have the structure

\[ \chi_{n/(pn±1)} = \prod_{j<k=1}^{N} (z_j - z_k)^p \chi_{±n}, \quad (2) \]

where \( \chi_{±n} \) is the wave function of IQHE state at \( \nu = n \) (with magnetic field pointing in the \( ±z \) direction), and \( p \) is an even integer. In other words, other than the fact that each electron has captured \( p \) vortices, FQHE states are the same as the IQHE states. The bound state of an electron and \( p \) vortices can be interpreted as a particle, called ‘composite fermion’ (CF), and the FQHE of electrons can be interpreted as the IQHE of CFs. In the limit of \( B \to ∞ \), when the FQHE states are maximally polarized, electrons are taken to be spinless in the construction of \( \chi_{±n} \). In the limit when the Zeeman energy is negligible, (but \( \hbar \omega_c \) is still large) \( \chi_{±n} \) contains \( n_{1\uparrow} \) spin-up and \( n_{1\downarrow} \) spin-down (where \( n = n_{1\uparrow} + n_{1\downarrow} \)) Landau bands occupied. For even \( n \), \( n_{1\uparrow} = n_{1\downarrow} = n/2 \) and the low-field state is spin-singlet. For odd \( n \) it has a non-zero spin. The CF states have been tested numerically for a large number of cases in both limits, and found to be extremely good representations of the actual Coulomb ground states \[14, 15\]. Furthermore, a straightforward generalization of the CF wave functions provides a complete and microscopically accurate description of the entire low-energy Hilbert space of states at arbitrary filling factors \[14\].

The wave functions of the type in Eq.(2) can be written only for odd-denominator filling factors. The spin-singlet wave function \( \chi_{1/2} \) is the simplest generalization of these wave functions to an even-denominator fraction. It also lends itself to a CF interpretation, since it contains vortices bound to electrons in the state \( \chi_2 \). The difference from the states of Eq.(2) is that now two kinds of vortices are attached to each electron of \( \chi_2 \): one is seen by all other electrons, while the other is seen only by electrons of the same spin. Note that it is the electron spin that allows us to write a CF wave function at a half-integral filling factor, which brings out the important role of spin in the case of even-denominator FQHE.

Motivated by the success of the CF theory, we study \( \chi_{1/2} \) in this paper using finite size exact diagonalization techniques. Since we are interested in a singlet state, we set the Zeeman energy to zero in all our calculations. We start with a short-range interaction model, defined
by the pseudopotential parameters

\[ [V_0, V_1, V_2, \ldots] = [\alpha, 1, 0, 0, \ldots] \ . \]  \hspace{1cm} (3)

The only variable in this model is \( \alpha = V_0/V_1 \). Short-range-interaction models have proved quite successful in reproducing the phenomenology of the FQHE \[14\]; for example, the model of eq.(3) produces FQHE at \( n/(2n \pm 1) \) for fully polarized electrons \[17\]. The reason is that incompressible states are not very sensitive to the details of interaction. We will show that at \( \nu = 1/2 \) the LESS state of this model possesses the properties of an incompressible state.

Another advantage of this model is that its ground state is known exactly for \( \alpha = 0 \), where it is precisely given by the HR wave function. In numerical studies, it is found that the HR ground state is valid roughly for \( \alpha < 1.0 \), i.e., for interactions that have an attractive core. We will now show that the LESS state of this model for \( \alpha > 1.0 \) is well described by the lowest LL projection of the CF trial wave function \( \chi_{1/2} \).

We investigate the nature of the LESS state numerically. Our numerical calculations are performed in the spherical geometry \[10\], in which \( N \) electrons move on the surface of a sphere under the influence of a radial magnetic field produced by a magnetic monopole at the center. The flux through the sphere is given by \( N_\phi \hbar c/e \) where \( N_\phi \) is an integer due to Dirac quantization condition. The state \( \chi_{1/2} \) occurs when

\[ N_\phi = 2N - 4 \ . \]  \hspace{1cm} (4)

Clearly, in the limit of large \( N \), the filling factor \( N/N_\phi \) is 1/2. We work with eight electrons. The total size of the Hilbert space in the lowest LL is 1,562,275. However, due to the symmetry of the problem, it is sufficient to work in the sector with \( L_z = S_z = 0 \), where \( L_z \) and \( S_z \) are the \( z \) components of the total orbital angular momentum and the total spin, respectively. In this sector, the size of the Hilbert space is 21,773, which is numerically manageable by Lanczos techniques. For an eight electron system, we find, coming from above, that there is a transition from a non-singlet ground state to a singlet ground state at \( \alpha = 3.2 \), and the ground state remains singlet for \( \alpha < 3.2 \).

