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Landau level mixing and particle-hole symmetry breaking for spin transitions in fractional quantum Hall effect

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The spin transitions in the fractional quantum Hall effect provide a direct measure of the tiny energy differences between differently spin polarized states, and thereby serve as an extremely sensitive test of the quantitative accuracy of the theory of the fractional quantum Hall effect, and, in particular, of the role of Landau level mixing in lifting the particle-hole symmetry. We report on an accurate quantitative study of this physics, evaluating the effect of Landau level mixing in a non-perturbative manner using a fixed-phase diffusion Monte Carlo method. We find excellent agreement between our calculated critical Zeeman energies and the experimentally measured values. In particular, we find, as also do experiments, that the critical Zeeman energies for fractional quantum Hall states at filling factors $\nu = 2 - n/(2n \pm 1)$ are significantly higher than those for $\nu = n/(2n \pm 1)$, a quantitative signature of the lifting of particle-hole symmetry due to Landau level mixing.

The role of particle-hole symmetry in the lowest Landau level (LLL) as well as its breaking due to Landau level (LL) mixing has come into renewed focus in the contexts of the competition between the Pfaffian and the anti-Pfaffian wave functions for the $\nu = 5/2$ fractional quantum Hall (FQH) effect [1–9] and of the nature of the composite-fermion (CF) Fermi sea at $\nu = 1/2$ [10–24]. LL mixing also affects various observable quantities in FQH effect, and a lack of its quantitative understanding has been one of the major impediments towards the goal of an accurate comparison between theory and experiment. The effect of LL mixing has been treated in a perturbative approach [4–9], but the extent of its validity for typical experiments has remained unclear, because the relevant parameter controlling the strength of LL mixing, namely the ratio of the Coulomb interaction to the cyclotron energy $\kappa = (e^2/\epsilon\ell)/\hbar\omega_c$, is typically ~ 1 and sometimes as high as ~ 2 . (Here $\ell = \sqrt{\hbar c/eB}$ is the magnetic length, ϵ is the dielectric constant of the background material, and $\omega_c = eB/m_b c$ is the cyclotron frequency.)

We study in this work the effect of LL mixing through the non-perturbative method of fixed-phase diffusion Monte Carlo [25–27]. We focus here on the phase transitions between differently spin polarized FQH states as a function of the Zeeman energy, which are an ideal testing ground for the role of LL mixing, both because a wealth of experimental information exists for the critical energies where such transitions occur [28–40], and because they depend sensitively on LL mixing [40, 41]. The critical Zeeman energy E_Z^{crit} , quoted below in terms of the dimensionless ratio $\alpha_Z^{\text{crit}} = E_Z^{\text{crit}}/(e^2/\epsilon\ell)$, is a direct measure of the tiny energy differences between differently spin polarized states, and thus serves as an extremely sensitive test of the quantitative accuracy of the theory.

In particular, a longstanding puzzle has been that the observed values of α_Z^{crit} for spin transitions at the filling factor $\nu = 2 - n/(2n \pm 1)$ are significantly higher than those at $\nu = n/(2n \pm 1)$. Because particle-hole symmetry in a system confined to the LLL guarantees that the transitions at ν and $2 - \nu$ occur at the same α_Z^{crit} , it is clear that LL mixing, which breaks particle-hole symmetry, is responsible for the effect. Surprisingly, for heterojunction samples, α_Z^{crit} for spin transitions at the filling factor $\nu = 2 - n/(2n \pm 1)$ are higher even than the theoretical values for systems with zero width and zero LL mixing, which is counterintuitive because the corrections due to finite width and finite LL mixing are both expected to weaken the interaction and thus reduce α_Z^{crit} .

If fixed-phase DMC can be demonstrated to provide a quantitative account of these experiments, it will not only reveal the role of Landau level mixing in a quantitative fashion but, in principle, also enable an investigation of the effect of LL mixing on various other issues, including the 5/2 Pfaffian/anti-Pfaffian state and the 1/2 CF Fermi sea, in a non-perturbative approach.

