

## Effects of Landau Level Mixing on the Fractional Quantum Hall Effect in Monolayer Graphene

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We report results of exact diagonalization studies of the spin- and valley-polarized fractional quantum Hall effect in the  $N = 0$  and  $N = 1$  Landau levels in graphene. We use an effective model that incorporates Landau level mixing to lowest order in the parameter  $\kappa = ((e^2/\epsilon\ell)/(\hbar v_F/\ell)) = (e^2/\epsilon v_F \hbar)$ , which is magnetic field independent and can only be varied through the choice of substrate. We find Landau level mixing effects are negligible in the  $N = 0$  Landau level for  $\kappa \lesssim 2$ . In fact, the lowest Landau level projected Coulomb Hamiltonian is a better approximation to the real Hamiltonian for graphene than it is for semiconductor based quantum wells. Consequently, the principal fractional quantum Hall states are expected in the  $N = 0$  Landau level over this range of  $\kappa$ . In the  $N = 1$  Landau level, fractional quantum Hall states are expected for a smaller range of  $\kappa$  and Landau level mixing strongly breaks particle-hole symmetry, producing qualitatively different results compared to the  $N = 0$  Landau level. At half filling of the  $N = 1$  Landau level, we predict the anti-Pfaffian state will occur for  $\kappa \sim 0.25$ – $0.75$ .

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*Introduction.*—The fractional quantum Hall effect (FQHE) occurs when electrons are confined to two dimensions and placed in a uniform perpendicular magnetic field at electron densities  $\rho$  such that the filling factor  $\nu = 2\pi\ell^2\rho$  is a rational fraction ( $\ell = \sqrt{\hbar c/eB}$  is the magnetic length) and the temperature is low (typically on the order of a kelvin) [1]. For densities  $\rho \sim 10^{11}/\text{cm}^2$ , the magnetic field strength  $B$  must typically be from several up to tens of teslas. A plateau is observed in the Hall resistance with  $R_{xy} = h/fe^2$ , for a rational number  $f$ , along with a concomitant vanishing of the longitudinal resistance  $R_{xx} = 0$ . Since the electrons in graphene move in a two-dimensional layer of negligible width and interact through a Coulomb interaction with a dielectric constant on the order of 1, they would appear to realize a nearly perfect setting for the FQHE. Instead, the FQHE in graphene has remained puzzling [2,3] since the initial experimental observations [4,5], even though early calculations predicted that the FQHE in graphene would be nearly identical to the FQHE in semiconductor heterostructures in the lowest electronic Landau level (LL) [6–9]. Despite the fact that the single particle dispersion is linear (relativistic) in graphene and quadratic in semiconductor heterostructures, the Haldane pseudopotentials in the  $N = 0$  LL for both systems are identical in the absence of LL mixing.

On closer inspection, LL mixing—not taken into account in previous theoretical studies—may be very different in graphene than in semiconductors. Landau level mixing occurs when electrons in the fractionally filled  $N$ th LL have

a substantial probability amplitude of making virtual transitions to higher and lower LLs. This tendency is characterized by the ratio between the Coulomb interaction energy and the cyclotron energy; i.e., the LL mixing parameter  $\kappa$  is defined as

$$\kappa = \begin{cases} \frac{e^2/\epsilon\ell}{\hbar\omega} \sim \frac{2.5}{\sqrt{B[\text{tesla}]}} & \text{GaAs semiconductor} \\ \frac{e^2/\epsilon\ell}{\hbar v_F/\ell} = \frac{e^2}{\epsilon v_F \hbar} & \text{graphene,} \end{cases}$$

where  $\omega = eB/mc$ . In semiconductors,  $\kappa$  is inversely proportional to the magnetic field strength  $B$  and therefore can, in principle, be made small with a sufficiently large magnetic field. Traditionally, this was a primary motivation for ignoring LL mixing effects in these systems. In graphene,  $\kappa$  has no magnetic field dependence and only depends on material properties, namely, the Fermi velocity  $v_F$  and the dielectric constant  $\epsilon$ . For a suspended graphene sheet  $\kappa \approx 2.2$  and for graphene placed on substrates such as  $\text{SiO}_2$ ,  $\kappa \approx 0.9$ , or boron nitride,  $\kappa \approx 0.5$ – $0.8$  [10,11]. Clearly, LL mixing cannot safely be ignored, particularly in freestanding graphene where the FQHE was first experimentally observed.

