THE COMPOSITE FERMION PICTURE FOR N ELECTRONS ON A HALDANE SPHERE: HUND'S RULE FOR MONOPOLE HARMONICS

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The mean field composite Fermion (MFCF) picture has been qualitatively successful when applied to electrons (or holes) in the lowest Landau level. Because the energy scales associated with Coulomb interactions and with Chern–Simons gauge field interactions are different, there is no rigorous justification of the qualitative success of the MFCF picture. Here we show that the behavior of the electron pseudopotential for the lowest monopole harmonic shell is opposite to that of the spherical harmonics of atomic physics. As a consequence, states with low total angular momentum L usually form the low energy sector in the spectrum, in contrast to Hund's rule of atomic physics. Which state with small L is the ground state depends on the number of multiplets of a given L and on their fractional parentage from states of given pair angular momentum. The MFCF prediction for the low energy sector can be thought of as the equivalent of Hund's rule governing monopole harmonics of the totally spin polarized system. It can be rigorously justified for an arbitrary number of electrons only by comparison with detailed numerical studies and experiment.

For N electrons on a Haldane sphere [1] (containing at the center a magnetic monopole of charge $2S\,hc/e$), the single particle states fall into angular momentum shells with $l_n = S + n$, $n = 0, 1, \ldots$ The nth shell is $2l_n + 1$ fold degenerate. The composite Fermion (CF) [2] transformation attaches to each electron a flux tube of strength $2p_0$ flux quanta oriented opposite to the original magnetic field. If the added flux is treated in a mean field approximation, the resulting effective magnetic field seen by one CF is $B^* = B - 2p_0\,(hc/e)\,n_s$ (n_s is the number of electrons per unit area). An effective CF filling factor ν_0^* ($\nu_0^{*\,-1} = \nu_0^{-1} - 2p_0$) and an effective monopole strength $2S^*$ ($2S^* = 2S - 2p_0(N-1)$) seen by one CF can also be defined. $|S^*|$ plays the role of the angular momentum of the lowest CF shell [3]. States belonging to the Jain sequence occur when ν_0^* is an integer. For such integral CF fillings, the ground state is a Laughlin [4] incompressible liquid state with angular momentum $L = 0$. If ν_0^* is not an integer, a partially occupied CF shell will contain $n_{\rm QE}$ quasielectrons (or $n_{\rm QH}$ quasiholes). In the MFCF picture these states form a degenerate band of angular momentum multiplets with energy $n_{\rm QE}\varepsilon_{\rm QE}$ where $\varepsilon_{\rm QE}$ is the energy of a single quasielectron (or $n_{\rm QH}\varepsilon_{\rm QH}$ for quasiholes). The degeneracy results from the neglect of QP–QP interactions in the MFCF approximation [5].

Hierarchy states [6] outside the Jain sequence are obtained (when ν_0^* is not equal to an integer) by reapplying the CF transformation to residual quasiparticles in the partially filled CF shell. In comparing the predictions of the CF hierarchy picture with numerical results for states containing three or four quasiparticles, it is found that the MF approximation is often qualitatively incorrect. Before worrying about the reapplication of the MFCF approach to residual quasiparticles in a partially filled CF shell, it is very useful to ask why the MFCF picture applied directly to electrons (or holes) in a partially filled shell gives qualitatively correct results. In light of the different energy scales describing Coulomb interactions and Chern–Simons gauge field interactions, the justification cannot lie in a cancellation between these interactions.

