Half-filled 2D bilayers in a strong magnetic field: Revisiting the $\nu = 1/2$ fractional quantum Hall effect

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We examine the quantum phase diagram of the fractional quantum Hall effect in the lowest Landau level in half-filled bilayer structures as a function of tunneling strength and layer separation. Using numerical exact diagonalization we investigate the important question of whether this system supports a fractional quantum Hall effect described by the non-Abelian Moore-Read Pfaffian state in the strong tunneling regime. We find that, although it is in principle possible, it is unlikely that the non-Abelian FQH exists in the lowest Landau level. We establish that all so far observed FQHE states in half-filled lowest Landau level bilayers are most likely described by the Abelian Halperin 331 state.

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Two important developments have rekindled interest in the phenomena of even-denominator incompressible fractional quantum Hall (FQH) states in bilayer semiconductor structures. The first is the recent intriguing experimental observation by Luhman et al. [1] of two distinct even-denominator (filling factors $\nu = 1/2$ and $1/4$) FQH states in a very wide ($\sim 600\,\text{Å}$) single quantum well (WQW) structure at very high ($> 40\,\text{T}$) magnetic fields. The second development, motivated by implications for fault-tolerant topological quantum computation [2], is the great deal of recent theoretical and experimental interest in the possible non-Abelian nature of the $\nu = 5/2$ second Landau level (SLL) FQH state in the single-layer system [3]. This leads to the interesting as well as important question whether a non-Abelian $\nu = 1/2$ FQH state, i.e., the analog of the possibly non-Abelian $\nu = 5/2 = 2 + 1/2$ SLL single-layer state, can exist in the lowest Landau level (LLL) under experimentally observable conditions. This question has a long history [4] in the theoretical literature going back to the early 1990s. Motivated by these considerations we revisit the $\nu = 1/2$ FQHE in bilayer structures (with each layer having $\nu = 1/4$ on average) by theoretically investigating the quantum phase diagram for the LLL $\nu = 1/2$ bilayer FQH state using the FQH spherical system finite size exact diagonalization technique. We obtain an approximate quantum phase diagram for the spin-polarized $\nu = 1/2$ bilayer FQH system in the LLL in the parameter space of inter-layer separation ($d$), inter-layer tunneling strength ($t$) or, equivalently, the symmetric-antisymmetric gap energy, and the width or thickness ($w$) of the individual wells (for simplicity, we assume the two wells to be identical). We take the system to be fully spin-polarized since all experimental $\nu = 1/2$ FQH states appear to be fully spin-polarized.

Our main findings are: (i) the recently observed WQW $\nu = 1/2$ FQHEs [1,2] are strong-pairing Abelian Halperin 331 FQH states [4] which, however, sit close to the boundary between the Abelian 331 and the weak-pairing non-Abelian Pfaffian (Pf) FQH state [5], and (ii) it may be conceivable, as a matter of principle, to realize the LLL $\nu = 1/2$ Pfaffian non-Abelian FQHE in very thick bilayers, but as a matter of practice, this is unlikely since the $\nu = 1/2$ FQHE gap is extremely small (perhaps zero) in the parameter regime where the Pf is more stable than the 331 phase. Our findings about the fragility of the LLL $\nu = 1/2$ non-Abelian Pf state are consistent with recent conclusions [6,7], but our main focus in the current work is in understanding the $\nu = 1/2$ bilayer quantum phase diagram treating $t$, $d$, and $w$ as independent tuning parameters of the system Hamiltonian.

Before presenting our results, we discuss the context of our theoretical investigation. The proposed Moore-Read Pf state is a weak-pairing single-layer FQH state at $\nu = 1/2$ which, in principle, applies to any orbital LL (i.e., LLL as well as SLL). Thus, as a matter of principle the $\nu = 1/2$ LLL single-layer Pf FQHE is certainly a possibility although it has never been observed experimentally. The best existing numerical work [8,9] indicates that either the single-layer $\nu = 1/2$ LLL Pf state does not exist in nature or if it exists, does so only in rather thick 2D layers with an extremely small FQH excitation gap, making it impossible or very difficult to observe experimentally. By contrast, the single-layer $\nu = 5/2$ SLL FQHE is observed routinely, albeit at low temperatures ($\lesssim 100\,\text{mK}$), in high mobility ($\gtrsim 10^6\,\text{cm}^2/\text{Vs}$) samples, and with a rather small (but experimentally accessible) activation gap ($\sim 100\text{-}500\,\text{mK}$). In fact, it has been pointed out that the experimental $\nu = 5/2$ FQHE is always among the strongest (along with the $\nu = 7/3$ and $8/3$ FQHE) observed FQH states in the SLL.

