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

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The effect of Landau level (LL) mixing on the $\nu=5/2$ fractional quantum Hall state is studied directly in a minimal, yet still numerically tractable, approximation. Specifically, the inter-LL excitations with one unit of cyclotron energy are included in the exact diagonalization of a small yet representative number of electrons on a sphere. Significant reduction of the excitation gap found already in this simple model indicates that LL mixing must play an important role in more realistic systems, with a full spectrum of allowed inter-LL excitations. This suggests a possible route to the explanation of the troubling discrepancy between earlier calculations and experiments. On the other hand, even within our limited approach the LL mixing is found to considerably reduce overlaps with the Moore-Read wave function, raising the question of the actual realization of non-Abelian quasiparticles (QPs) at $\nu=5/2$. In view of the discussed limitations of exact numerics, conclusive resolution of this question will probably require an experiment directly probing the QP statistics.

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I. INTRODUCTION

Discovery[1] of the fractional quantum Hall (FQH) effect in a half-filled first excited Landau level (LL_1) demonstrated the possibility for incompressible quantum liquid (IQL) states outside of the "standard" hierarchy[2,3] described below. Laughlin states[2] occur at the fractional LL fillings $\nu \equiv 2\pi\varrho\lambda^2=(2p+1)^{-1}$ (where ϱ is the electron concentration, λ is the magnetic length, and p is an integer). The simple form of Laughlin many-body wave functions 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 (under some conditions[5]) form "daughter" IQL states with their own QPs, giving rise to an entire IQL hierarchy.[3] The most stable IQL states, occurring at $\nu=s(2ps\pm1)^{-1}$ (s being another integer), appear naturally in Jain's composite fermion (CF) model[6] involving the concepts of flux attachment and an effective magnetic field. All Laughlin and Jain states are characterized by odd-denominator filling fractions ν and fractional QP charge $q=e(2ps\pm1)^{-1}$.

For the even-denominator IQL state observed at $\nu=\frac{5}{2}$, Moore and Read (MR) proposed[7] a different, paired wave function, and predicted that its QPs obeyed non-Abelian statistics. The MR state has been studied in great detail[8–11] and interpreted by two complementary[12] pictures: as a Laughlin state of tightly bound electron pairs[13,14] or a superfluid of weakly bound CF pairs.[15–17]

The first numerical calculations for interacting electrons in a partially filled LL_1 were carried out by Morf.[18] They seemed to confirm that a half-filled LL_1 has a spin-polarized incompressible ground state accurately described by the MR wave function. However, subsequent experiments[19–22] revealed minute excitation gaps $\Delta\sim0.1-0.45$ 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-two-dimensional (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 wave function. It has become very important in the context of topological quantum computation, whose recent proposals[23–26] take advantage of the non-Abelian 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 is a minimum-level approach. With the single-electron states labeled by the LL index n and the angular momentum m, it includes the scattering processes $(n,m;n',m')\leftrightarrow(n+1,m+\delta m;n',m'-\delta m)$ with an arbitrary δm. These terms are expected to be most important at sufficiently small Coulomb-to-cyclotron energy ratios β. However, such approximation is notably weaker than the first-order perturbation scheme in β, by neglecting similar terms with higher combinations of LLs. The neglected terms have smaller β (by having both smaller Coulomb matrix elements and a higher cyclotron energy difference), but are also of the first order. Therefore, our limited approximation can only give a qualitative account of the LL mixing. However, a strong effect obtained in this model predicts quite conclusively a strong effect in a corresponding real system.

We apply the above procedure to the $\nu=\frac{1}{3}$, $\frac{2}{5}$, and $\frac{5}{2}$ states and evaluate the excitation energy gaps Δ and (in the last case) the overlap ξ with the MR wave function. At $\beta\sim1$ (relevant for the experiments at $\nu=\frac{5}{2}$), we find a strong reduction in both Δ and ξ. Unfortunately, the calculations including excitations to higher LLs are beyond our capabilities. Our conclusion concerning the gap reduction gives qualitative support to the work of Morf and d'Ambrumenil,[27] who however included LL mixing in a different way,[28] using a screened interaction that is strictly valid only for $\nu\gg1$. Furthermore, our prediction of strong deviation from the MR wave function supports the recent proposals[29–31] for new