We compare the LESS state of the above model (which is also the ground state for \( \alpha < 3.2 \)) with three trial wave functions. One is HR hollow-core wave function \( \chi_{1/2}^{HR} \), which is
the exact ground state of the above one parameter model when $\alpha = 0$. (This wave function also occurs at $N_\phi = 2N - 4$). The second trial wave functions is the lowest LL projection of our trial wave function $\chi_{1/2}$:

$$\mathcal{P}_\chi \chi_{1/2} = \mathcal{P} \left[ \prod_{j<k=1}^{N} (z_j - z_k) \right] \left[ \prod_{j<k=1}^{N/2} (z_j - z_k) \right] \left[ \prod_{j<k=N/2+1}^{N} (z_j - z_k) \right] \chi_2 ,$$

where $\mathcal{P}$ is the projection operator. Unlike $\chi_{1/2}$, this projected wave function does not vanish when two electrons of opposite spin approach one another, and is not expected to be very accurate in the limit of $\alpha \to \infty$. To redress this problem, we construct the following ‘hard-core’ trial wave function:

$$\mathcal{P}_\infty \chi_{1/2} = \left[ \prod_{j<k=1}^{N} (z_j - z_k) \right] \mathcal{P} \left[ \prod_{j<k=1}^{N/2} (z_j - z_k) \right] \left[ \prod_{j<k=N/2+1}^{N} (z_j - z_k) \right] \chi_2$$

This explicitly vanishes when any two electrons coincide, regardless of their spin, and is expected to be more appropriate in the limit of $\alpha \to \infty$. The projection is carried out using techniques described elsewhere [14].

The overlap between the hollow-core and the hard-core trial wave functions is quite small (0.0377), which is not surprising given their distinct physical origins. For $\alpha << 1.1$, the LESS state is expected to be close to the HR hollow-core wave function. Our numerical calculations show that for $\alpha >> 1.1$, the hard-core trial wave function is indeed a good representation of the LESS state. [For example, the overlap between the true LESS state with the hard-core trial wave function is 0.96 for $\alpha = 10$.] Thus, we have a good understanding of the two extreme limits of the one-parameter short range model. Fig.1 shows how the various overlaps vary as a function of $\alpha$ in the regime where the LESS state is the global ground state. The hard-core state does better than the hollow-core state for $\alpha \geq 1.1$. This is the region where the interaction at short distances is repulsive; $\alpha < 1.1$ effectively corresponds to an attractive core. Interestingly, in the intermediate regime, $0.7 < \alpha < 2.7$, the ground state is best described by the simply projected state $\mathcal{P}_\chi \chi_{1/2}$. Thus, a remarkably good description of the short-ranged model is possible in the entire parameter regime. The fact that the LESS state is well approximated by these trial wave functions also implies that it is incompressible, as these trial wave functions describe incompressible states.
Unfortunately, we do not know of a realistic model which exhibits singlet FQHE at $\nu = 1/2$. The following calculations provide some insight into the relevance of our results to the real case with the Coulomb interaction. First of all, the LESS state of the Coulomb interaction (which is not the ground state) is quite close to the CF trial wave function (overlap of 0.82 with the hard-core wave function). The question is if it can be made to be the ground state. In Fig. 2, we show the behavior of the ground state for an interaction \([\alpha V_1, V_1, V_2, ...]\), in which all $V_i$, are set at their Coulomb values (at $\nu = 1/2$), which we will call 'modified Coulomb interaction'. The physical Coulomb interaction corresponds to $\alpha = 2.0$. Here also we see that the global ground state is spin-singlet for up to $\alpha = 1.4$, at value a crossover occurs a ground state which is compressible ($L = 1$), and the LESS state becomes an excited state. Similar to the short-range model, the LESS state is best described by the hollow core state for $\alpha < 1.1$, whereas for $\alpha > 1.1$ it is quite well described by the CF states.