The Diffusion Monte Carlo (DMC) method [42, 43] solves the many-body Schrödinger equation by noting that its imaginary time ($t \rightarrow it$) version can be interpreted as a diffusion equation. The wave function Φ of interest plays the role of the density of diffusing particles, which is valid when Φ is always positive, such as for Bose systems in their ground states. In order to treat Fermi statistics, a fixed-node approximation is used which does not allow diffusion through the nodal surface. The fixed-node DMC, suitable for real wave function, cannot be applied directly to FQH systems, which, due to the broken time-reversal symmetry, produce complex valued eigenfunctions for interacting fermions. For such systems, a fixed-phase approximation was introduced by Ortiz,

Ceperley and Martin [25] who express the wave function as $\Phi(\mathcal{R}) = |\Phi(\mathcal{R})|e^{i\varphi_T(\mathcal{R})}$, and solve the appropriate Schrödinger equation for the real non-negative wave function $|\Phi(\mathcal{R})|$ by DMC. Here $\mathcal{R} = (\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$ denotes the coordinates collectively, and the phase $\varphi_T(\mathcal{R})$ is fixed with the help of an initial “trial” or “guiding” wave function $\psi_T(\mathcal{R}) = |\psi_T(\mathcal{R})|e^{i\varphi_T(\mathcal{R})}$. The DMC algorithm gives the lowest energy consistent with the prescribed trial phase $\varphi_T(\mathcal{R})$ and the accuracy of the results depends on the choice of $\varphi_T(\mathcal{R})$. It was found by Güçlü and Umrigar[44] that the Coulomb eigenstate of the LLL subspace is an excellent choice for ψ_T , i.e., LL mixing does not significantly alter the phase. We will therefore choose for our fixed-phase DMC the phases of the wave functions of the CF theory, which are known to accurately represent the actual Coulomb eigenstates [45, 46].

We follow the method presented by Melik-Alaverdian, Bonesteel and Ortiz [26, 27], who have generalized the fixed-phase DMC method to the spherical manifold [47]. The electrons are confined to the surface of a sphere [48] of radius R_0 with a magnetic monopole of strength Q at the center, producing a total flux of $2Q\phi_0$. In order to simulate the diffusion process conveniently, a stereographic projection is employed to represent electrons positions by planar coordinates $\mathbf{r} = (x, y) = (\cos\phi, \sin\phi)\cot(\theta/2)$, where θ and ϕ are the usual spherical angles. The Hamiltonian is then written as

$$H = \frac{1}{2m_b} \sum_i D(\mathbf{r}_i)[-i\hbar\nabla_i + e\mathbf{A}(\mathbf{r}_i)]^2 + V(\mathcal{R}), \quad (1)$$

where $D(\mathbf{r}_i) = (1 + r_i^2)^2/4R_0^2$. The vector potential $\mathbf{A} = -\frac{\hbar c Q}{eR} \cot\theta\hat{\phi}$ produces a radial magnetic field $B = 2Q\phi_0/4\pi R_0^2$ in the Haldane gauge. At filling factor $\nu = \frac{n}{2pn\pm 1}$, for trial function $\psi_T(\mathcal{R})$ we choose the wave functions of the CF theory (suppressing the spin part) [45, 46]

$$\Psi_{n/(2pn\pm 1)} = \mathcal{P}_{\text{LLL}}\Phi_{\pm n_\uparrow}\Phi_{\pm n_\downarrow}\Phi_1^{2p} \quad (2)$$

Here Φ_n is the wave function for n filled Landau levels, $\Phi_{-n} \equiv [\Phi_n]^*$, and \mathcal{P}_{LLL} denotes LLL projection, performed below using the method in Refs. [46, 49–51]. The state of spinful composite fermions with n_\uparrow spin-up and n_\downarrow spin-down filled Λ levels (CF LLs) is denoted as $(n_\uparrow, n_\downarrow)$, with $n = n_\uparrow + n_\downarrow$.

