Landau level mixing in the $\nu = 5/2$ fractional quantum Hall state

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The $\nu = 5/2$ fractional quantum Hall state is studied numerically, directly including the effects of electron scattering between neighboring Landau levels. Significant reduction of the excitation gap caused by the LL mixing explains the discrepancy between earlier calculations and experiments. On the other hand, LL mixing also considerably reduces overlaps with the Moore–Read wavefunction, raising a question of the actual realization of nonabelian quasiparticles in present experiments.

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I. INTRODUCTION

Discovery of the fractional quantum Hall (FQH) effect in a half-filled first excited Landau level (LL)1,2 demonstrated the possibility for incompressible quantum liquid (IQL) states outside of the “standard” hierarchy described below. Laughlin states3 occur at the fractional LL fillings $\nu \equiv 2\pi \rho \lambda^2 = (2p+1)^{-1}$ (where $\rho$ is electron concentration, $\lambda$ is the magnetic length, and $p$ is an integer). The simple form of Laughlin many-body wavefunctions suggested that their low energy could be understood in terms of the avoidance of pair states with the smallest relative pair angular momentum (and largest repulsion).4 The quasiparticles (QPs) of the Laughlin states can (un-)form “daughter” IQL states with their own QPs, giving rise to an entire IQL hierarchy.5

The most stable IQL states, occurring at $\nu = s(2p_s \pm 1)^{-1}$ ($s$ being another integer), appear naturally in Jain’s composite fermion (CF) model6 involving the concepts of flux attachment and an effective magnetic field. All Laughlin and Jain states are characterized by odd-denominator filling fractions $\nu$ and fractional QP charge $q = e(2p_s \pm 1)^{-1}$. For the even-denominator IQL state observed at $\nu = \frac{5}{2}$, Moore and Read (MR) proposed1 a different, paired wavefunction, and predicted that its QPs obeyed nonabelian statistics. The MR state has been studied in great detail and interpreted by two complementary pictures: as a Laughlin state of tightly bound electron pairs10,11 or a superfluid of weakly bound CF pairs12,13.

The first numerical calculations for interacting electrons in a partially filled LL were carried out by Morf.14 They seemed to confirm that a half-filled LL has a spin-polarized incompressible ground state accurately described by the MR wavefunction. However, the subsequent experiments15,16,17,18 revealed minute excitation gaps $\Delta \sim 0.1 - 0.45$ K in the real $\nu = \frac{5}{2}$ states, up to $20\times$ smaller than predicted from numerics. The fact that only a small part of this discrepancy could be attributed to the finite width of the quasi-2D electron layer or to the weak disorder posed a challenge for the theoretical models. It also raised a fundamental question of whether the actual, experimentally realized $\nu = \frac{5}{2}$ states are indeed adequately described by the MR wavefunction. It has become very important in the context of topological quantum computation, whose recent proposals19,20,21 take advantage of the nonabelian QP statistics. This fundamental question is the main subject of our present paper.

We directly include LL mixing in exact diagonalization by adding states containing a single cyclotron excitation to the Hilbert space of a partially filled spin-polarized LL. This can be regarded as a first-order approximation in the Coulomb-to-cyclotron energy ratio $\beta$. We apply this procedure to the $\nu = \frac{1}{2}, \frac{2}{5}$, and $\frac{3}{5}$ states and evaluate the excitation energy gaps $\Delta$ and (in the last case) the overlap $\rho$ with the MR wavefunction. At $\beta \sim 1$ (relevant for the experiments at $\nu = \frac{5}{2}$), where our first-order results are only qualitative, we find a strong reduction in both $\Delta$ and $\rho$. Unfortunately, the calculations including excitations to higher order in $\beta$ are beyond our capabilities. Our conclusion concerning the gap reduction gives qualitative support to the work of Morf and d’Ambrumenil,22 who however included LL mixing in a different way, using a screened interaction that is strictly valid only for $\nu \gg 1$. Furthermore, our prediction of strong deviation from the MR wavefunction supports the recent proposals23 for new experiments aimed at determining directly the QP statistics at $\nu = \frac{5}{2}$ (rather than merely at determining the incompressibility).

