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Excitations of the Moore–Read $\nu = \frac{5}{2}$ State: Three-Body Correlations and Finite-Size Effects on a Sphere

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Correlations in partially filled electron and composite fermion Landau levels are studied numerically. Insight into the nature of the correlations is obtained by using model pair pseudopotentials. Energy spectra of a model short-range three-body repulsion are calculated. Moore–Read ground state at the half-filling and its quasielectron, quasihole, magnetoroton, and pair-breaking excitations are all identified. The quasielectron/quasihole excitations are described by a composite fermion model for Laughlin-correlated electron pairs. Comparison of energy spectra and wavefunction overlaps obtained for different pseudopotentials suggests that finite-size effects can be important in numerical diagonalization studies on a sphere.

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1. Introduction

Laughlin correlations [1] among electrons in the lowest Landau level (LL_0) imply maximum possible avoidance of pair states with the smallest relative angular momentum $\mathcal{R}_2$. They are responsible for the most prominent fractional quantum Hall (FQH) states at filling factors $\nu = n(2pn \pm 1)^{-1}$ [2, 3]. However, FQH states with different, non-Laughlin correlations occur as well, e.g., in higher electron LL's (LL_n with $n \geq 1$) [4] or in composite fermion (CF) LL's [5]. The correlations are determined by the pseudopotential [6] defined as the pair interaction energy V_2 as a function of $\mathcal{R}_2$. A "harmonic" pseudopotential* produces no correlations (i.e.,

*A harmonic pseudopotential is linear in average squared separation $\langle r^2 \rangle$. On a sphere it is linear in $L_2(L_2+1)$, where l and $L_2 = 2l - \mathcal{R}_2$ are the single-particle and pair angular momenta, respectively. On a plane (i.e. for $2l \to \infty$), it is linear in $\mathcal{R}_2$.

each multiplet with the same total angular momentum L has the same energy E) [7]. Often, the essential correlations associated with an actual interaction can be reproduced by a simple "model" pseudopotential in which the harmonic part is neglected, and an anharmonicity is introduced at a few lowest values of $\mathcal{R}_2$. For example, the Laughlin wavefunction [1] at the filling factor $\nu = \frac{1}{3}$ is an exact $E = 0$ eigenstate of $V_2(\mathcal{R}_2) = \delta_{\mathcal{R}_2,1}$.

We use an exact diagonalization on a Haldane sphere [2] to study eigenstates of a model two-body pseudopotential $U_\alpha(\mathcal{R}_2) = (1-\alpha)\, \delta_{\mathcal{R}_2,1} + \frac{1}{2}\alpha\delta_{\mathcal{R}_2,3}$. For$\alpha = 0$ and 1, the low-energy states avoid having a large pair amplitude $\mathcal{G}_2$ [6] at $\mathcal{R}_2 = 1$ and 3, respectively. For $\alpha \sim \frac{1}{2}$, amplitudes for pairs with $\mathcal{R}_2 = 1$ and 3 are comparable. Because U_α is subharmonic at $\mathcal{R}_2 = 1$ for $\alpha \geq \frac{1}{2}$, Laughlin correlations cannot be responsible for the observed $\nu = \frac{5}{2}$ and $\frac{3}{8}$ FQH states (corresponding to half-filled LL_1 and CF-LL_1, respectively). Proposed trial wavefunctions include Halperin [8] and Haldane–Rezayi [9] states with Laughlin correlations between spin-triplet and spin-singlet pairs, respectively, and the Moore–Read [10] state that can be defined as the $E = 0$ ground state of a short-range three-body repulsion [11]. These paired states were investigated in detail [12–14]. However, which model best fits different experimental situations is not certain.

In this note we concentrate on the half-filled LL_1. Because the pair–pair interaction does not conserve $\mathcal{R}_2$ of each individual pair, its pseudopotential is not well defined [15]. Therefore, Laughlin correlations among the pairs invoked in Halperin and Haldane–Rezayi pairing models cannot be rigorously established. In fact, it has been incorrectly assumed [11] that such pairing results for pseudopotentials attractive at short range rather than "harmonically" repulsive like $U_{\frac{1}{2}}$. On the other hand, the Moore–Read wavefunction correctly describes the ground state for an interaction with a very special short-range behavior, while the pseudopotentials in experimental systems depend on sample parameters (e.g., layer width w). Earlier diagonalization studies indicated that realistic Coulomb pseudopotentials in LL_1 are slightly too weak at short range to support the Moore–Read state [14]. This suggests that it is not quite as accurate a description of the $\nu = \frac{5}{2}$ state as the Laughlin wavefunction is of the $\nu = \frac{1}{3}$ state.