Instead of studying a single-layer 2D system we concentrate on the spin-polarized bilayer system assuming an arbitrary tunneling strength $t$ (proportional to the symmetric-antisymmetric gap) and an arbitrary layer separation $d$. We numerically obtain the quantum phase
diagram at \( \nu = 1/2 \) for this bilayer system in the \( t-d \) space, concentrating entirely on the Pfaffian and the 331 FQHE phases. Our focus on the bilayer spin-polarized \( \nu = 1/2 \) FQHE is consistent with the experimental fact that the incompressible \( \nu = 1/2 \) FQHE has so far been observed only in effective bilayer structures. The goal is to carry out an extensive comparison with all existing bilayer \( \nu = 1/2 \) FQH experimental observations to ascertain any hint of a Pfaffian \( \nu = 1/2 \) state for large values of \( t \). It is obvious that our model system is an effective bilayer (single-layer) \( \nu = 1/2 \) system for small (large) values of \( t \), and therefore by studying the quantum phase diagram as a function of \( t \) (and \( d \)) we hope to shed light on the possible existence of a single-layer \( \nu = 1/2 \) FQHE in real systems. Recent FQHE experiments at \( \nu = 1/2 \) for large values of the tunneling strength make it imperative that a theoretical analysis be carried out to achieve a proper qualitative understanding of the experimental situation [1,2].

We use a simple model Hamiltonian incorporating both finite tunneling and finite layer separation for our bilayer FQH system:

\[
\hat{H} = \sum_{i<j}^{N} V_{\text{intra}}(|\mathbf{r}_i - \mathbf{r}_j|) + V_{\text{intra}}(|\mathbf{\tilde{r}}_i - \mathbf{\tilde{r}}_j|) + V_{\text{inter}}(|\mathbf{r}_i - \mathbf{\tilde{r}}_j|) - t \hat{S}_z ,
\]

(1)

where \( \mathbf{r}_i(\mathbf{\tilde{r}}_i) \) is the position of the \( i \)-th electron in the right(left) layer. In Eq. (1), \( V_{\text{intra}}(r) = e^2/(\kappa \sqrt{r^2 + w^2}) \) and \( V_{\text{inter}}(r) = e^2/(\kappa \sqrt{r^2 + d^2}) \) are the intralayer and interlayer Coulomb interaction incorporating a finite layer width \( w \) and a center-to-center interlayer separation \( d \) (\( > w \) by definition). The \( x \)-component of the pseudospin operator \( \hat{S}_x \) controls the tunneling between the two quantum wells with large \( t \) denoting strong tunneling. We numerically diagonalize \( \hat{H} \) in the spherical geometry assuming specific values of \( w, d, \) and \( t \) (each expressed throughout in dimensionless units using the magnetic length \( l = (\hbar/eB)^{1/2} \) as the length unit and the Coulomb energy \( e^2/(\kappa l) \), where \( \kappa \) is the background dielectric constant, as the energy unit). Following the standard well-tested procedures [4, 8, 9] used extensively in the FQHE literature, we calculate the overlap between the exact numerical \( N \) electron ground state wavefunction of the Coulomb Hamiltonian defined by Eq. (1) and the candidate \( N \) electron variational states which are the Halperin 331 strong-pairing [6] and the Moore-Read Pfaffian weak-pairing [7] wavefunctions:

\[
\Psi_{331} = \prod_{i<j}^{N/2} (z_i - z_j)^3 \prod_{i<j}^{N/2} (\bar{z}_i - \bar{z}_j)^3 \prod_{i,j}^{N} (z_i - \bar{z}_j)
\]

(2)

\[
\Psi_{\text{Pf}} = \text{Pf} \left\{ \frac{1}{z_i - z_j} \right\} \prod_{i<j}^{N} (z_i - z_j)^2,
\]

(3)

respectively, where \( z = x - iy \) is the electron coordinate in the plane. We ensure that (i) the ground state is homogeneous, i.e., has zero total orbital angular momentum, and (ii) there is a gap, the FQH excitation gap, separating the ground state from all excited states. The results shown in this paper all use an \( N = 8 \) electron system, but larger systems show the same qualitative features. Since the theoretical techniques are standard, we do not give the details, concentrating instead on the results and their implications for \( \nu = 1/2 \) FQHE experiments.

The calculated overlap and gap determine the nature of the FQHE and its strength at \( \nu = 1/2 \) in our theory. We operationally define the system to be in the 331 (Pf) phase depending on the overlap with the 331 (Pf) state being the larger of the two. We emphasize that our work is a comparison between these two incompressible states only, and we cannot comment on the possibility of some other state (i.e., neither 331 nor Pf) being the ground state. We do, however, rule out the possibility that the real system has a compressible ground state (without manifesting FQHE), e.g., a composite fermion sea, not considered in our calculation.