II. MODEL

We use Haldane’s spherical geometry,24 convenient for the exact study of liquid states with short-range correlations. On a sphere of radius $R$, the normal magnetic field $B$ is produced by a Dirac monopole of strength $2Q = 4\pi R^2 B/\phi_0$, defined here in the units of flux quantum $\phi_0 = \hbar c/e$. Using a magnetic length $\lambda = \sqrt{\hbar c/eB}$, this can be rewritten as $Q\lambda^2 = R^2$. The series of LLs labeled by $n = 0, 1, 2, \ldots$ are represented by shells of angular momentum $l = Q + n$ and degeneracy $g = 2l + 1$. The cyclotron energy is $\hbar \omega_c = \hbar c B/\mu c$ (counted from the lowest LL), where $\mu$ is the effective mass. The orbitals $\psi_{nm}(\theta, \phi)$ are called monopole harmonics.

The $\mathcal{N}$-electron Hamiltonian matrix is calculated in the configuration-interaction basis $|i_1, \ldots, i_N\rangle$. Here, the composite indices $i = [n, m, \sigma]$ also include spin, and the
FIG. 1: (color online) (a) Energy spectrum (energy $E$ as a function of angular momentum $L$) of $N = 12$ electrons in a LL shell of angular momentum $l = 25/2$, corresponding to an isolated, half-filled first excited LL. (b) Excitation gap $\Delta$ extracted from the spectra similar to (a), plotted as a function of the electron number $N$; $w$ is the width of the 2D electron layer and $\lambda$ is the magnetic length.

expressions for two-body Coulomb matrix elements (also in layers of finite widths $w$) can be found for example in Ref. 27. At a given LL filling (defined by $N$ and $g$, the basis states can be classified by $\Delta E = \hbar \omega_c \sum_{\lambda} n_k - \varepsilon_{\text{min}}$, i.e., the total cyclotron energy measured from the lowest possible value $\varepsilon_{\text{min}}$ allowed by the Pauli exclusion principle (e.g., $\varepsilon_{\text{min}} = 0$ at $\nu \leq 2$, or $\varepsilon_{\text{min}} = (N - 2g) \hbar \omega_c$ at $2 < \nu \leq 4$). Alternatively, the total number of cyclotron excitations $K = \Delta E / (\hbar \omega_c)$ can be defined.

The exact numerical diagonalization in the Hilbert space restricted to $N = 0$ means including Coulomb scattering within only one, partially filled LL, and neglecting the LL mixing. For $\nu = \frac{5}{2}$ this reduces the $N$-particle problem to $N = N - 2g$ electrons confined to an isolated LL$_1$. A typical numerical spectrum is shown in Fig. 1(a). The non-degenerate ground states with a gap generally appear in finite-size systems with even values of $N$ (they are known to be paired$^{14}$ at $2l = 2N + 1$ or (equivalent via the $N \rightarrow g - N$ particle-hole conjugation) at $2l = 2N - 3$, both extrapolating to $N/g \rightarrow \frac{1}{2}$ for large $N$. As shown in Fig. 1(b), the excitation gap $\Delta$ rather weakly depends on $N$, allowing one to estimate the value $\Delta \approx 0.02 e^2/\lambda$ for an infinite (planar) system.$^{13,14}$

Unfortunately, this value is not confirmed by the experiments. The gaps measured from the thermal activation of longitudinal conductance range from 0.001 to 0.004 $e^2/\lambda$, depending on the electron mobility$^{15,16,17,18}$ with extrapolation to a disorder-free system not exceeding $\sim 0.006 e^2/\lambda$. As shown in Fig. 1(b) for $w = \lambda$ (i.e., $w = 11.4$ nm at $B = 5$ T), this discrepancy cannot be explained by a finite width of the electron layer.

An obvious advantage of the $K = 0$ approximation is that calculations can be done for sufficiently large values of $N$ to eliminate finite-size errors. It could be trivially justified by a small ratio of Coulomb and cyclotron energies, $\beta = (e^2 \lambda^{-1}) / (\hbar \omega_c) = \lambda / a_B$ (with the Bohr radius $a_B = \hbar^2 / \mu e^2$). However, $\beta > 1$ at the fields $B \sim 5$ T typically used in FQH experiments at $\nu = \frac{5}{2}$.