Recently, we constructed an effective Hamiltonian for the FQHE in graphene that fully incorporates Landau level mixing [11]. This effective Hamiltonian for electrons fractionally filling the  $N$ th LL was produced by integrating out all other LLs to first order in  $\kappa$  (following Ref. [12]) and is characterized by Haldane pseudopotentials

$$\begin{aligned}
H(\kappa) &= \sum_{i<j} V_{\text{eff}}(\kappa, |\mathbf{r}_i - \mathbf{r}_j|) + \sum_{i<j<k} V_{3\text{body}}(\kappa, \mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) \\
&= \sum_{\alpha} V_{\alpha}^{(2)}(N, \kappa) \sum_{i<j} \hat{P}_m(m_{ij}) \\
&\quad + \sum_{\beta} V_{\beta}^{(3)}(N, \kappa) \sum_{i<j<k} \hat{P}_{ijk}(m_{ijk}), \tag{1}
\end{aligned}$$

where  $\hat{P}_{ij}(m_{ij})$  and  $\hat{P}_{ijk}(m_{ijk})$  project electrons  $i$  and  $j$  or  $i, j$ , and  $k$  onto states with relative angular momentum  $m_{ij}$  or  $m_{ijk}$ , respectively.  $V_{\alpha}^{(2)}(N, \kappa)$  and  $V_{\beta}^{(3)}(N, \kappa)$  are the  $\kappa$  dependent two- and three-body effective Haldane pseudopotentials [13,14]. (Similar to Ref. [11], we use planar geometry pseudopotentials throughout this work.) The expansion to lowest order in  $\kappa$  is especially interesting because, in addition to renormalizing the two-body Coulomb interaction, it generates three-body terms that explicitly break particle-hole symmetry. The most important aspects of this effective Hamiltonian are (i) in the  $N = 0$  LL the three-body terms vanish due to particle-hole symmetry, which is an exact symmetry only in this LL, (ii) the two-body corrections are numerically small for  $N = 0$ , and (iii) the size and character of the LL mixing corrections make the FQHE unlikely for  $N \geq 2$ . (See Ref. [11] for more details, especially Fig. 11.)

In this work, we have performed numerical exact diagonalization of Eq. (1) in the spherical geometry in the  $N = 0$  and  $N = 1$  LLs, focusing on filling factor  $\nu = 1/3, 2/3$ , and  $1/2$ . The first two are representative of well-understood fractions in GaAs and are almost certainly Abelian [15–17] while the third is still not completely understood in GaAs but is suspected to be non-Abelian in the  $N = 1$  LL [18–20]. In our calculations  $N_e$  electrons are placed on a spherical surface of radius  $\sqrt{N_{\Phi}/2}$  with a radial magnetic field produced by a magnetic monopole of strength  $N_{\Phi}/2$  at the center ( $N_{\Phi}$  is required by Dirac to be an integer). The relationship between the magnetic field strength and the number of particles is  $N_{\Phi} = N_e/\nu - S$ , where  $S$  is a topological quantum number known as the “shift” [21] and the filling fraction is  $\nu = \lim_{N_e \rightarrow \infty} N_e/N_{\Phi}$ . A fractional quantum Hall (FQH) state will possess rotational invariance (total angular momentum  $L = 0$ ) and an energy gap that remains finite in the thermodynamic limit. Particle-hole symmetry plays a central role in the  $N = 1$  LL since the three-body terms that emerge from LL mixing break this symmetry. Hence, particle-hole conjugated states may have very different physics (the particle-hole conjugate relationship is found through  $N_h = N_{\Phi} + 1 - N_e$ ).

Since we are focusing on  $\nu = 1/3, 2/3$ , and  $1/2$  we will compare the exact ground states of Eq. (1) with the Laughlin [15] state at  $\nu = 1/3$  and its particle-hole conjugate at  $\nu = 2/3$  and the Moore-Read (MR) Pfaffian [18] and anti-Pfaffian [22,23] states at  $\nu = 1/2$ . These FQH states correspond to shifts of  $S = 3$  and  $0$  for the Laughlin

$1/3$  and  $2/3$  states, respectively, and  $S = 3$  and  $-1$  for the MR Pfaffian and anti-Pfaffian, respectively.