Our goal is to compute the critical Zeeman energy where a FQH system undergoes a transition from a fully spin-polarized (FP) state into either a partially spin-polarized (PP) or a spin-singlet (SS) state. We first obtain the per particle interaction energies $E_{(n_\uparrow, n_\downarrow)}$ of the states $(n_\uparrow, n_\downarrow)$. The dimensionless critical Zeeman energy α_Z^{crit} for the transition between two successive states $(n_\uparrow, n_\downarrow)$ and $(n_\uparrow - 1, n_\downarrow + 1)$ is given by

$$\alpha_Z^{\text{crit}} = (n_\uparrow + n_\downarrow) \left[\frac{E_{(n_\uparrow, n_\downarrow)} - E_{(n_\uparrow - 1, n_\downarrow + 1)}}{e^2/\epsilon\ell} \right]. \quad (3)$$

Many previous studies [41, 51–53] have used variational Monte Carlo (VMC) to evaluate α_Z^{crit} using the LLL wave functions of Eq. 2. (For other approaches, see Refs. 54–57.) To study the effect of LL mixing, we perform DMC as a function of κ , which, for parameters appropriate for electron-doped GaAs ($\epsilon = 12.5$, electron band mass $m_b = 0.067m_e$), is given by $\kappa \approx 2.6/\sqrt{B[T]} \approx 1.28\sqrt{\nu/(\rho/10^{11}\text{cm}^{-2})}$, where ρ is the areal density. The DMC result reduces to VMC result in the limit of $\kappa = 0$.

The non-zero transverse width of GaAs-Al_xGa_{1-x}As heterojunctions and quantum wells also has a quantitative effect, producing an effective two-dimensional interaction dependent on the transverse wave function $\xi(z)$:

$$V^{\text{eff}}(r) = \frac{e^2}{\epsilon} \int dz_1 \int dz_2 \frac{|\xi(z_1)|^2 |\xi(z_2)|^2}{[r^2 + (z_1 - z_2)^2]^{1/2}}, \quad (4)$$

where z_1 and z_2 denote the coordinates perpendicular to the 2D plane, and $r = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$. $V^{\text{eff}}(r)$ is less repulsive than the ideal 2D interaction $e^2/\epsilon r$ at short distances. In this work, we calculate the critical Zeeman energy using $V^{\text{eff}}(r)$ to include the effect of the finite transverse width. A realistic $\xi(z)$ for each density and geometry is obtained by solving the Schrödinger and Poisson equations self-consistently through the local density approximation [58]. Note that the finite-width correction the VMC results depends on the density through $\xi(z)$.

In the following, we show our numerical results for α_Z^{crit} in the thermodynamic limit and compare them with those obtained from transport experiments. We have used two methods to perform extrapolation to $N \rightarrow \infty$. In Method I, we extrapolate the energy difference to the thermodynamic limit. For this purpose, we correct for the finite size deviation of the density from its asymptotic value by multiplying the finite-size energy with a factor $(2Q\nu/N)^{1/2}$ [59], and, if needed, also interpolate the energy to the appropriate particle number. In Method II, we extrapolate the density-corrected per particle energies of SS, FP or PP states to thermodynamic limit separately, and then obtain α_Z^{crit} according to Eq. (3). The results quoted below are obtained from Method I unless specified otherwise [47]. The errors shown below arise primarily from the extrapolation; the statistical error from Monte Carlo sampling is comparatively negligible.

We first study the FQH states with fillings $\nu = \frac{n}{2n+1}$. Critical Zeeman energies α_Z^{crit} for $\nu = 2/5, 3/7$ and $4/9$ are shown in Fig. 1 for an ideal 2D system with width $w = 0$, for GaAs-Al_xGa_{1-x}As quantum wells with widths $w = 30$ and 50 nm, and also for a GaAs-Al_xGa_{1-x}As heterojunction (HJ). α_Z^{crit} calculated from DMC and VMC are plotted as a function of density ρ with solid and dashed lines respectively. The value of κ is shown at the upper x-axis. For quantum wells, α_Z^{crit} from VMC (no LL mixing) decreases with increasing w or ρ . The behavior