To include LL mixing, we expand the Hilbert space by adding the $K = 1$ states, i.e., allow excitation of up to one electron to a higher LL. This can be regarded as a kind of first-order perturbation scheme in $\beta$. However, note that such coupling of the entire $K = 0$ and $K = 1$ subspaces is more than a first-order perturbation on the specific $K = 0$ eigenstates. The basis is shown schematically in Fig. 2(a) and (b). At $\nu = \frac{5}{2}$, the underlying, filled lowest LL gives rise to more types of excitations than at $\nu < 1$. Generally, the inter-LL excitations can be decomposed into addition of an electron or a hole to a specific LL in the presence of a correlated state of the initial $N$ electrons. There are two distinct cases, depending on the target LL: (i) Addition to (or removal from) the LL occupied by the incompressible liquid. This causes creation of several fractionally charged QPs. At $\nu = \frac{1}{2}$ or $\frac{5}{2}$, they are well known Laughlin/Jain QPs, with a simple and intuitive picture in the CF model. However, the nature and dynamics of the QPs at $\nu = \frac{5}{2}$ are not nearly as well understood. (ii) Addition to (or removal from) a different LL. This makes the added/removed electron distinguishable from the correlated electrons. This problem resembles coupling of a Laughlin liquid to a (positive) valence hole$^{22}$ or a (negative) trion.$^{22}$ However, coupling of the $\nu = \frac{5}{2}$ state to a foreign charge is far less understood.

Since all three types of $K = 1$ excitations must be included in the calculation on the same footing, even this limited account of LL mixing boosts the space dimension from $\sim 10^3$ to $\sim 4 \times 10^5$ for $N = 8$ at $2l = 17$. This precludes similar calculations for larger systems or further inclusion of the $K > 1$ excitations. On one hand, this makes the present results somewhat susceptible to finite-size errors (although Fig. 1(b) may suggest that $N = 8$, i.e., four pairs, is already a representative system) and
accurate only up to the first-order perturbation in β. On the other hand, a much larger number of $K = 1$ excitations at $\nu > 2$ than at $\nu < 1$ suggests that the effects of LL mixing should be more important at $\nu = \frac{5}{2}$ than in Laughlin or Jain liquids of the lowest LL.

### III. RESULTS AND DISCUSSION

We focus on two features of the $\nu = \frac{5}{2}$ state: the excitation gap and the overlap with the MR wavefunction. The results of calculations of the gap $\Delta$ for $N = 8$ and $K \leq 1$ in a 2D layer of zero width are shown in Fig. 2(c).

As argued above and anticipated from experiments, the gap reduction $\Delta/\Delta_0$ (where $\Delta_0$ is the result for $K = 0$) is noticeably greater at $\nu = \frac{5}{2}$ than at both $\nu = \frac{3}{2}$ or $\frac{5}{2}$. On the other hand, the fact that the gap at $\nu = \frac{1}{2}$ is reduced more than at $\nu = \frac{2}{2}$ can be related to the smaller QP charge in the latter case ($q = e/5$ versus $e/3$).

Since the low-energy response of a liquid involves formation and interaction of the QPs, the harsh β ≪ 1 criterion for the accuracy of the isolated-LL approximation may be relaxed to $\beta^* \ll 1$. Here, $\beta^* = (q^2 \lambda^{-1}/(\hbar \omega_c) = (q/e)^{3/2}/\beta$ involves the Coulomb energy scale of the QPs. Indeed, when the gaps in the weak-perturbation regime are plotted as a function of $\beta^*$ as in Fig. 2(d), the data for $\nu = \frac{5}{2}$ and $\frac{5}{2}$ falls close to the same line, $1 - \Delta/\Delta_0 \approx 3\beta^*$. Taking $q = e/4$ for the $\nu = \frac{5}{2}$ state results in a much (about $3\times$) steeper curve. This indicates that the response of the $\nu = \frac{5}{2}$ state to the perturbation associated with the LL mixing at a finite $\beta$ is (due to a richer inter-LL excitation spectrum) relatively stronger than the response of Laughlin or Jain states in the lowest LL.

Furthermore, if the experiments on all three electron liquids were to be carried out at similar concentrations (corresponding to a maximum mobility), the difference between them will be additionally magnified by a difference in $\beta$ corresponding to different $\nu$. For example, for $g = 2.3 \times 10^{11}$ cm$^{-2}$ we obtained gap reduction of 8.5%, 2.5%, and 35% at $\nu = \frac{1}{2}$, $\frac{3}{2}$, and $\frac{5}{2}$, respectively.

In the above discussion we have established the following. (i) Realistic estimates of the excitation gap at $\nu = \frac{5}{2}$ must include the LL mixing, whose effect at this filling is much stronger than for Laughlin or Jain states in the lowest LL. (ii) The gap reduction caused by LL mixing is already significant in the $K \leq 1$ approximation. (iii) It is plausible that the full account of the LL mixing might reconcile experimental results in the limit of vanishing disorder with the numerics. Unfortunately, calculations for $K > 1$ and $N \geq 8$ are beyond our present capabilities.