2. Model

For electrons confined to a spherical surface in a shell of angular momentum l, $V_2(\mathcal{R}_2)$ is simply an expectation value of the Coulomb interaction for an electron pair in LL_n with a total angular momentum $L_2 = 2l - \mathcal{R}_2$. For CF quasiparticles (QP's), $V_2(\mathcal{R}_2)$ can be obtained from the numerical diagonalization of the Coulomb interaction for small electron systems which contain two Laughlin QP's [6]. Results for $V_2(\mathcal{R}_2)$ in LL_0, LL_1, CF-LL_0, and CF-LL_1 can be found in the literature [7, 16–18]. Numerical results for small systems on a sphere are qualitatively correct, provided that the range of the interaction (or correlation length), scaled with a magnetic length $\lambda = \sqrt{hc/eB}$, is small compared to radius of the sphere R.

Correlations in a specific many-body multiplet $|L, \beta\rangle$ are conveniently described by a pair amplitude function $\mathcal{G}_2(\mathcal{R}_2)$ equal to the number of pairs with a given value of $\mathcal{R}_2$ divided by the total number of pairs $\binom{N}{2}$ [7]. The total interaction energy of a multiplet is given by $E(L, \beta) = \binom{N}{2} \sum_{\mathcal{R}_2} \mathcal{G}_2(\mathcal{R}_2) V_2(\mathcal{R}_2)$.

3. Results and discussion

3.1. Two-body correlations

In Fig. 1 we display $\mathcal{G}_2(1)$ and $\mathcal{G}_2(3)$ for the lowest $L = 0$ states of the model pseudopotential $U_\alpha(\mathcal{R}_2)$. The values of N and $2l$ were chosen to correspond to the known families of incompressible $\nu = \frac{1}{2}$ and $\frac{1}{3}$ ground states in LL_1 and in CF-LL_1, corresponding to the total electron filling factors $\nu = \frac{5}{2}$, $\frac{7}{3}$, $\frac{3}{8}$, and $\frac{4}{11}$. It is clear that Laughlin correlations with $\mathcal{G}_2(1) \ll \mathcal{G}_2(3)$ occur for $\alpha \sim 0$, and an opposite relation $\mathcal{G}_2(3) \ll \mathcal{G}_2(1)$ holds for $\alpha \sim 1$. For $\alpha \sim \frac{1}{2}$ (corresponding to electrons in LL_1) the situation is not so simple because $V_2(\mathcal{R}_2)$ is nearly harmonic at short range, and the correlations cannot be expressed in terms of avoidance of a single value of $\mathcal{R}_2$. However, the Moore–Read state is known [11] to be an exact $E = 0$ ground state of a short-range *three-body* repulsion. This suggests that a careful investigation of three-body correlations might be useful.

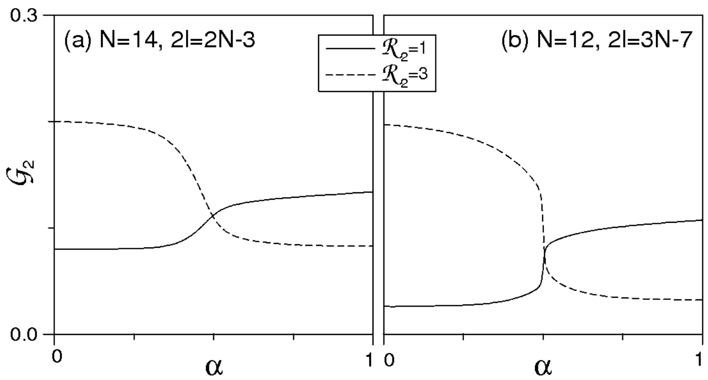

Fig. 1. Dependence of pair amplitudes $\mathcal{G}_2$ on parameter α of pair interaction U_α, obtained for the lowest $L = 0$ states of N particles at $2l = 2N - 3$ (a) and $3N - 7$ (b), corresponding to a $\frac{1}{2}$- and $\frac{1}{3}$-filled shell, respectively.