The single particle states for an electron on a Haldane sphere are called monopole harmonics [7] and denoted by $|l_n, m\rangle$, where $l_n = S + n$ and $-l_n \le m \le l_n$. The single particle energies depend only on S and n, and for the fractional quantum Hall (FQH) effect, only the lowest shell with $n = 0$, which is completely spin polarized, need be considered. The many electron states $|m_1, m_2, \ldots, m_N\rangle$ can be written as $c^\dagger_{m_1} c^\dagger_{m_2} \ldots c^\dagger_{m_N} |0\rangle$ where $|0\rangle$ is the vacuum state. The object of numerical studies is to diagonalize the electron-electron interaction within the subspace of the $(2S+1)![N!(2S+1-N)!]^{-1}$ many particle states of the lowest shell. The numerical calculations for Laughlin condensed states or states containing a small number of Laughlin quasiparticles [4] become difficult when the number of electrons N exceeds 10. The calculations give the eigenvalues E as a function of the total angular momentum L, and the numerical results always show one or more L multiplets forming a low energy sector (or low energy band).

It has been demonstrated [3,8] that the CF picture correctly predicts the low lying band of multiplets by simply noting that when the N electrons are converted to N composite Fermions, the angular momentum of the lowest shell goes from l_0 to $l_0^* = l_0 - p(N-1)$, where $2p$ is the number of flux quanta attached to each CF. A very fundamental question which is not well understood is, "Why does the MFCF picture do so well in describing not just the Jain sequence of incompressible states, but also the low lying band of multiplets for any value of $2S$?" The problem of N

Fermions in a shell of angular momentum l is very familiar from atomic and nuclear physics [9]. In this note we concentrate on the similarities and differences between the problems of N electrons in the lowest angular momentum shell of a Haldane sphere and N electrons in an atomic shell of the same angular momentum l. First, because of the magnetic monopole of magnitude $2S(hc/e)$, where $2S$ is an integer, the monopole harmonics $|l_n, m\rangle$ have angular momentum $S+n$ ($n = 0, 1, 2, \ldots$) which can be integral or half-integral. The spherical harmonics have $S = 0$, so l must be an integer. For FQH systems (i.e. $\nu < 1$) we are interested in the lowest angular momentum shell with $l_0 = S$. Second, the Zeeman splitting is large compared to the Coulomb interaction, so only totally spin polarized states of FQH systems need be considered. In fact, even if the Zeeman splitting vanished, the exchange energy would result in the maximum possible spin polarization for the lowest energy multiplet as prescribed by Hund's first rule. Because the total spin is always equal to $\frac{1}{2}N$ and only the lowest shell is occupied, the total (spin *plus* orbital) angular momentum J is never of concern. It is simply the sum of L and $\frac{1}{2}N$. Third, for FQH systems, calculations with N values up to 10 and l values up to 27/2 have been performed [10]. In atomic systems, l values up to 3 (f-states) and N values up to 7 are usually the maximum values studied.

The key rule, especially for the maximally polarized systems, is Hund's second rule. It states that the largest allowable L value consistent with the first rule (maximum possible spin) will be the ground state. This is certainly not the case for FQH systems. Many Laughlin incompressible states at $L = 0$ are ground states, and states containing 1, 2, 3, ... quasiparticles always have allowed L values that are much smaller than $L_{\rm MAX} = \frac{1}{2}N(2l - N + 1)$. What causes this difference?

In Fig. 1 we display the Coulomb pseudopotential for a pair of electrons in single particle angular momentum states $l = 1$ through 5, as a function of the pair angular momentum $\mathbf{L}_{12} = \mathbf{l}_1 + \mathbf{l}_2$. For monopole harmonics ($l = S$, $n = 0$) $V(L_{12})$ increases with increasing L_{12}. For atomic shells (spherical harmonics) just the opposite occurs – the repulsion decreases with increasing L_{12} (for the h-shell and higher, $V(L_{12})$ begins to increase beyond some relatively large value of L_{12}, but this is never of concern in atomic physics).