We first show in Fig. 1(a) our numerically calculated FQHE quantum phase diagram (QPD) for the bilayer \( \nu = 1/2 \) system in the \( t-d \) space with the color coding indicating the numerical FQH gap strength and the dashed line separating the 331 phase from the Pf phase (i.e., the overlap with 331 (Pf) larger than the dashed line). The dashed line is only an operational phase boundary within our calculation since all we know is that the 331 (Pf) has higher (lower) overlap above (below) this line. The calculated overlap for each phase, i.e., 331 (Pf) above (below) the dashed line, varies between \(~0.6\) and \(~0.96\) for our \( 8 \)-particle system. We show the QPD for three values of the layer width parameter (a) \( w = 0 \); (b) \( w = 0.6 \); (c) \( w = 2.4 \). The zero- (Fig. 1(a)) and the intermediate-width (Fig. 1(b)) results are of physical relevance whereas the (unrealistically) large width results (Fig. 1(c)) are provided only for completeness (since this is the regime where the Pf state dominates over the 331 state in the QDP). We note that we are using the simplistic Zhang-Das Sarma (ZDS) model [10] for describing the well width effect, and crudely speaking \( w = 1 \) in the ZDS model corresponds roughly to \( w_{\text{WQW}} \approx 6 \) where \( w_{\text{WQW}} \) is the corresponding physical quantum well width. For a single WQW, where the effective bilayer is created by the self-consistent potential of the electrons themselves, our model \( w \) is typically much less than the total width \( W \) of the WQW—very roughly speaking \( w \sim W/6 \), and \( d \sim W/2 \). As emphasized above, we treat \( t \), \( d \), and \( w(< d) \) as independent
double-quantum-well (single-WQW) structures. We note that the single triangle on the Pf side of the QPD does not manifest showing FQHE are within the large solid circles in (a) with the lower smaller (upper larger) circles indicating experiments in figures that the Pf state becomes more dominant, albeit with very small FQH excitation gap, for larger values of $\nu$.

FIG. 1: (color online) Quantum phase diagram (QPD) and FQHE gap (color coded) versus layer separation $d$ and tunneling strength $t$ for widths (a) $w = 0$, (b) $w = 0.6$, and (c) $w = 2.4$. For the QPD, the 331 and Pf phases (as discussed in the text) are separated by a dashed black line and labeled appropriately. The FQHE gap is given as a contour plot with color coding given by the color-bar from dark to light, i.e., white being a largest value of 0.4 and black being value of 0. The asterisks, triangles, circles, and squares correspond to the different experiments in Refs. 12, 11, 5 and 1, respectively. Only experimental points showing FQHE are within the large solid circles in (a) with the lower smaller (upper larger) circles indicating experiments in double-quantum-well (single-WQW) structures. We note that the single triangle on the Pf side of the QPD does not manifest any experimental FQHE indicating that the theoretical gap may be overestimated for the Pf state. It is obvious from the figures that the Pf state becomes more dominant, albeit with very small FQH excitation gap, for larger values of $w$.

In Fig. 1 we have put as discrete symbols all existing $\nu = 1/2$ bilayer experimental data (both for double quantum well systems and single wide quantum wells) in the literature, extracting the relevant parameter values (i.e., $d$ and $t$) from the experimental works 1, 5, 11, and 12. Because of the ambiguity and uncertainty in the definition of $w$, we have put the data points on all three QPDs shown in Fig. 1 although the actual experimental width values correspond to only Figs. 1(a) and (b).

Results shown in Fig. 1 bring out several important points of physics not clearly appreciated earlier in spite of a great deal of theoretical exact diagonalization work on $\nu = 1/2$ bilayer FQHE: (i) It is obvious that large (small) $t$ and small (large) $d$, in general, lead to a decisive preference for the existence of $\nu = 1/2$ Pf (331) FQHE. The fact that large $t$ values would preferentially lead to the Pf state over the 331 state is, of course, expected since the system becomes an effective one-component system for large tunneling strength. (ii) What is, however, not obvious, but apparent from the QPDs shown in Fig. 1 is that the FQH gap (given in color coding in the figures) is maximum near the phase boundary between 331 and Pf. (iii) Another non-obvious result is the persistence of the 331 state for very large (essentially arbitrarily large!) values of the tunneling strength $t$ as long as the layer separation $d$ is also large--thus having a large $t$ by itself, as achieved in the Luhman et al. experiments 1, is not enough to realize the single-layer $\nu = 1/2$ Pf FQHE, one must also have a relatively small value of layer separation $d$ so that one is below the phase boundary (dashed line) in Fig. 1. The explanation for the Luhman experimental $\nu = 1/2$ FQHE being a 331 state, as can be seen in Fig. 1 is indeed the fact that both $t$ and $d$ are large in these samples making 331 a good variational state. (iv) An important aspect of Fig. 1 is that the Pf FQHE gap tends to be very small--this is particularly true for larger values of $w$, where the Pf overlap is larger. This implies, as emphasized by Storni et al. 9, that the observation of a $\nu = 1/2$ Pf state is unlikely since the activation gap would be extremely (perhaps even vanishingly) small. (v) For larger values of $w$ (and large $t$), our calculated QPD is dominated by the Pf state--particularly for the unrealistically large width $w = 2.4$ (corresponding to $w_{QW} \sim 14$) where all the experimental $d$ and $t$ values fall in the Pf regime of the phase diagram. We emphasize, however, that this Pf-dominated large-$w$ (and large-$t$) regime will be difficult (perhaps even impossible) to access experimentally since the FQH gap would be apparently extremely small as in Fig. 1.