The criterion for the avoidance of a specific pair state at $\mathcal{R}_2$ is that it corresponds to the dominant positive anharmonic term of $V_2(\mathcal{R}_2)$ [7]. The three-body states are also labeled by relative (with respect to the center of mass) angular momentum $\mathcal{R}_3 = 3, 5, 6, \ldots$, and larger $\mathcal{R}_3$ means a larger average area spanned by the three particles. Since no degeneracies appear in the $V_3(\mathcal{R}_3)$ spectrum for $\mathcal{R}_3 < 9$, its low-$\mathcal{R}_3$ part can be considered a three-body pseudopotential analogous to $V_2(\mathcal{R}_2)$. The results obtained for different pair interactions are shown in

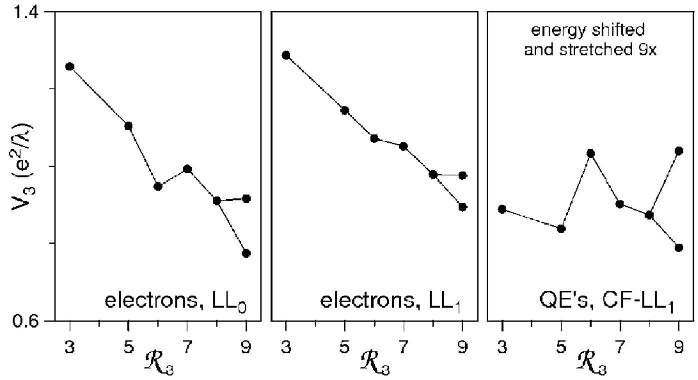

Fig. 2. Triplet interaction pseudopotentials $V_3(\mathcal{R}_3)$ for various pair pseudopotentials. λ is the magnetic length.

Fig. 2. The nonmonotonic behavior of $V_3(\mathcal{R}_3)$ in frame (c) most likely precludes the tendency to avoid the $\mathcal{R}_3 = 3$ triplet state in the quasielectron (QE) systems. On the other hand, the monotonic character of $V_3(\mathcal{R}_3)$ in frame (b) might lead to the avoidance of the same $\mathcal{R}_3 = 3$ triplet state in a partially filled LL_1. The dependence of $V_3(\mathcal{R}_3)$ on $V_2(\mathcal{R}_2)$ can be captured by calculating the leading V_3 coefficients for the model pair pseudopotential U_α. Only around $\alpha \sim \frac{1}{2}$ is $V_3(\mathcal{R}_3)$ a superlinear (i.e., superharmonic) function for small $\mathcal{R}_3$.

3.2. Three-body correlations

The hypothesis of the avoidance of the $\mathcal{R}_3 = 3$ triplets in partially filled LL_1 can be tested using "triplet amplitude" $\mathcal{G}_3(\mathcal{R}_3)$. It is defined in analogy to the pair amplitude, as an expectation value of the operator $\widehat{\mathcal{P}}_{ijk}(\mathcal{R}_3, \beta_3)$ projecting a many-body state Ψ onto the subspace with three particles ijk being in an eigenstate $|\mathcal{R}_3, \beta_3\rangle$ (here, β_3 distinguishes different multiplets at the same $\mathcal{R}_3$; it can be omitted for $\mathcal{R}_3 < 9$). The triplet amplitudes are normalized, $\sum_{\mathcal{R}_3,\beta_3} \mathcal{G}_3(\mathcal{R}_3, \beta_3) = 1$, and satisfy an additional sum rule:

$$L(L+1) + \frac{N(N-3)}{2} l(l+1) = \frac{N(N-1)}{6} \sum_{\mathcal{R}_3,\beta_3} \mathcal{G}_3(\mathcal{R}_3, \beta_3) L_3(L_3+1), \quad (1)$$

where $L_3 = 3l - \mathcal{R}_3$ is the total triplet angular momentum. Energy of Ψ is $E = \binom{N}{3} \sum_{\mathcal{R}_3,\beta_3} \mathcal{G}_3(\mathcal{R}_3, \beta_3)\, V_3(\mathcal{R}_3, \beta_3)$.