We consider only fully spin- and valley-polarized states so our results apply to experimental configurations in which spin and valley degeneracy are explicitly broken, for example, by the substrate or in bilayer graphene [24–27]. However, the single particle dispersion in bilayer graphene is quadratic compared to the linear dispersion in monolayer graphene; thus, we caution the reader that our results might only be qualitatively applicable there. Reference [25] provided an explanation for the recent experimental observation of a  $1/2$ -filled FQHE in bilayer graphene [24] but was unable to distinguish MR Pfaffian from anti-Pfaffian. Perhaps our work can shed some light on that question. Our results also apply to those states in which spin and valley polarization occurs spontaneously—or nearly spontaneously, since weak  $SU(4)$  symmetry-breaking effects are present [28,29]. It is beyond the scope of the present work to study physics that leads to spin and valley polarization or to study states not fully polarized [30–32]. The three-body terms in Eq. (1), while not increasing the Hilbert space dimension, drastically decrease the sparsity of the Hamiltonian matrix. While adding spin is possible and will be done in a future study [33], adding spin and valley degrees of freedom is numerically prohibitive. It is likely only possible to consider system sizes on the order of six particles while including both effects. Hence, these two effects, in the context of exact diagonalization, will have to await further studies and/or further numerical and theoretical breakthroughs.

Before describing our results, we describe the connection between the filling factor  $\nu$  in our calculations and the observed Hall conductance  $\sigma_{xy} = f(e^2/h)$ . We model electrons with filling fraction  $\nu$  in the  $N$ th LL by considering electrons at  $\nu$  in the  $N = 0$  LL and account for  $N \neq 0$  by modifying the Haldane pseudopotentials appropriately. Because of particle-hole symmetry about  $N = 0$ , the Hall conductance  $f$  is related to the Landau level  $N$  and its fractional filling  $\nu$  according to  $f = 4N - 2 + k + \nu$ . The factor of 4 is due to the spin and valley degrees and  $k = 0, 1, 2, 3$  labels the possible spin and valley quantum numbers within a LL. Therefore, our results for  $\nu = 1/3$  and  $N = 0$  apply to  $f = -(5/3), -(2/3), 1/3, 4/3$ , and for  $N = 1$  the corresponding  $f$ 's are  $f = 7/3, 10/3, 13/3, 16/3$ . Meanwhile, our results for  $\nu = 2/3$  and  $N = 0$  apply to  $f = -(4/3), -(1/3), 2/3, 5/3$  and for  $N = 1$  the corresponding  $f$ 's are  $f = 8/3, 11/3, 14/3, 17/3$ . Finally,  $\nu = 1/2$  corresponds, in the  $N = 0$  LL to  $f = -(3/2), -(1/2), 1/2, 3/2$  and, in the  $N = 1$  LL, to  $f = 5/2, 7/2, 9/2, 11/2$ . On the hole side, for  $N = -1$ , one simply transforms all  $f \rightarrow -f$ .

*Results.*—We first report our results and then provide justification. We conclude that (i) LL mixing has a large qualitative effect on the FQHE in the  $N = 1$  LL. The  $\nu = 1/3$  FQHE ( $f = 7/3, 10/3, 13/3, 16/3$ ) survives

even with strong LL mixing, but the particle-hole conjugate state at  $\nu = 2/3$  ( $f = 8/3, 11/3, 14/3, 17/3$ ) does not. We predict a FQHE state in the  $\nu = 1/2$  filled  $N = 1$  LL that is likely in the universality class of the anti-Pfaffian state [22,23]. (ii) The FQHE in the  $N = 0$  LL of graphene is nearly identical to the FQHE in the  $N = 0$  LL in semiconductor heterostructures even in the presence of strong LL mixing. Amusingly, the FQHE in the  $N = 0$  LL in graphene is more like the minimal theoretical model than semiconductor systems: graphene has no finite-thickness modification of the Coulomb potential, and LL mixing does not generate three-body terms as a result of particle-hole symmetry. As such, the  $\nu = 1/2$  case is found to be, as in semiconductor heterostructures, a composite fermion Fermi sea [17,34,35].