In discussing Fig. 1 further, we mention that our 331 (Pf) regimes not only have the wavefunction overlap with the corresponding 331 (Pf) state being larger than the other, but also the calculated expectation value $\langle \hat{S}_x \rangle \approx 0 (4)$ in the 331 (Pf) regime. Thus, our QPD is consistent with both the overlap and the pseudo-spin calculation as obtained from exact diagonalization.

We now discuss the published experimental results in light of our theoretical QPD. First, we note that most of the existing experimental points fall on the 331 side of the phase diagram which is consistent with our QPD in Fig. 1. In particular, only samples on the 331 side of the QDP with reasonably large FQH gaps, i.e., the data points close to the phase boundary, exhibit experimental FQHE. By contrast, the one data point (in Figs. 1(a) and (b)) on the Pf side of the phase boundary does not manifest any observable FQHE in spite of its location being in a regime of reasonable FQH excitation gap according
to our phase diagram. This is consistent with the finding of Storni et al. \[9\] that the \( \nu = 1/2 \) FQH Pf gap in a single-layer system is likely to be vanishingly small in the thermodynamic limit. It is, therefore, possible that much of the Pf regime in our QPD has a much smaller excitation gap than what we obtain on the basis of our \( N = 8 \) particle diagonalization calculation. We refer to Storni et al. \[9\] for more details on the theoretical status of the single-layer LLL \( \nu = 1/2 \) FQHE.

For a more detailed view of the \( \nu = 1/2 \) bilayer FQHE, we show in Figs. 2(a) and (b), respectively, our calculated FQHE gap as a function of \( t \) (for a few fixed \( d \) values) and as a function of \( d \) (for a few fixed \( t \) values). In each figure, we also depict the line separating the 331 (smaller \( t/\)larger \( d \)) and the Pf (larger \( t/\)smaller \( d \)) regimes in the phase diagram. The qualitatively interesting point is, of course, the non-monotonicity in the FQHE gap as a function of \( t \) or \( d \) with a maximum close (but always on the 331 side) to the phase boundary. The non-monotonicity in the FQHE gap as a function of \( t \) (but not \( d \)) was earlier pointed out, but our result that the peak lies \textit{always} on the 331 side of the phase boundary is a new result. We emphasize that the FQHE gap peak lying always on the 331 side of the phase boundary is strong evidence that the 331 phase is the dominant FQH phase in \( \nu = 1/2 \) systems. We believe that the only chance of observing the \( \nu = 1/2 \) Pf FQHE is to look on the Pf side of phase boundary at fairly large values of \( d \) and \( t \). This is in sharp contrast to the SLL \( \nu = 5/2 \) bilayer FQHE where we recently showed that there are two sharp ridges far away from each other in the \( d-t \) space corresponding to the \( \nu = 5/2 \) Pf and 331 bilayer phases \[13\]. We note that for unrealistically large \( w \) (Fig. 1(c)), Pf dominates over 331 but the FQHE gap becomes extremely small everywhere.

We conclude by commenting on the nature of the quantum phase transition (QPT) between the 331 and the Pf phases in the \( d-t \) space. It may appear at first sight that our work implies a continuous QPT from the strong-pairing 331 to the weak-pairing Pf state with increasing (decreasing) \( t \) (\( d \)). This is, however, deceptive since all we are doing is \textit{comparing these two phases} using a finite size diagonalization study for discrete values of \( t \) and \( d \). It is entirely possible that a completely different phase, e.g. a compressible composite fermion Fermi liquid phase, has lower energy and intervenes between the 331 and Pf phases so that the system goes from 331 to Pf (or vice versa) through two first-order transitions. There is independent numerical evidence that the compressible composite fermion sea indeed has a lower ground state energy than the Pf state in a single-layer \( \nu = 1/2 \) (but not \( 5/2 \)) system which corresponds to the large \( t \) (and small \( d \)) regime in our QPD. This would indicate first order transitions in going from 331 to the Pf (if it exists) through the compressible phase. What we have shown here is that if the \( \nu = 1/2 \) bilayer Pf phase exists at all, then it would manifest most strongly in wide samples and close to the phase boundary with the 331 phase, but will have an extremely small FQHE excitation gap.

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