In Fig. 3 we plot the leading amplitudes $\mathcal{G}_3(\mathcal{R}_3)$ as a function of α, calculated in the lowest $L = 0$ states of the FQH systems used earlier. Clearly, all triplet amplitudes significantly depend on α, but we especially want to point out the following three features for $\mathcal{R}_3 = 3$: (i) at $\nu = \frac{1}{2}$, the tendency to avoid $\mathcal{R}_2 = 1$ pairs at $\alpha \sim 0$ is *not* synonymous with the avoidance of $\mathcal{R}_3 = 3$ triplets; (ii) $\mathcal{G}_3(3)$ *vanishes* for $\alpha \approx \frac{1}{2}$ at $\nu = \frac{1}{2}$; (iii) $\mathcal{G}_3(3)$ *increases* when α increases beyond $\frac{1}{2}$ in all frames.

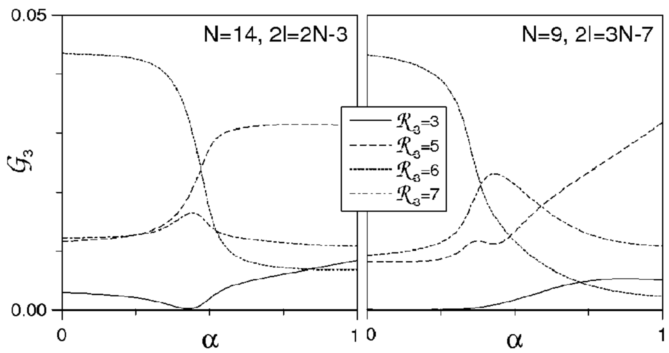

Fig. 3. Dependence of triplet amplitudes $\mathcal{G}_3$ on parameter α of pair interaction U_α, obtained for the lowest $L = 0$ states of N particles in the same FQH states as used in Fig. 1.

Observation (iii) confirms the suspicion based on the form of $V_3(\mathcal{R}_3)$ in Fig. 2c that, against an earlier assumption [11], the Halperin paired state [8] is not an adequate description for systems with subharmonic pseudopotentials at short range. In particular, such a model appears inappropriate for the QE's in CF-LL_1 (i.e., in the FQH states at $\nu = \frac{3}{8}$ and $\frac{4}{11}$). Instead of Halperin's pairing, grouping into larger clusters most likely occurs.

We have evaluated the value α_0 at which $\mathcal{G}_3(3)$ drops (nearly) to zero at $2l = 2N - 3$ for different $N \leq 14$, but it is difficult to reliably estimate α_0 on a plane. However, other evidence [19] suggests that α_0 is close to $\frac{1}{2}$ for $N \to \infty$. Since $U_{\frac{1}{2}}$ accurately models Coulomb interaction in LL_1, the $\mathcal{R}_3 > 3$ correlations are expected to accurately describe experimental FQH systems at $\nu \sim \frac{5}{2}$.

3.3. Spectra of three-body repulsion

To study excitations of the Moore–Read state, a simple model three-body repulsion $W(\mathcal{R}_3) = \delta_{\mathcal{R}_3,3}$ can be used [12, 13], which induces exactly the right type of correlations ($\mathcal{R}_3 > 3$). In Fig. 4a we present the energy spectrum for $N = 14$ and $2l = 2N - 3$. There is exactly one $E = 0$ state in the spectrum at $L = 0$ (at $2l < 2N - 3$ every state has $E > 0$, and at $2l > 2N - 3$ there is more than one $E = 0$ state). This fact makes the Moore–Read an extension of the Laughlin idea for the $\nu = \frac{1}{3}$ state at $2l = 3N - 3$ being the only state in its Hilbert space with no pair amplitude at $\mathcal{R}_2 = 1$. Just as the avoidance of more than one pair state generated the whole $\nu = \frac{1}{3}, \frac{1}{5}, \ldots$ sequence, the avoidance of not pairs, but triplets gives rise to incompressibility at new values of ν.