*Graphene FQHE in half-filled Landau levels.*—In Figs. 1(a)–1(c) we show the numerical wave function overlap between the exact ground state of the effective Hamiltonian in Eq. (1) for  $\nu = 1/2$  in the  $N = 0$  and  $N = 1$  LLs and the Moore-Read Pfaffian ( $N_\Phi = 2N_e - 3$ ) and anti-Pfaffian ( $N_\Phi = 2N_e + 1$ ) wave functions as a function of the LL mixing parameter  $\kappa$ . For  $N = 0$  we do not consider the overlap with the anti-Pfaffian wave function since there are no particle-hole symmetry breaking three-body terms; i.e., the MR Pfaffian and anti-Pfaffian are degenerate. For the lowest LL [Fig. 1(a)] the overlap is relatively insensitive to LL mixing until approximately

$\kappa \sim 2$  when it increases slightly before collapsing to zero. In fact, this behavior and others not shown are consistent with previous results for  $\nu = 1/2$  in the lowest LL of semiconductor systems [35]. In contrast, in the  $N = 1$  LL [Fig. 1(b)], LL mixing increases the overlap between the ground state and the anti-Pfaffian to a maximum above 0.93 while the overlap with the MR Pfaffian monotonically decreases. The latter phenomenon is the opposite of what happens in the case of GaAs in the  $N = 1$  LL [36]. The dramatic effect of the LL mixing induced three-body terms can be seen if one considers only the two-body terms in Eq. (1). In that case, the behavior is qualitatively similar to the  $N = 0$  LL [Fig. 1(c)].

Next we calculate the FQHE energy gap (for a presumed paired state) for a far-separated quasiparticle and quasihole pair (an exciton), which is the difference between the lowest energy at  $L = N_e/2$  for  $N_e/2$  even and  $L = N_e/2 - 1$  for  $N_e/2$  odd and the absolute ground state at  $L = 0$ . If the ground state does not have  $L = 0$  the gap is taken to be zero. This method avoids some aliasing problems inherent in finite sized FQHE studies and is a useful alternative to a computation comparing ground state energies for different values of flux  $N_\Phi$  [37]. But even with this method we still ignore the  $N_\Phi = 21$  state when calculating the gap since it is aliased with an Abelian composite fermion state [16,17]. Interestingly, the FQHE energy gap is a nonmonotonic function of  $\kappa$ ; a maximum is obtained around  $\kappa \sim 0.5 \sim 0.7$  [Fig. 1(d)].

*Graphene FQHE in 1/3- and 2/3-filled Landau levels.*—Figures 2(a) and 2(b) show the overlap between the Laughlin wave function or its particle-hole conjugate and the exact ground state of Eq. (1) at  $\nu = 1/3$  or  $2/3$  in the  $N = 0$  and  $N = 1$  LLs, i.e.,  $N_\Phi = 3N_e - 3$  or  $N_\Phi = 3N_e/2$ , respectively. Again, for  $N = 0$  we only show overlaps with the Laughlin wave function at  $1/3$

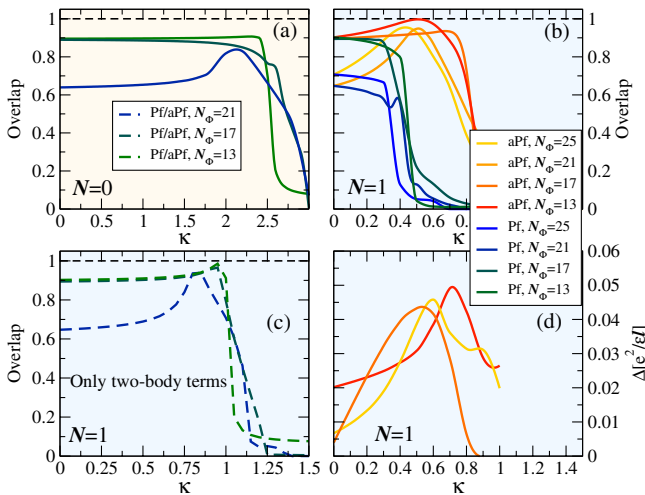


FIG. 1 (color online). The wave function overlaps between the exact ground state of Eq. (1) and the MR Pfaffian and anti-Pfaffian as a function of LL mixing ( $\kappa$ ) for the (a)  $N = 0$  and (b)  $N = 1$  LLs. The FQHE energy gap (exciton energy, i.e., a far separated quasiparticle and quasihole) for the  $N = 1$  LL in units of  $e^2/\epsilon\ell$  as a function of  $\kappa$  is shown in panel (d). Note that the  $N_\Phi = 21$  system is aliased with a composite fermion state at  $\nu = 4/9$ ; hence, these results are ambiguous and not included. Finally, panel (c) shows wave function overlaps in the  $N = 1$  LL for the exact ground state of Eq. (1) excluding any particle-hole symmetry breaking three-body terms demonstrating its qualitative similarity with the  $N = 0$  LL.