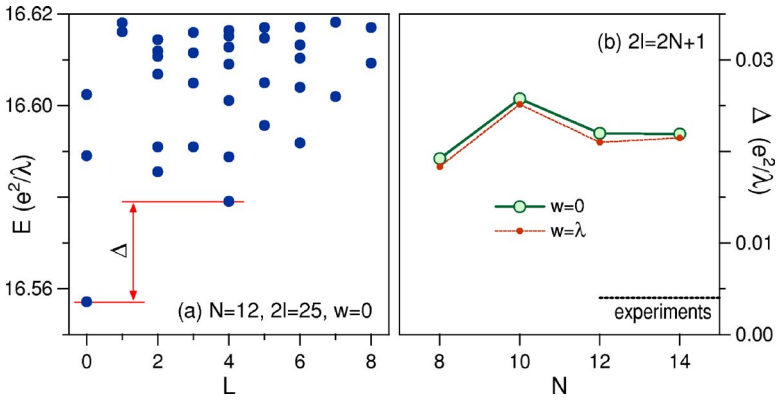

FIG. 1. (Color online) (a) Energy spectrum (energy E as a function of angular momentum L) of $N=12$ electrons in a LL shell of angular momentum $l=25/2$, corresponding to an isolated, half-filled first excited LL. (b) Excitation gap Δ extracted from spectra similar to (a), plotted as a function of the electron number N; w is the width of the 2D electron layer and λ is the magnetic length.

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,[3] 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 $2Q=4\pi R^2B/\phi_0$, defined here in units of the flux quantum $\phi_0=hc/e$. 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 $n\hbar\omega_c=n\hbar eB/\mu c$ (counted from the lowest LL), where μ 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 $|i_1,\ldots,i_{\mathcal{N}}\rangle$. Here, the composite indices $i=[n,m,\sigma]$ also include spin, and the expressions for two-body Coulomb matrix elements (also in layers of finite widths w) can be found for example in Ref. 32. At a given LL filling (defined by $\mathcal{N}$ and g), the basis states can be classified by $\Delta\mathcal{E}=\hbar\omega_c\Sigma_k n_k-\mathcal{E}_{\min}$, i.e., the total cyclotron energy measured from the lowest possible value $\mathcal{E}_{\min}$ allowed by the Pauli exclusion principle [e.g., $\mathcal{E}_{\min}=0$ at $\nu\leqslant 2$, or $\mathcal{E}_{\min}=(\mathcal{N}-2g)\hbar\omega_c$ at $2<\nu\leqslant 4$]. Alternatively, the total number of cyclotron excitations $K=\Delta\mathcal{E}/(\hbar\omega_c)$ can be defined.

The exact numerical diagonalization in the Hilbert space restricted to $K=0$ means including Coulomb scattering within only one, partially filled LL, and neglecting the LL mixing. For $\nu=\frac{5}{2}$ this reduces the $\mathcal{N}$-particle problem to $N=\mathcal{N}-2g$ electrons confined to an isolated LL_1. A typical numerical spectrum is shown in Fig. 1(a). The nondegenerate ground states with a gap generally appear in finite-size systems with even values of N (they are known to be paired[7]) at $2l=2N+1$ or (equivalent via the $N\to g-N$ particle-hole conjugation) at $2l=2N-3$, both extrapolating to $N/g\to\frac{1}{2}$ for large N. As shown in Fig. 1(b), the excitation gap Δ rather weakly depends on N, allowing one to estimate the value $\Delta\approx 0.02e^2/\lambda$ for an infinite (planar) system.[17,18]

Unfortunately, this value is not confirmed by the experiments. The gaps measured from the thermal activation of longitudinal conductance range from $0.001e^2/\lambda$ to $0.004e^2/\lambda$, depending on the electron mobility,[19–22] with extrapolation to a disorder-free system not exceeding $\sim 0.006e^2/\lambda$. 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 the 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 $\mathcal{N}$ 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., we allow excitation of up to one electron to a higher LL. The basis is shown schematically in Figs. 2(a) and 2(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

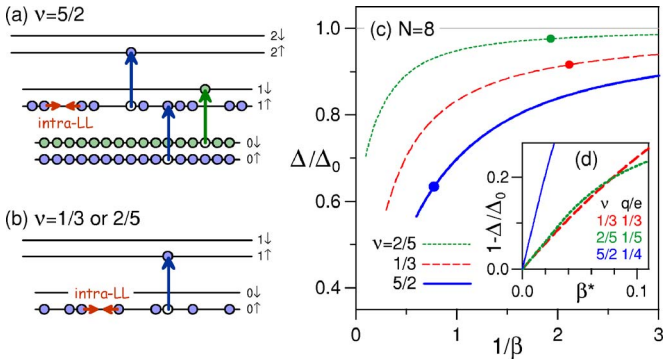

FIG. 2. (Color online) (a), (b) Comparison of inter-LL excitations with up to one unit of cyclotron energy in the $\nu=5/2$ state and in Laughlin or Jain liquids at $\nu<1$. (c) Reduction of the excitation gap of different quantum Hall states due to LL mixing, plotted as a function of the cyclotron-to-Coulomb energy ratio β^{-1}. Δ and Δ_0 are gaps calculated for $N=8$ and $2l=16$, 21, and 17 (for $\nu=2/5$, 1/3, and 5/2). The full dots correspond to the electron concentration $\varrho=2.3\times 10^{11}$ cm^{-2}. (d) Gap reduction $1-\Delta/\Delta_0$ as a function of parameter β^* in which Coulomb energy $q^2\lambda_q^{-1}$ involves different fractional charge quanta q (indicated) appropriate for different liquids.