An antisymmetric state containing N Fermions of angular momentum l can be written $\left|l^N, L\alpha\right\rangle$, and it can be expressed as [9]

$$\left|l^N, L\alpha\right\rangle = \sum_{L_{12}} \sum_{L'\alpha'} G_{L\alpha,L'\alpha'}(L_{12}) \left|l^2, L_{12}; l^{N-2}, L'\alpha'; L\right\rangle , \qquad (1)$$

where $G_{L\alpha,L'\alpha'}(L_{12})$ is called the coefficient of fractional grandparentage. In Eq. (1), $\left|l^2, L_{12}; l^{N-2}, L'\alpha'; L\right\rangle$ is a state of angular momentum L. It is antisymmetric under permutation of particles 1 and 2, which have pair angular momentum L_{12}, and under permutation of particles 3, 4, ..., N, which have angular momentum L'. The label α (or α') distinguishes independent orthogonal states with the same angular momentum L (or L').

It is not difficult to prove the operator identity

$$\hat{L}^2 + N(N-2)\,\hat{l}^2 = \sum_{\rm pairs} \hat{L}_{ij}^2 . \qquad (2)$$

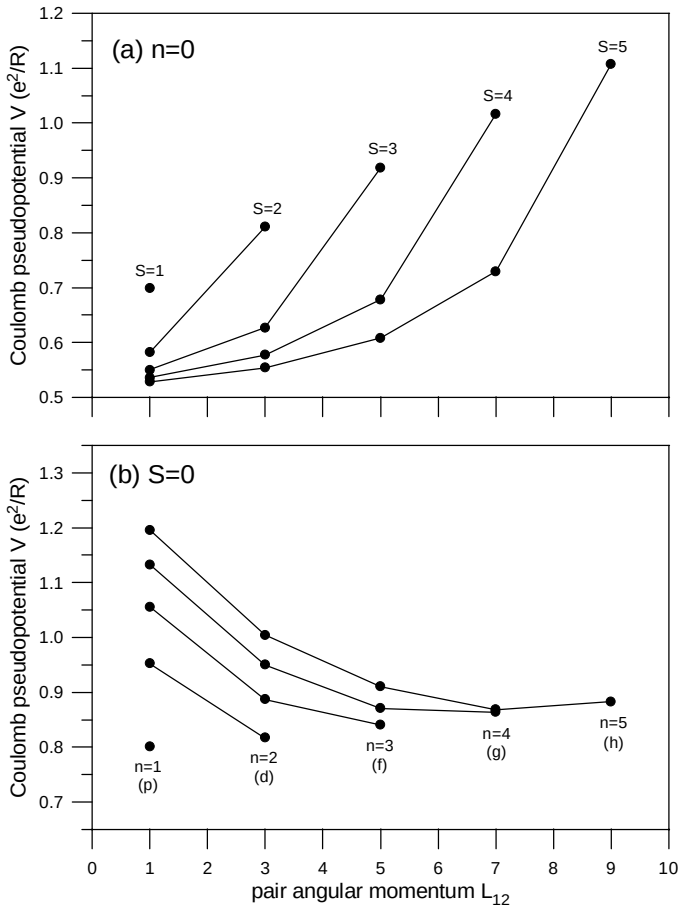

Figure 1. The pseudopotential for a pair of electrons of total angular momentum L_{12} as a function of $l = S + n$. Energy is measured in units of e^2/R, where R is the radius of the sphere. (a) monopole harmonics, $n = 0$; (b) spherical harmonics, $S = 0$, calculated for a radial wavefunction which localizes the electrons at radius R.

Here $\hat{L} = \sum_i \hat{l}_i$ and $\hat{L}_{ij} = \hat{l}_i + \hat{l}_j$. If we take diagonal matrix element of Eq. (2) between states $\left|l^N, L\alpha\right\rangle$, we obtain

$$\left\langle l^N, L\alpha\right| \sum_{\text{pairs}} \hat{L}_{ij}^2 \left|l^N, L\alpha\right\rangle = L(L+1) + N(N-2)\, l(l+1). \tag{3}$$