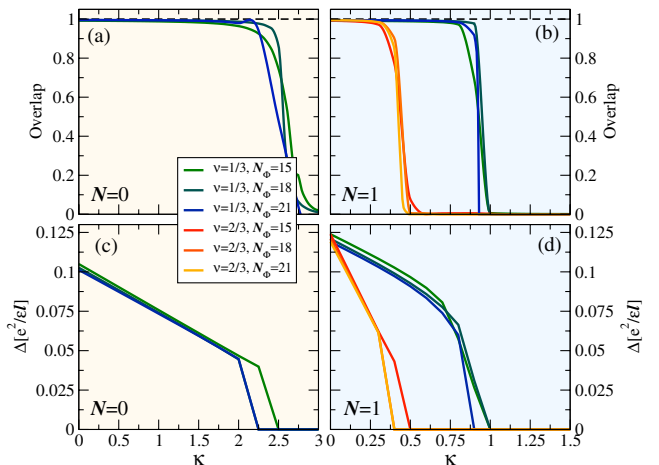


FIG. 2 (color online). The wave function overlaps between the exact ground state of Eq. (1) and the Laughlin state as a function of LL mixing ( $\kappa$ ) for the (a)  $N = 0$  and (b)  $N = 1$  LLs. Panels (c) and (d) show FQHE excitation gaps (defined in the text) for the  $N = 0$  and  $N = 1$  LLs in units of  $e^2/\epsilon\ell$  as a function of  $\kappa$ .

since there are no three-body terms present to break particle-hole symmetry. The overlap remains very large ( $\sim 0.99$ ) until  $\kappa \approx 2$  where it abruptly drops to zero. In the  $N = 1$  LL, we find that LL mixing breaks particle-hole symmetry for modest values of  $\kappa$  and the overlaps with the Laughlin wave function at  $1/3$  and  $2/3$  markedly diverge; the  $1/3$  overlap remains  $\sim 0.99$  until  $\kappa \sim 1$  while the  $2/3$  overlap remains large only until  $\kappa \sim 0.4$ .

In Figs. 2(c) and 2(d) we calculate the FQHE energy gap as the difference between the lowest energies at  $L = N_e$  and  $L = 0$  (unpaired excitation). The gap decreases monotonically with  $\kappa$  for  $N = 0$  until collapsing to zero around  $\kappa \sim 2$  coinciding with the  $\kappa$  where the overlap vanishes. For  $N = 1$  we find that the gap decreases monotonically with  $\kappa$  until the overlaps and gaps collapse to zero simultaneously. The  $1/3$  state survives much stronger LL mixing (to  $\kappa \sim 1$ ) while the  $2/3$  state does not (the overlap and gap vanish at  $\kappa \sim 0.4$ ).

*FQHE gaps in the thermodynamic limit and experimental comparison.*—Last, we show the FQHE gaps extrapolated to the thermodynamic limit for  $\nu = 1/3, 2/3$ , and  $1/2$  in the  $N = 0$  and  $N = 1$  LL (Fig. 3). If  $\kappa = e^2/ev_F\hbar$  is varied in an experiment, by changing the dielectric constant  $\epsilon$ , then the energy gap must be plotted in units of the changing scale  $e^2/\epsilon\ell$  (or else the scale must be held constant by simultaneously varying  $B$ ). Consider two examples. (1) In Ref. [4], the energy gap of  $f = 1/3$  was measured to be  $\Delta_{\text{exp}} \sim 60$  K at  $B = 14$  T in a suspended sample with  $\kappa = 2.2$ . As shown in Fig. 3, the calculated gap is  $\Delta_{\text{calc}} \sim 0.035e^2/\epsilon\ell$ . Since  $\epsilon = 1$  for a suspended sample, this corresponds to  $\Delta_{\text{calc}} \sim 85$  K,