The analogy to the Laughlin $\nu = \frac{1}{3}$ state goes beyond the incompressible ground state. The low-energy excitations clearly form a band that resembles the magnetoroton curve [13]. In frame (b) we overlay data obtained for $N = 6$ to 14 and plot it as a function of wavevector $k = L/R$. The continuous character of this band and the minimum at $k \approx 1.5\lambda^{-1}$ are clearly visible.

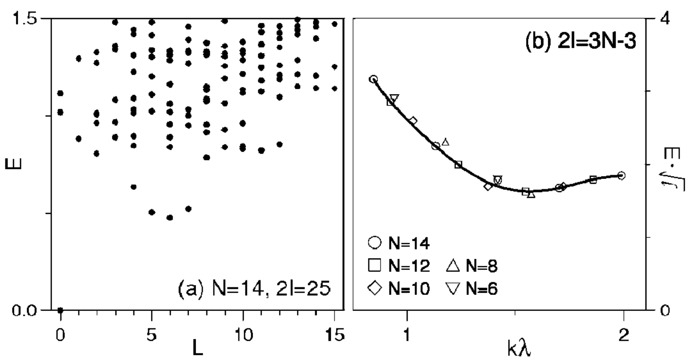

Fig. 4. (a) Energy spectrum $E(L)$ of $N = 14$ particles interacting through triplet pseudopotential $W(\mathcal{R}_3)$, at the Moore–Read value of $2l = 2N - 3 = 25$. (b) Energy dispersion $E(k)$ for the excited magnetoroton band. λ is the magnetic length.

An increase in $\mathcal{G}_2(1)$ for $\alpha \geq \frac{1}{2}$ in Fig. 1a as compared to the Laughlin correlated state at $\alpha = 0$ might indicate pairing. If the pairs had Laughlin correlations [8], novel FQH states would result. However, until now such correlations have not been established in any realistic FQH system. Since only for $N = 6$, 10, and 14 (but not for $N = 8$ or 12) do the $L = 0$ ground states occur for QE's, this picture seems inadequate in CF-LL_1 [15]. However, for half-filled LL_1, large values of $\mathcal{G}_2(1)$ and, *at the same time*, the vanishing of $\mathcal{G}_3(3)$ supports this idea in the Moore–Read state. By effectively acting like a short-range three-body repulsion W, Coulomb repulsion in LL_1 allows grouping electrons into pairs, but yields Laughlin correlations among them. This can be modeled by a fictitious flux attachment in a standard way.

The CF model describing Laughlin-correlated pairs with $\mathcal{R}_2 = 1$ and $L_2 = 2l-1$ works in the following way: 7 flux quanta (4 to account for the Pauli principle, 4 to model correlations among the pairs, and -1 to convert bosons to fermions) are attached to each of the $N_2 = \frac{1}{2}N$ pairs, giving an effective angular momentum $l_0^* = (2l-1) - \frac{7}{2}(N_2 - 1)$ of the lowest CF-pair shell (CFP-LL_0). For $2l = (2N-3) \pm \Delta$, its degeneracy is $g_0^* \equiv 2l_0^* + 1 = N_2 \pm 2\Delta$. When $\Delta = 0$, the CFP's completely fill CFP-LL_0 giving an $L = 0$ ground state. The magnetoroton band describes a QH–QE excitation between the CFP-LL_0 and CFP-LL_1 shells. The quasihole (QH) and QE angular momenta are $l_0^* = \frac{1}{2}(N_2 - 1)$ and $l_1^* = l_0^* + 1$, respectively, giving a QE–QH band with $1 \leq L \leq N_2$. The lower-L states of this band merge with the continuum, but those at larger L are clearly visible in Fig. 4a.