The left hand side is simply $\frac{1}{2}N(N-1)$ times the average value of the square of the pair angular momentum in the state $\left|l^N, L\alpha\right\rangle$. Clearly, states with higher L have higher values of this quantity. The left hand side of Eq. (3) can be expressed as

$$\left\langle l^N, L\alpha\right| \sum_{\text{pairs}} \hat{L}_{ij}^2 \left|l^N, L\alpha\right\rangle = \frac{1}{2}N(N-1) \sum_{L_{12}} \mathcal{G}_{L\alpha}(L_{12})\; L_{12}(L_{12}+1), \tag{4}$$

where

$$\mathcal{G}_{L\alpha}(L_{12}) = \sum_{L'\alpha'} \left|G_{L\alpha, L'\alpha'}(L_{12})\right|^2 . \tag{5}$$

From the orthonormality of the functions $\left|l^N, L\alpha\right\rangle$,

$$\sum_{L_{12}} \sum_{L'\alpha'} G^*_{L\alpha,L'\alpha'}(L_{12})\, G_{L\beta,L'\alpha'}(L_{12}) = \delta_{\alpha\beta} \tag{6}$$

and

$$\sum_{L_{12}} \mathcal{G}_{L\alpha}(L_{12}) = 1. \tag{7}$$

The energy of the state $\left|l^N, L\alpha\right\rangle$ is given by

$$E_\alpha(L) = \sum_{L_{12}} \mathcal{G}_{L\alpha}(L_{12})\, V(L_{12}). \tag{8}$$

It is noteworthy that the average value of $\sum_{\text{pairs}} \hat{L}^2_{ij}$ is independent of which multiplet α is being considered. In view of Eqs. (3), (4), and (8), it is not surprising that in atomic physics, where $V(L_{12})$ decreases rapidly with L_{12}, Hund's second rule holds. For states with $L = L_{\text{MAX}}$ only a single multiplet ever appears, and it has the highest value of the average pair angular momentum. Despite this strong indication that, in atomic systems, the state with the largest allowed value of L (consistent with the maximum value of the total spin) has the lowest energy, Hund's rule is considered an empirical rule, that can be rigorously justified only by numerical calculations.

For the case of monopole harmonics, $V(L_{12})$ rises very rapidly with increasing L_{12}. Therefore, low energy states must somehow be able to avoid having large grandparentage in states with large values of L_{12}. In a previous paper we have demonstrated analytically that this is true for three electron systems [11]. For the monopole harmonics the general trend is to have $N_L^{-1} \sum_\alpha E_\alpha(L)$, the average $E(L)$ for all multiplets with angular momentum L, increase with increasing L. However, when the single particle angular momentum, l, increases beyond some value for an N-particle system, several multiplets of the same L begin to appear. In Tab. 1 we present as an example the number of independent multiplets of angular momentum L, as a function of $l_0 = S$, for a system of six electrons. The values of S go from 0 to 15/2, and L from 0 to 15 (the table uses $2S$ and $2L$ to avoid printing half-integers and only values of $2L$ up to 23 have been included), If the pseudopotential were given by $\tilde{V}(L_{12}) = A + B\, L_{12}(L_{12}+1)$, all of the different multiplets with the same value of L would be degenerate because of Eqs. (3)–(8), and L_{MIN}, the smallest allowed L-multiplet, would be the ground state. The difference between $\tilde{V}(L_{12})$ and the actual pseudopotential $V(L_{12})$ leads to a lifting of this degeneracy (different multiplets repel one another). The splittings caused by $V(L_{12}) - \tilde{V}(L_{12})$ can become large when N_L, the number of times the multiplet L occurs, is large. In this case, a state with L larger than L_{MIN} can become the ground state since the actual values of $E_\alpha(L)$ depend on how the values of $\mathcal{G}_{L\alpha}(L_{12})$ are distributed, not just on the average value of $\hat{L}^2_{12}$ for that value of L. For example, the lowest energy multiplet with $2L = 3$ and $2S = 14$ is lower in energy than the multiplets at $2L = 1$ and 2, because it is one of 12 multiplets as compared to only 6 and 4 at $2L = 1$ and 3, respectively. Knowing which multiplet is the ground state or which multiplets form the "low energy band" without performing detailed numerical calculation is a considerably more difficult task than it was for spherical harmonics.