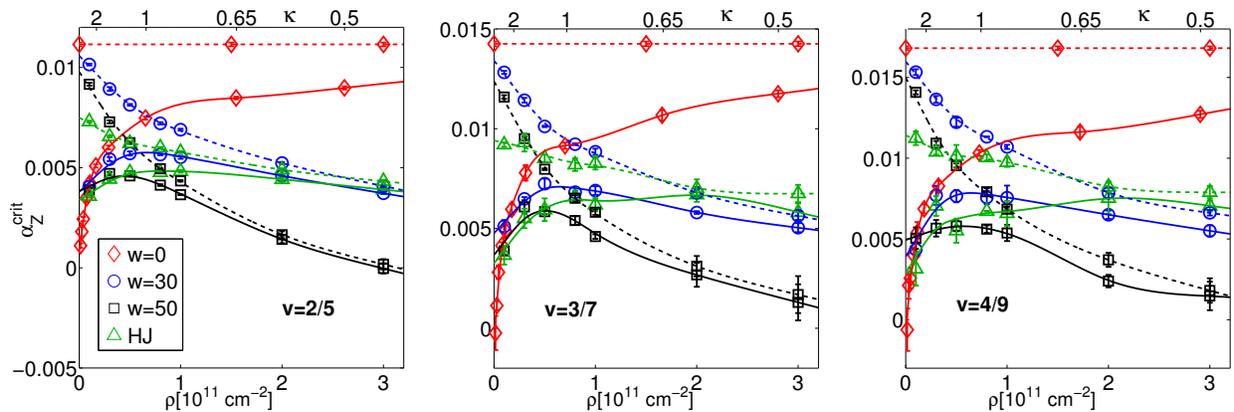


FIG. 1. (Color online) The theoretical critical Zeeman energies $\alpha_Z^{\text{crit}} = E_Z^{\text{crit}}/(e^2/\epsilon\ell)$ for $\nu = 2/5$ (left), $3/7$ (middle), $4/9$ (right) are shown with empty symbol with error bars, calculated from both DMC (solid line) and VMC (dashed line), for ideal 2D system ($w = 0$), quantum wells with widths $w = 30\text{nm}$ and 50nm , and heterojunction (HJ). The symbols ρ denotes the electron density. The solid lines for quantum wells and heterojunction display a “hill” shape, where, roughly speaking, LL mixing correction dominates on the left of the “hill” (at small ρ) and finite width correction on the right (at large ρ).

of the α_Z^{crit} from DMC, which includes the correction due to LL mixing, is more complicated. At large ρ (small κ), the DMC results are close to the VMC results for each width. On the other hand, with decreasing ρ (increasing κ), the DMC results are increasingly lower than the VMC results. For $\kappa \gtrsim 2$ the DMC results are largely insensitive to w , implying that the dominating correction here is due to LL mixing. We note that we have not included in our calculations any physics relating to an instability of the FQH effect at large κ [60].

One of the main messages of our calculation is that LL mixing and finite-width corrections significantly reduce the critical Zeeman energy at $\nu = \frac{n}{2n+1}$, by a factor of 2 or more for the experimental systems. This is consistent with the fact that, in typical experiments, the FQH states at $\nu < 1/2$ are fully spin polarized even with zero tilt of magnetic field. The transitions at $\nu = 2/5, 3/7$ have been seen by Kang *et al.* [32] in transport experiments only by significantly decreasing the Landé factor g_0 with the application of hydrostatic pressure.

For FQH states at $\nu = \frac{n}{2n-1}$, where the composite fermions are in a negative effective magnetic field, the wave functions of non-fully spin polarized states in Eq. 2, evaluated with the projection method in Ref. [49, 51] are not as accurate as those for $n/(2n+1)$ and are known to produce, for $w = 0$ and $\kappa = 0$, values of α_Z^{crit} that are off by up to a factor of two relative to the exact results [41]. For example, for $\nu = 2/3$, the value of $\alpha_Z^{\text{crit}} = 0.0082(1)$ obtained from the wave functions in Eq. 2 is much lower than the value $0.0183(5)$ obtained from exact diagonalization (ED) for $\kappa = 0$ at $w = 0$. The reason is because our projection method [49, 51] slightly overestimates the probability of spatial coincidence of electrons in the non-fully polarized states, and thereby overestimates their energies. (The “hard-core” projection of Ref. [61] produces very accurate wave functions, but is not amenable

to numerical evaluations.) Fortunately, we find that for $\kappa \gtrsim 2$ the results are insensitive to slight differences in the initial trial wave function ψ_T because of the relatively large modification due to LL mixing. Taking again the example of $\nu = 2/3$, for $\kappa = 1.91$, both the exact wave function and the wave function in Eq. 2 produce $\alpha_Z^{\text{crit}} \approx 0.0090$ (see Fig. 3 and Fig. S1 in the Supplementary Material [47]).