In Fig. 5 we present the spectra obtained for even values of N and $2l = (2N - 3) \pm 1$. At $2l = (2N - 3) + 1$, there is always a band of $E = 0$ states at $L = N_2,\ N_2 - 2,\ \ldots$ [13], corresponding to two QH's in CFP-LL_0 of degeneracy $g_0^* = N_2 + 2$. The first excited band above the two-QH states contains an additional QE–QH pair. At $2l = (2N - 3) - 1$ no states can have $E = 0$, but the lowest band contains two QE's in CFP-LL_1 of degeneracy $g_1^* = N_2$. Indeed, in spectrum (b),

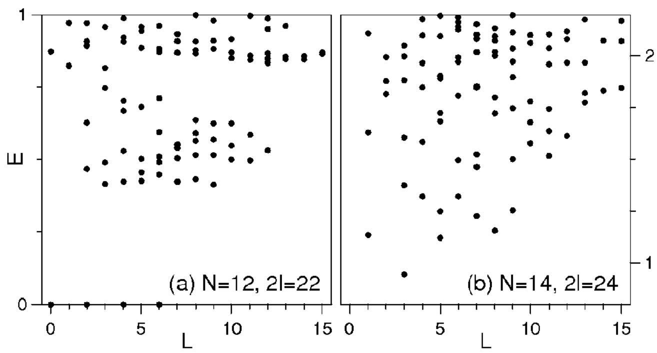

Fig. 5. The same as Fig. 4a but for (a) $2l = 2N - 2$ and (b) $2l = 2N - 4$, corresponding to two QH's and two QE's in the Moore–Read state, respectively.

the low-energy band at $L = N_2 - 2,\ N_2 - 4, \ldots$ can be found.

The CFP model cannot describe pair-breaking excitations, generally expected to be neutral fermions. They can be identified in the spectra for odd N and $2l = 2N - 3$ [11], as shown in Fig. 6a. For any odd value of N, the lowest band occurs at $L = \frac{5}{2},\ \frac{7}{2}, \ldots,\ \frac{1}{2}N$, that seems to describe dispersion of an excitonic state of two QP's of opposite charge. This becomes more convincing in Fig. 6b, where the data obtained for different N is plotted together as a function of wavevector k, and a clear magnetoroton-type minimum appears at $k \approx 1.0\ \lambda^{-1}$.

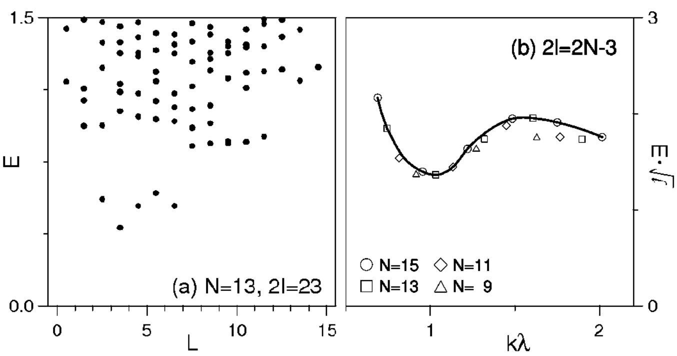

Fig. 6. (a) The same as Fig. 4a but for an odd number of particles $N = 13$ and $2l = 2N - 3 = 23$. (b) Energy dispersion $E(k)$ for the pair-breaking band. λ is the magnetic length.