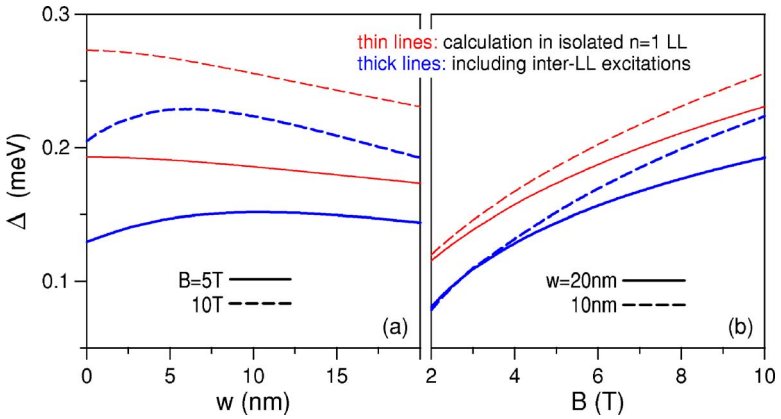

FIG. 3. (Color online) Dependence of the excitation gaps Δ calculated at $\nu=5/2$ (for $N=8$) with and without LL mixing, on the 2D layer width w (a) and the magnetic field B (b).

removal from) the LL occupied by the incompressible liquid. This causes creation of several fractionally charged QPs. At $\nu=\frac{1}{3}$ or $\frac{2}{5}$ they are the well-known Laughlin or 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 or removed electron distinguishable from the correlated electrons. This problem resembles coupling of a Laughlin liquid to a (positive) valence hole[33,34] or a (negative) trion.[35] 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]. 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 wave function. The results of calculations of the gap Δ for $N=8$ and $K\leqslant 1$ in a 2D layer of zero width are shown in Fig. 2(c). As argued above and anticipated from experiments, the gap reduction Δ/Δ_0 (where Δ_0 is the result for $K=0$) is noticeably greater at $\nu=\frac{5}{2}$ than at both $\nu=\frac{1}{3}$ and $\frac{2}{5}$. On the other hand, the fact that the gap at $\nu=\frac{1}{3}$ is reduced more than at $\nu=\frac{2}{5}$ 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 $\beta\ll 1$ criterion for the accuracy of the isolated-LL approximation may be relaxed to $\beta^*\ll 1$. Here, $\beta^*=(q^2\lambda_q^{-1})/(\hbar\omega_c)=(q/e)^{5/2}\beta$ involves the Coulomb energy scale of the QPs. Indeed, when the gaps in the weak-perturbation regime are plotted as a function of β^* as in Fig. 2(d), the data for $\nu=\frac{1}{3}$ and $\frac{2}{5}$ fall 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 β 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 β corresponding to different ν. For example, for $\varrho=2.3\times 10^{11}$ cm^{-2} we obtained gap reduction of 8.5%, 2.5%, and 35% at $\nu=\frac{1}{3}$, $\frac{2}{5}$, 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 $K\leqslant 1$ 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 $N\geqslant 8$ are beyond our present capabilities.

The dependence of gap Δ 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 wave functions $\chi(z)\psi_{nm}(\theta,\phi)$ 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 Δ discrepancy.

Let us now turn to the question of equivalence of the $\nu=\frac{5}{2}$ state realized in experiment and the model MR wave function. There is a subtle difference between the half-filled state and odd-denominator liquids like $\nu=\frac{1}{3}$ or $\frac{2}{5}$. In the latter states, it is not merely incompressibility but also the form of correlations and many-body wave function 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