Thus, if by tuning some parameters, the singlet state could be made the ground state, FQHE would result at $\nu = 1/2$. What will make the ground state singlet? It is possible that there will be a level crossing transition to a singlet ground state as LL mixing is increased. Unfortunately, calculations with 4 or 6 electrons are not reliable because of finite size effects, while for an eight particle system, it is not possible for us to carry out a direct numerical investigation of the effect of LL mixing due to the enormously large Hilbert space. However, the following points support our belief. (i) As shown by Rezayi and Haldane \[18\], LL mixing effectively renormalizes the pseudopotentials $V_m$ in such a way that $V_0$ is reduced more rapidly than the others. Consider a situation in which all $V_i, i \neq 0$, are held fixed at their Coulomb values, while the ‘contact’ pseudopotential, $V_0$, is reduced. Clearly, this does not affect the energy of the fully polarized state, but reduces the energy of the singlet eigenstates. Therefore, it is plausible that if the contact interaction is reduced sufficiently, the singlet state may become the ground state \[19\]. This is explicitly seen to be true in the extreme limit when $V_m = [0, 1, 0, 0, ...]$. In this case, there is a unique zero energy singlet ground state, given exactly by HR trial wave function \[3\]. (ii) Now let us consider the other extreme limit of infinite hard-core repulsion, when the pseudopotential parameters are given by $V_m = [\infty, 1, 0, 0, ...]$. The ground state in the lowest LL is not singlet for this model. Let
us now include two LLs, and vary the LL separation to govern the LL mixing [20]. When the LL spacing is zero, it can be proven that there is again a unique zero energy singlet ground state given by our trial wave function $\chi_{1/2}$ (see Appendix). Thus, even for very large $V_0$, LL mixing can produce a singlet ground state. This is a rather remarkable result, since, in general, strong short-range repulsion favors fully polarized states. We also find that in the two LL model the hard core interaction mimicks the Coulomb interaction quite faithfully. In our 4 electron calculation, the Coulomb ground state with zero LL spacing has an overlap of 0.96 with $\chi_{1/2}$. Unfortunately, for 6 and 8 electrons the Hilbert space of the 2 LL problem is prohibitively large, which prevents us from studying the effects of LL mixing. But, clearly, as the LL mixing is increased by reducing the LL spacing, there is an explicit level crossing transition to a singlet ground state in this model.

We parenthetically note here that we had claimed in Ref[8] that in the two LL model the ground state of the hard-core Hamiltonian of Eq.(3) at $\hbar \omega_c = 0$ (which is our trial wave function) is adiabatically connected to the ground state at $\hbar \omega_c = \infty$. Clearly, this is not correct, since the ground state at $\hbar \omega_c = \infty$ is not even spin-singlet. Our calculation shows, however, that the $\hbar \omega_c = 0$ ground state evolves adiabatically into the LESS state at $\hbar \omega_c = \infty$.

We have also investigated the finite width effects on the ground state of the system. We looked at the simplest case of a square well potential, as well as the case where there is a small potential barrier in the center of the well, which leads to an effective double layer system [21]. It was found that finite width does not stabilize the spin-singlet state in either case. Even though finite width gives the desired effect of reducing the ratio $V_0/V_1$, it also makes the effective interaction more long-ranged, which in turns lowers the critical ratio of $V_0/V_1$ at which the crossover to a spin-singlet state occurs.

In conclusion, we have proposed the following scenario for the FQHE at $\nu = 1/2$. The lowest energy state in the spin-singlet sector is ‘incompressible’, and is well represented by a CF trial wave function for repulsive interactions. However, it is not the global ground state for most parameters, which is the reason why FQHE at half-integral filling factor is not observed. We propose that half-integral FQHE will occur for those parameters for which the singlet state becomes the overall ground state. This is the main result of our work.
Now we investigate the relevance of $\chi_{1/2}$ to the FQHE at $\nu = 5/2$. As mentioned earlier, we still work at $\nu = 1/2$ (i.e in the lowest LL), but choose the pseudopotentials appropriate for $\nu = 5/2$. In this case the physical interaction corresponds to $\alpha = 1.45$. Fig. 3 shows the behavior of the LESS state. Unfortunately, the CF states, even though showing the same pattern as for $1/2$, have quite a poor overlap with the LESS state. This is mainly due to the relatively large value of $V_2$ in the second LL. We have checked that a ratio $V_2/V_1 \leq 0.8$ is needed to make the CF states relevant. The Coulomb ratios of $V_2/V_1$ are 0.766 at $1/2$ and 1.083 at $5/2$. This also explains why Fig.3 is so different from the short-range model results. At $5/2$ the crossover from a spin-singlet to a spin-polarized ground state (not shown in Fig.3) occurs at $\alpha = 1.2$, Note however that the HR state shows quite a good overlap with the ground state up to $\alpha = 1.1$. The level crossing occurs relatively much closer to the Coulomb value in $5/2$ than in $1/2$, making it easier for LL mixing (or some other mechanism) to produce incompressibility. Unlike at $1/2$, the incompressible state at $5/2$ is likely to be better described by the HR state than the CF states. Note also that, rather unexpectedly, the HR state has a very small overlap at $\alpha = 0$.