3.4. Finite-size effects

Earlier studies using Coulomb pseudopotential in LL_1 [11, 14, 17] showed $L = 0$ ground states with a gap at $2l = 2N - 3$ but there were no clear indications of the QP or pair-breaking excitations identified in the spectra of W [12, 13]. A major problem with the calculations on a sphere is the size-dependence of the critical value α_0 at which $\mathcal{R}_3 = 3$ is avoided. It is clear from the analysis of squared overlaps $\zeta_u(\alpha) = |\langle\phi_\alpha|\psi_u\rangle|^2$ of the eigenstates ϕ_α of U_α with the eigenstates ψ_u of various other interactions u: three-body repulsion W and electron and QE pair pseudopotentials V_2 in LL_0, LL_1, and CF-LL_1. The exact Moore–Read eigenstate of W turns out to be an excellent ground state of U_α at $\alpha \approx 0.425$. So is the ground state of Coulomb pair interaction in LL_1, but at a different $\alpha \approx 0.5$. The disagreement between these two values of α does not disappear in wide samples (e.g., $|\langle\psi_W|\psi_{LL1}\rangle|^2 = 0.48$, 0.58, and 0.71 for $w/\lambda = 0$, 1.75, and 3.5, respectively). This raises the question of whether the Moore–Read trial state and its QP excitations actually occur in the FQH $\nu = \frac{5}{2}$ state. Fortunately, the disagreement appears to be largely artificial. The size-dependence of α_0 can be traced to that of the pair amplitudes $\mathcal{G}_2(\mathcal{R}_2)$ of the triplet eigenstates at $\mathcal{R}_3 = 3$, 5, 6,..., directly caused by the surface curvature. This curvature causes α_0 to be smaller than the value $\frac{1}{2}$ appropriate for the Coulomb pseudopotential in LL_1. As $N \to \infty$, we expect $\alpha_0 \to \frac{1}{2}$ in agreement with the behavior of $V_2(\mathcal{R}_2)$ in the same limit. Then the energy spectra of $V_2(\mathcal{R}_2)$ in LL_1 and of $W(\mathcal{R}_3)$ should become similar. We surmise that: (i) Finite-size calculations on a sphere using Coulomb pair interaction do not correctly reproduce correlations of an infinite $\nu = \frac{5}{2}$ state. They use pseudopotentials corresponding to $\alpha \approx \frac{1}{2}$, different from $\alpha_0 < \frac{1}{2}$ leading to the avoidance of $\mathcal{R}_3 = 3$. The $\alpha = \alpha_0 = \frac{1}{2}$ coincidence is probably recovered for $N \to \infty$ which would mean that the real, infinite systems at $\nu = \frac{5}{2}$ do have the "$\mathcal{R}_3 > 3$" correlations while the correlations in finite systems are different and size-dependent. (ii) In finite systems, correct "$\mathcal{R}_3 > 3$" correlations are recovered if the pair pseudopotential is appropriately enhanced at short range. (iii) Assuming that the $\alpha = \alpha_0 = \frac{1}{2}$ coincidence is restored in infinite systems, the equivalence of Coulomb and W interactions at half-filling is not limited strictly to the Moore–Read ground state. The $(\pm e/4)$-charged QP's and the pair-breaker identified in the spectra of W accurately describe the low-energy excitations in the real $\nu = \frac{5}{2}$ systems.

4. Conclusion

We have studied two- and three-body correlations in partially filled degenerate shells for various interactions between the particles. Variation of the relative strength of two leading pair pseudopotentials drives the correlations through three regimes. The intermediate regime, corresponding to the nearly harmonic pseudopotential at short range, describes correlations among electrons in LL_1, particularly in the $\nu = \frac{5}{2}$ FQH state.

In contrast to the correlations between electrons in LL_0 or between Laughlin QE's in CF-LL_1 (whose pseudopotentials are strongly super- and subharmonic at short range, respectively), the intermediate regime is not characterized by a simple avoidance of just one pair eigenstate corresponding to the strongest anharmonic repulsion. Instead, we have shown that near half-filling the low-energy states for such interactions have simple three-body correlations. They consist of the maximum avoidance of the triplet state with the smallest relative angular momentum $\mathcal{R}_3 = 3$. In particular, at exactly half-filling, this corresponds to the fact [11] that the Moore–Read ground state is the $E = 0$ eigenstate of a model short-range three-body repulsion W with the only pseudopotential parameter at $\mathcal{R}_3 = 3$. The Moore–Read ground state is a three-body analog of the Laughlin $\nu = \frac{1}{3}$ state with $\mathcal{R}_2 > 1$. It is separated by a finite excitation gap from a magnetoroton band with a minimum at $k \approx 1.5\lambda^{-1}$. Its elementary excitations are the $(\pm e/4)$-charged QP's and the pair-breaker. The bands of few-QP states near half-filling are well described by a CF picture appropriate for Laughlin pair–pair correlations.

Finally, the problem of numerical calculations on a sphere associated with the surface curvature is addressed. It is found that finite-size models using Coulomb interaction between electrons do not correctly reproduce correlations of the $\nu = \frac{5}{2}$ FQH state due to the distortion of triplet wavefunctions. Overlaps with the Moore–Read-like correlated states are small. However, it is argued that the $\nu = \frac{5}{2}$ FQH state observed experimentally is described much better by the Moore–Read trial state than could be expected from the calculation of overlaps in small systems. Consequently, the origin of its incompressibility is precisely the avoidance of the $\mathcal{R}_3 = 3$ triplet state, and its elementary excitations are the $(\pm e/4)$-charged QP's and the pair-breaker.

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