Fig. 2 shows the comparison between experimental data (filled symbol) and theoretical results (empty symbols) for α_Z^{crit} for many states at $\nu = n/(2n \pm 1)$. The theoretical results are obtained with DMC for the specific experimental parameters (ρ, w). The black empty circles show the α_Z^{crit} obtained from ED with $\kappa = 0$ and $w = 0$, taken from Ref. [41]. The experimental values for α_Z^{crit} are significantly lower than the ED values, but in reasonably good agreement with our DMC results.

The corrections due to LL mixing enter in a more dramatic manner when one compares the spin transitions between the filling factor regions $0 < \nu < 1$ and $1 < \nu < 2$. Experiments have found (see Fig. 3 of Ref. 40) that the α_Z^{crit} 's for the latter are significantly higher than those for the former. As noted above, the difference arises from, and thus is a measure of, the breaking of the particle-hole symmetry by LL mixing. To address this issue, we find it most convenient (for reasons of computational cost) to study the spin transitions at $\nu = 2/3$ and $\nu = 4/3$. To obtain accurate results, we use for our ψ_T the exact $\kappa = 0$ Coulomb wave functions for the SS states at $2/3$ and $4/3$, Eq. 2 for $2/3$ FP state, and $\Phi_{1\uparrow}\Psi_{1/3\downarrow}$ for the $4/3$ PP state. For SS states, we can only calculate for small systems as the exact states contain a large number of Slater determinants. Fig. 3 shows the α_Z^{crit} for $\nu = 4/3$ (green circle) and $\nu = 2/3$ (blue square) obtained from the extrapolation Method II. The value of α_Z^{crit} at $\kappa = 0$ is approximately consistent with the exact value 0.0175 [41], giving

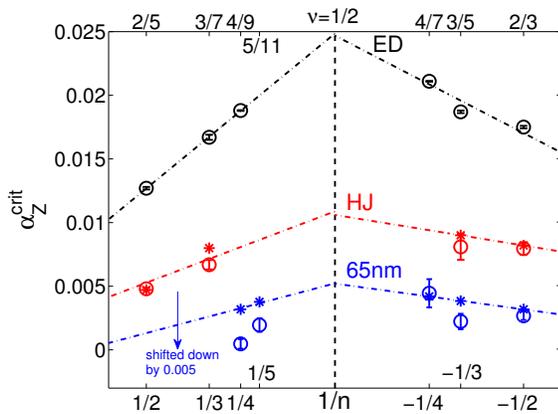


FIG. 2. (Color online) Comparison between experimental values (stars) and theoretical DMC values (empty circles) of $\alpha_Z^{\text{crit}} = E_Z^{\text{crit}}/(e^2/\epsilon\ell)$ for a $w = 65\text{nm}$ quantum well (blue) from Liu *et al.* [40], and heterojunctions (red) from Engel *et al.*[30] and Kang *et al.*[32]. (For the experiment of Kang *et al.*, we estimate the value of the Landé factor g_0 by assuming that it changes linearly and passes through zero at a pressure of roughly 18 Kbar [62].) The filling factors $\nu = n/(2n+1)$ are shown on top and $1/n$ at the bottom. The black circles show the results obtained from exact-diagonalization (ED) without including any LL mixing or finite-width corrections [41] (these do not involve DMC calculation). The results for 65nm quantum well are shifted down by 0.005 for ease of depiction. The dashed lines are a guide to the eye. For heterojunction, some other experimental values (theoretical predictions) of α_Z^{crit} are 0.0109 [0.0076(4)] [29] and 0.0078 [0.0065(4)] [30] at $\nu = 2/3$, and 0.0081[0.0080(20)] [30] at $\nu = 3/5$; these are not shown on the figure to avoid clutter.

ν	$d(\alpha_Z^{\text{crit}})/d\kappa$	
	perturbative	non-perturbative (DMC)
2/5	-0.0023	-0.0043
3/7	-0.0025	-0.0050
2/3	-0.0135	-0.0057
4/3	0.0339	0.0184

TABLE I. This table compares the values of $d(\alpha_Z^{\text{crit}})/d\kappa$ at $\kappa = 0$ obtained from the perturbative and the non-perturbative DMC calculations.

us confidence in our calculated α_Z^{crit} with relatively small system sizes. The main message of Fig. 3 is that the α_Z^{crit} at 4/3 is substantially higher than that at 2/3 for the typical experimental value of $\kappa \approx 1-2$. Note that we only show the zero-width results, because the extrapolation of finite-width results to thermodynamic limit has a poor statistics for such small systems [47]. We also show in Fig. 3 the experimental data from GaAs-Al_xGa_{1-x}As heterojunction samples, because these have the smallest effective width, with solid symbols for $\nu = 2/3$ (light blue) and $\nu = 4/3$ (green). The agreement with the $w = 0$ results is very good, which is not surprising because we know from Fig. 1 that at relatively large κ ($\gtrsim 2$), α_Z^{crit} is not very sensitive to the width w .