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**APPENDIX**

Let us give the proof of the following theorem.

**Theorem:** In the 2LL Hilbert space of $0 \uparrow, 0 \downarrow, 1 \uparrow, 1 \downarrow$ Landau bands, assuming all of them to be degenerate at zero energy, the spin-singlet state $\chi_{1/2}$ is the unique zero energy ground state at $\nu = 1/2$ of the model interaction

$$V_{TK}(r) = \infty \delta(r) + \lambda \nabla^2 \delta(r),$$

which is equivalent to the infinite hard-core repulsion defined in the text.

**Proof:** All states with zero energy must vanish at least as fast as $r^2$ as two electrons, at a distance $r$, approach one another. We now show that at $\nu = 1/2, \chi_{1/2}$ is the only state with this property. (i) Since only two LLs are available, one of the zeros as the $j$ and $k$ electrons
are brought close to each other must be of the form \((z_j - z_k)\). Thus the wave function must contain a factor \(\chi_1 = \prod_{j<k=1}^{N}(z_j - z_k)\).

(ii) Due to Pauli principle, when two electrons with the same spin approach each other, the wave function must vanish at least as fast as \(r^3\). Thus the state must contain another factor \(\chi_{1;1} = \prod_{r<s=1}^{N/2}(z_r - z_s) \prod_{p<q=N/2+1}^{N}(z_p - z_q)\).

(iii) Thus the most general form of a state that is confined to the lowest LLs and vanishes at least as fast as \(r^2\) is

\[ \chi_{1/2} = \chi_1 \chi_{1;1} \chi_\nu \]

where \(\chi_\nu\) must be within the lowest two LLs. Further note that \(\chi_\nu\) must vanish when any two electrons coincide; for electrons with opposite spins it must vanish because we want the wave function to vanish at least as fast as \(r^2\) as any two electrons come close, and for electrons with the same spins it must vanish due to Pauli principle. The largest value that \(\nu\) can assume is \(\nu = 2\) where \(\chi_\nu\) is the state with two filled LLs of spinless electrons. The product \(\chi_{1/2}\) is then the unique wave function at \(1/2\) which vanishes at least as fast as \(r^2\) when two electrons approach each other. It is therefore the unique zero energy ground state for the above hard-core model interaction.
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**Figure Captions**

Fig.1. Overlap of the exact ground state of the short range model defined in the text with the hollow-core state $\chi_{1/2}^{HR}$ (dashed line), the hard-core state $\mathcal{P}_\infty\chi_{1/2}$ (dotted line), and with the simply projected state $\mathcal{P}\chi_{1/2}$ (solid line). The calculation in this figure as well as those in Figs. 2 and 3 was done for an 8 electron system, and at zero Zeeman energy.

Fig.2. Overlap of the exact ground state of the modified Coulomb model in the lowest LL ($\nu = 1/2$) with the hollow-core state $\chi_{1/2}^{HR}$ (dashed line), the hard-core state $\mathcal{P}_\infty\chi_{1/2}$ (dotted line), and with the simply projected state $\mathcal{P}\chi_{1/2}$ (solid line). The actual Coulomb interaction occurs at $\alpha = 2.0$.

Fig.3. Overlap of the lowest energy spin-singlet eigenstate of the modified Coulomb model in the first LL ($\nu = 5/2$) with the hollow-core state $\chi_{1/2}^{HR}$ (dashed line), the hard-core state $\mathcal{P}_\infty\chi_{1/2}$ (dotted line), and with the simply projected state $\mathcal{P}\chi_{1/2}$ (solid line). This state is the ground state for $V_0/V_1 < 1.2$. The actual Coulomb interaction occurs at $\alpha = 1.45$. 

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