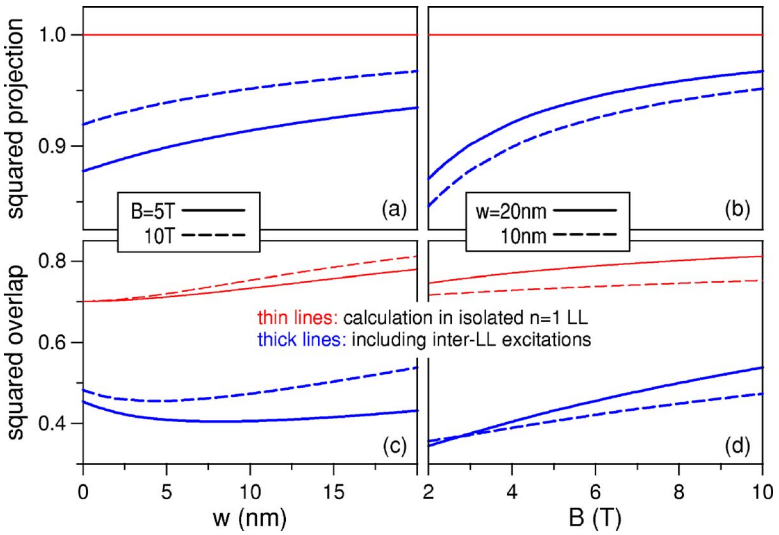

FIG. 4. (Color online) Dependence of the squared projection onto the LL_1 (top) and the squared overlap with the Moore-Read wave function (bottom) of the $\nu=5/2$ ground states calculated for $N=8$ with and without LL mixing, on the 2D layer width w (left) and the magnetic field B (right).

electron-electron pseudopotentials, but the exact form of the wave function 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 wave functions sharing the same symmetry: the MR state, which can be defined as an exact ground state of a short-range three-body repulsion,[13] and a clustered state characterized[36] by the maximum avoidance of the next to the lowest value of the relative pair angular momentum $\mathcal{R}=3$. The MR state is anticipated for the pair repulsion which is nearly harmonic at short range (i.e., with the pseudopotential decreasing linearly through $\mathcal{R}=1$, 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 parameters[18] and surface curvature,[14] raising the question of whether the $\nu=\frac{5}{2}$ FQH state and the MR model state are indeed (qualitatively) equivalent.

How does LL mixing affect this problem? In the top frames of Fig. 4 we plot the squared projection $|\mathcal{P}_{K=0}\Psi|^2$ onto the LL_1 (i.e., onto the $K=0$ subspace) of the same ground states Ψ whose gaps are shown in Fig. 4. It depends on w and B, but it is always significantly higher than Δ/Δ_0 or the (not shown) squared overlap with the $K=0$ ground state, in consequence of the coupling between intra- and inter-LL excitations in the $K\leqslant 1$ space. In the bottom frames we plot the squared overlap $\xi^2=|\langle \mathrm{MR}|\Psi\rangle|^2$ 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.[14] 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 wave function 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[29–31] irreplaceable. For comparison with Fig. 4, squared projections and overlaps calculated for Laughlin and Jain states in the lowest LL are much higher (all above 0.95 within the same range of w and B).

Let us close by recalling the important limitations of our numerical approach. (i) The Hilbert space used in exact diagonalization includes the most important but not all two-body scattering processes that are of the first order in the Coulomb-to-cyclotron energy ratio β. This is justified by the expectation that the neglected terms may affect the magnitude of LL mixing effects, but not the conclusion that these effects are significant. (ii) Only one system size was studied for $\nu=\frac{5}{2}$. Smaller systems are not representative and larger systems yield too large Hamiltonian matrices. However, we were able to compare data similar to Fig. 2(b) for Laughlin and Jain states of different electron numbers and found regular and weak size dependence in both cases, validating the qualitative conclusions. On the other hand, regular size dependence in Fig. 1(b) supports taking the $N=8$ case as a representative finite system for $\nu=\frac{5}{2}$. (iii) The stability of the MR state at $\nu=\frac{5}{2}$ is known to depend sensitively on the exact form of the interaction pseudopotential at short range (and thus, indirectly, on the quantum well width w, electron number N in a finite-size calculation, etc.). Therefore, the absolute values of the overlaps ξ in Figs. 4(c) and 4(d) cannot be interpreted as reliable estimates for realistic infinite systems. However, a strong decrease in ξ due to LL mixing is probably a genuine effect, and so is the strong admixture of higher LLs in the $\nu=\frac{5}{2}$ ground state shown in Figs. 4(a) and 4(b). The question of whether LL mixing changes qualitatively the nature of the QPs at $\nu=\frac{5}{2}$ has not been resolved.

IV. CONCLUSION

We studied the effect of LL mixing on the $\nu=\frac{5}{2}$ FQH state. The effect is more pronounced in this state than in the incompressible liquids of the lowest LL such as $\nu=\frac{1}{3}$ or $\frac{2}{5}$ (even at the same magnetic field) due to the richer inter-LL excitation spectrum. We found strong reduction of the $\nu=\frac{5}{2}$ excitation gap in the numerical calculation carried out within a restricted Hilbert space of a small number of electrons. This result suggests that the LL mixing might be at origin of the the troubling disparity between the previous numerics (which ignored this effect) and the available experiments. Our prediction agrees qualitatively with Ref. 27 which in-

cluded LL mixing in a different way. Finally, the LL mixing appears to significantly lower overlaps with the MR wave function. This result amplifies the need for the recently proposed[29–31] experiments, designed to probe directly the non-Abelian statistics of the QPs at $\nu=\frac{5}{2}$.

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