The dependence of gap $\Delta$ on the magnetic field $B$ and finite layer width $w$ are displayed in Fig. 3. Finite width was introduced to the model by the calculation of two-body Coulomb matrix elements using 3D wavefunctions $\chi(z)\psi_{nm}(\theta, \phi)$ with $\chi(z) \propto \cos(\pi z/w)$ for the normal direction. Remarkably, $\Delta(w)$ is nonmonotonic, with a maximum between $w = 5$ and 10 nm, depending on $B$. While the reduced gaps are still about twice larger than the experimental values, the inclusion of even only $K = 1$ excitations clearly improves the model. This suggests LL mixing as the main reason for the earlier $\Delta$ discrepancy.

Let us now turn to the question of equivalence of the $\nu = \frac{5}{2}$ state realized in experiment and the model MR wavefunction. There is a subtle difference between the half-filled state and odd-denominator liquids like $\nu = \frac{1}{2}$ or $\frac{5}{2}$. In the latter states, it is not merely incompressibility but also the form of correlations and many-body wavefunction that are robust against the variation of material, $w$, or $B$ — as long as the interaction pseudopotential is sufficiently strong (superharmonic) at short range, weak compared to the cyclotron energy, and strong compared to disorder. In contrast, the half-filled state remains incompressible for a wide class of electron–electron pseudopotentials, but the exact form of the wavefunction strongly depends on their details. This limits information that can be inferred about the nature of the state from the observation of its incompressibility.

The underlying reason is the competition of at least two distinct wavefunctions sharing the same symmetry: the MR state, which can be defined as an exact ground state of a short-range three-body repulsion, and a clustered state characterized by the maximum avoidance of the next to the lowest value of the relative pair angular momentum, $R = 3$. The MR state is anticipated for the pair repulsion which is nearly harmonic at short range (i.e., with the pseudopotential decreasing linearly through $R = 1$, 3, and 5), such as in the LL$_1$. However, the overlaps of the actual Coulomb eigenstates obtained from finite-size numerics (in the $K = 0$ approximation) with the MR state are sensitive to the interaction parameter and surface curvature, raising the question of whether the $\nu = \frac{1}{2}$ FQH state and the MR model state are indeed (qualitatively) equivalent.

How does LL mixing affect this problem? In the top frames of Fig. 3 we plot the squared projection $|P_{K=0}\Psi|^2$ onto the LL$_1$ (i.e., onto the $K = 0$ subspace) of the same ground states $\Psi$ whose gaps are shown in Fig. 3. It depends on $w$ and $B$, but it is always significantly higher than $\Delta/\Delta_0$ or the (not shown) squared overlap with the
FIG. 4: (color online) Dependence of the squared projection onto the LL[1] (top) and the squared overlap with the Moore–Read wavefunction (bottom) of the $\nu = \frac{5}{2}$ ground states calculated for $N = 8$ with and without LL mixing, on the 2D layer width $w$ (left) and the magnetic field $B$ (right).

$K = 0$ ground state, in consequence of the coupling between intra- and inter-LL excitations in the $K \leq 1$ space. In the bottom frames we plot the squared overlap $\xi^2 = |\langle MR | \Psi \rangle|^2$ with the MR state (more precisely, with its particle–hole conjugate at $2l = 2N+1$). The small values for the $K = 0$ calculation (here, 0.75 to 0.80) may be to some extent an artifact of spherical geometry.\(^\text{11}\) However, a significant drop caused by the LL mixing (e.g., from 0.78 to 0.43 for $w = 20$ nm and $B = 5$ T) suggests that the MR wavefunction may not be a very realistic description of the $\nu = \frac{5}{2}$ state in this range of parameters. This ambiguity and the difficulty with more realistic calculations make further experiments\(^\text{24}\) irreplaceable.

### IV. CONCLUSION

We studied the effect of LL mixing on the $\nu = \frac{5}{2}$ FQH state. This effect is more pronounced than in the incompressible liquids of the lowest LL such as $\nu = \frac{1}{3}$ or $\frac{5}{2}$ (even at the same magnetic field) due to the richer inter-LL excitation spectrum. The resulting reduction of the excitation gap explains the troubling disparity between previous numerics (without LL mixing) and the experiments. This prediction agrees qualitatively with Ref.\(^\text{22}\) which included LL mixing in a different way. Finally, the LL mixing significantly lowers overlaps with the MR wavefunction. This amplifies the need for the recently proposed\(^\text{23}\) experiments, designed to probe directly the nonabelian statistics of the QPs at $\nu = \frac{5}{2}$.