Table 1

Number of times the angular momentum multiplet L appears when $N = 6$ electrons of angular momentum $l_0 = S$ are combined in a totally antisymmetric state.

${}_2S^{2L}$	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
0		1		1																				
1	1																							
2		1		1																				
3	1		1		1																			
4				1																				
5	1																							
6				1																				
7	1		1		1		1																	
8		1		2	1	1	1	1		1														
9	2		2	1	3	1	3	1	2	1	1		1											
10		2	1	4	2	4	3	4	2	3	2	2	1	1		1								
11	3		4	3	6	3	7	4	6	4	5	2	4	2	2	1	1		1					
12		4	2	7	5	8	7	9	6	9	6	7	5	5	3	4	2	2	1	1		1		
13	4	1	7	5	11	7	13	9	13	10	12	8	11	7	8	5	6	3	4	2	2	1	1	
14		6	4	12	9	14	13	17	13	18	14	16	13	14	10	12	8	8	6	6	3	4	2	2
15	6	2	11	9	17	13	22	17	23	19	24	18	23	17	19	15	16	11	13	8	8	6	6	3

In the MFCF picture, the angular momentum l_0 of the lowest shell is replaced [2] by $l_0^* = l - (N-1)$. The allowed angular momenta L^* are obtained by placing N composite Fermions in the lowest CF angular momentum shells. This always results in a smaller maximum possible angular momentum $L^*_{\rm MAX}$. For example, if $2S \geq 3N-3$, $L^*_{\rm MAX} = \frac{1}{2}N(2S-3N-3)$; if $3N-3 \geq 2S \geq \frac{5}{2}N-4$, $L^*_{\rm MAX} = (2S-\frac{5}{2}N+4)(3N-3-2S)$; etc. At fillings corresponding to states in the Jain sequence $L^*_{\rm MAX} = 0$. For states containing several quasiparticles, a number of different L^* values less than or equal to $L^*_{\rm MAX}$ can occur. From the numerical calculations (and from experiment) it has been observed that the subset of allowed L^* multiplets obtained by placing N CF's into the lowest angular momentum shells form the low energy band of the original electron system. This is plausible because: (i) the allowed values of L^* are always small compared to the original $L_{\rm MAX}$ and therefore have a small expectation

value of $\sum_{\rm pairs} \hat{L}_{ij}^2$, and (ii) electron L values which occur a relatively large number of times tend to form the low energy band of L^*'s. For the six electron system with a given $2S$, the allowed L^* values are those appearing in row with $2S^* = 2S - 10$. The table of multiplicities depends only on $|2S|$, so if $2S - 10$ is negative, it is simply replaced by its magnitude. Because of this, the $\nu = 2/3$ state occurs at $2S = 9$ and the $\nu = 2/5$ state at $2S = 11$.

We have evaluated the coefficients of fractional grandparentage, $\mathcal{G}_{L\alpha}(L_{12})$ for values of N up to eight and for many different values of $2S$. In all cases where the MFCF approximation is applied to the electrons (or to holes in a nearly filled level), we find that the grandparentage arising from large L_{12} is smaller for the lowest energy band multiplets than for neighboring multiplets.

To some extent this is not very surprising since in order for a state to have low energy, it is required by Eq. (8) to avoid large parentage $\mathcal{G}(L_{12})$ for large L_{12}. Rather than introduce a second energy scale $\hbar\omega_c^*$ and assume that there exists a large cancellation between Chern–Simons and Coulomb interactions, we regard the MFCF approximation as a prescription (similar to Hund's rule in atomic physics) that selects a low angular momentum subset of the set of allowed L-multiplets of N electrons, which has low grandparentage for the strongly repulsive part of the Coulomb interaction, and therefore low energy. Our arguments make this hypothesis plausible, but the proof (as with Hund's rule) lies in comparison with experiment (in this case the numerical experiment of exact diagonalization).

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