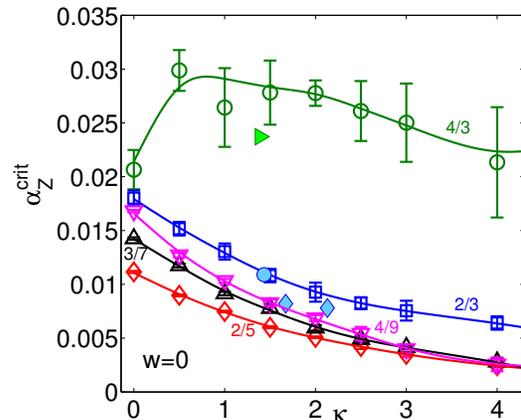


FIG. 3. (Color online) Theoretical critical Zeeman energies for $w = 0$ model as a function of the LL mixing parameter κ obtained from the DMC method for $\nu = 4/3$ (green circle), $2/3$ (blue square), $4/9$ (magenta downward triangle), $3/7$ (black upward triangle), and $2/5$ (red diamond). For the fractions $n/(2n+1)$, the wave functions of Eq. 2 are used to fix the phase. For $\nu = 2/3$ and $\nu = 4/3$ the exact Coulomb state in the LLL is used to fix the phase of the wave function. The solid lines are an approximate guide to the eye. The filled symbols indicate the experimental data from heterojunction samples at $\nu = 2/3$ (light blue) and $4/3$ (green), taken from Eisenstein *et al.* [29] (circle), Engel *et al.* [30] (diamond), and Du *et al.*[31] (rightward triangle).

It is natural to ask how well our results agree with those obtained from the perturbative approach in which the effect of LL mixing is incorporated within the LLL theory through an effective interaction, which contains perturbative corrections to the two-body interaction, and, minimally, also a three body interaction (because the two-body interaction does not break particle-hole symmetry). We discuss this issue for $w = 0$. As seen in Fig. 3, the perturbation theory is *in principle* valid for up to $\kappa \approx 1$ for the states $n/(2n \pm 1)$, and up to $\kappa \approx 0.5$ for the states at $2 - n/(2n \pm 1)$. In practice, one cannot keep all 2-body, 3-body and n -body terms in the calculation. We have evaluated α_Z^{crit} [47] using the interaction given by Peterson and Nayak[8], including corrections to the 2-body pseudopotentials $V_m^{(2)}$ for $m \leq 5$ and 3-body pseudopotentials $V_m^{(3)}$ for $m \leq 3$. Table I compares the perturbative $d(\alpha_Z^{\text{crit}})/d\kappa$ with that deduced from Fig. 3 at small κ . The two results are substantially different. For example, if the perturbative result is applied to $\kappa = 1.5$, it would produce $\alpha_Z^{\text{crit}} \sim 0.068$ and -0.003 for $\nu = 4/3$ and $2/3$, respectively, to be compared to the DMC values of $\alpha_Z^{\text{crit}} \sim 0.027$ and 0.012 . An exhaustive study of the quantitative importance of the terms left out in the perturbative study is outside the scope of the current study.

To conclude, we find that LL mixing substantially suppresses the critical Zeeman energies for the $\nu = \frac{n}{2n \pm 1}$ FQH states, and brings theory into satisfactory agree-

ment with experiment. We also find that LL mixing causes an enhancement of the critical Zeeman energy for $\nu = 2 - \frac{n}{2n \pm 1}$, as also seen experimentally. In addition to providing an accurate quantitative comparison between FQH theory and experiment, our work shows how the quantitative study of the spin physics can shed fundamental light on the role of LL mixing in breaking the particle-hole symmetry of the lowest LL.

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