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1. R. Willett, J. P. Eisenstein, H. L. Störmer, D. C. Tsui, A. C. Gossard, and J. H. English, Phys. Rev. Lett. 59, 1776 (1987).
2. R. B. Laughlin, Phys. Rev. Lett. 50, 1395 (1983).
3. F. D. M. Haldane, Phys. Rev. Lett. 51, 605 (1983).
4. F. D. M. Haldane, in The Quantum Hall Effect, edited by R. E. Prange and S. M. Girvin (New York: Springer-Verlag, 1987), Chap. 8, pp. 303–352.
5. A. Wójcik and J. J. Quinn, Phys. Rev. B 61, 2846 (2000).
6. J. J. Jain, Phys. Rev. Lett. 63, 199 (1989); Science 266, 1199 (1994); Phys. Today 53, No. 4, 39 (2000).
7. G. Moore and N. Read, Nucl. Phys. B 360, 362 (1991).
8. X.-G. Wen, Phys. Rev. Lett. 70, 355 (1993); C. Nayak and F. Wilczek, Nucl. Phys. B 479, 529 (1996); N. Read and E. Rezayi, Phys. Rev. B 54, 16864 (1996); E. Rezayi and F. D. M. Haldane, Phys. Rev. Lett. 84, 4685 (2000).
9. N. Read and D. Green, Phys. Rev. B 61, 10267 (2000).
10. M. Greiter, X.-G. Wen, and F. Wilczek, Phys. Rev. Lett. 66, 3205 (1991); Nucl. Phys. B 374, 567 (1992).
11. W. A. Wójcik and J. J. Quinn, Phys. Rev. B 71, 045324 (2005).
12. V. W. Scardola, K. Park, and J. K. Jain, Nature (London) 406, 863 (2000); K. C. Foster, N. E. Bonesteel, and S. H. Simon, Phys. Rev. Lett. 91, 168004 (2003).
13. C. Tóke and J. K. Jain, Phys. Rev. Lett. 96, 246805 (2006).
14. E. H. Rezayi, Phys. Rev. Lett. 80, 1505 (1998); R. H. Morf, N. d’Ambrumenil, and S. Das Sarma, Phys. Rev. B 66, 075408 (2002).
15. W. Pan, J.-S. Xia, V. Shvarts, D. E. Adams, H. L. Störmer, D. C. Tsui, L. N. Pfeiffer, K. W. Baldwin, and K. W. West, Phys. Rev. Lett. 83, 3530 (1999).
16. W. Pan, H. L. Störmer, D. C. Tsui, L. N. Pfeiffer, K. W. Baldwin, and K. W. West, Solid State Commun. 119, 641 (2001); Phys. Rev. Lett. 90, 016801 (2003).
17. J. P. Eisenstein, K. B. Cooper, L. N. Pfeiffer, and K. W. West, Phys. Rev. Lett. 88, 076801 (2002).
18. J. S. Xia, W. Pan, C. L. Vincente, E. D. Adams, N. S. Sullivan, H. L. Störmer, D. C. Tsui, L. N. Pfeiffer, K. W. Baldwin, and K. W. West, Phys. Rev. Lett. 93, 176809 (2004); J. Low Temp. Phys. 134, 579 (2004).
19. A. Yu. Kitaev, Annals Phys. 303, 2 (2003).
20. S. Das Sarma, M. Freedman, and C. Nayak, Phys. Rev. Lett. 94, 166802 (2005); Phys. Today 59, No. 7, 32 (2006).
21. N. E. Bonesteel, L. Hormozi, G. Zikos, and S. H. Simon, Phys. Rev. Lett. 95, 140503 (2005).
22. R. Morf and N. d’Ambrumenil, Phys. Rev. B 68, 113309 (2003).
23. I. L. Aleiner and L. I. Glazman, Phys. Rev. B 52, 11296 (1995).
24. A. Stern and B. I. Halperin, Phys. Rev. Lett. 96, 016802 (2006); P. Bonderson, A. Kitaev, and K. Shtengel, ibid. 96, 016803 (2006); E. Grosfeld, S. H. Simon, and A. Stern, ibid. 96, 226803 (2006).
25. A. Wójcik and J. J. Quinn, cond-mat/0609103.
26. X. M. Chen and J. J. Quinn, Phys. Rev. Lett. 70, 2130 (1993); E. I. Rashba and M. E. Portnoi, ibid. 70, 3315 (1993).
27. A. Wójcik, A. Gladysiewicz, and J. J. Quinn, Phys. Rev. B 73, 235338 (2006).
28 A. Wójc, D. Wodzinski, and J. J. Quinn, Phys. Rev. B 74, 035315 (2006).