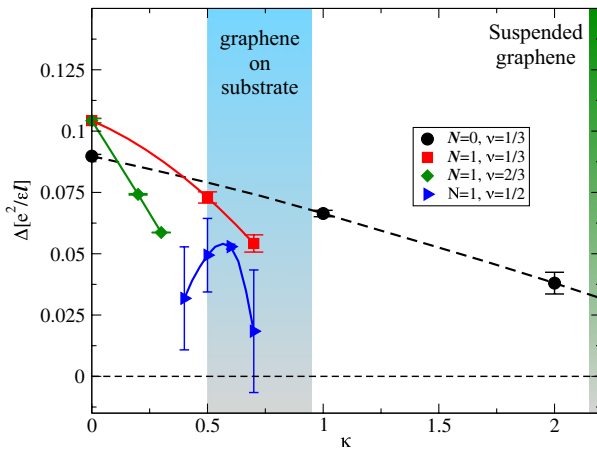


FIG. 3 (color online). FQHE energy gaps extrapolated to the thermodynamic limit as functions of  $\kappa$  for  $\nu = 1/3$  and  $2/3$  in the  $N = 0$  and  $N = 1$  LLs and  $\nu = 1/2$  in the  $N = 1$  LL. The  $1/3$  and  $2/3$  gaps decrease with  $\kappa$  while at  $\nu = 1/2$  the gap shows a maximum in  $\kappa$  at approximately the same value where the overlap with the anti-Pfaffian is maximum [see Fig. 1(b)]. The lines are merely a guide to the eye and the colored boxes indicate the approximate range of  $\kappa$  for graphene on a substrate (blue) and suspended graphene (green).

which differs from the experimental result by a factor of approximately 1.5. Considering that we have neglected the effects of disorder, this is an encouraging result. (2) In Ref. [2],  $\Delta_{\text{exp}} \sim 12$  K at  $B \sim 28$  T for  $f = 4/3$ . Taking  $\kappa = 0.5$  and  $\epsilon \sim 5$ , our calculations yield  $\Delta \sim 50$  K—a factor of about 5 too large. Perhaps this poorer estimate stems from different disorder characteristics of graphene on a substrate and/or the neglect of spin and valley degrees of freedom [31].

*Conclusions.*—Our conclusions are as follows. (i) When spin and valley degeneracy are broken, the FQHE in the  $N = 0$  LL of graphene is expected to be nearly identical to the  $B \rightarrow \infty$  minimal model of the FQHE (pure Coulomb Hamiltonian) as long as  $\kappa \leq 2$ . Thus, all of the known results in the  $N = 0$  LL for semiconductor systems transfer to graphene nearly perfectly even in the presence of LL mixing. (ii) The FQHE is expected in the  $N = 1$  LL for moderate values of  $\kappa$ —which might be expected on boron nitride and  $\text{SiO}_2$  substrates but not in suspended samples where LL mixing is too strong. We find strong particle-hole symmetry breaking in the  $N = 1$  LL, leading to stark differences between the  $1/3$  FQHE and the particle-hole symmetric partner at  $2/3$ ; i.e., the  $1/3$  state would exist in a system with  $\kappa = 0.7$  and the  $2/3$  state might not. (iii) Intriguingly, we find the anti-Pfaffian state to be stabilized in the  $N = 1$  LL for moderate values of  $\kappa \sim 0.25$ – $0.75$ . The MR Pfaffian, on the other hand, is disfavored by LL mixing.

While our results predict that the  $\nu = 1/3$  and  $2/3$  states will be related by symmetry in the  $N = 0$  LL and the latter will be suppressed in the  $N = 1$  LL, the experimental situation is more complicated. In the  $N = 0$  LL, odd-numerator states are generally suppressed. However, this is likely due to the presence of low-energy Skyrmion excitations in a spontaneously spin- and valley-polarized state [31,38,39]; however, LL mixing is known to generally effect Skyrmion excitations [40,41]. When the valley symmetry is explicitly broken, for example, by a substrate or with an applied electric field in a bilayer system, odd numerator states are strengthened. In the  $N = 1$  LL, the  $\nu = 7/3$  state is stronger than the  $\nu = 8/3$  state, in agreement with our calculations, yet the  $\nu = 11/3$  and  $10/3$  states have comparable gaps [2], similar to the experimental observations of the  $\nu = 7/3$  and  $8/3$  gaps in GaAs semiconductors. Last, we note that a  $1/2$ -filled FQH state has only been experimentally observed in bilayer graphene [24] and so far no experimental groups have definitively observed a  $1/2$ -filled state in the  $N = 1$  LL in monolayer graphene unlike in GaAs. We hope our work will motivate more experimental investigations in graphene.

The FQHE in graphene provides a diverse playground where interplay between LL mixing, disorder, and spin and valley degrees of freedom lead to rich and surprising physics. In this work, we have focused on the effects of LL mixing.

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