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Activation gaps for the fractional quantum Hall effect: realistic treatment of transverse thickness

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Abstract. The activation gaps for fractional quantum Hall states at filling fractions $\nu = n/(2n+1)$ are computed for heterojunction, square-quantum-well, and parabolic-quantum-well geometries, using an interaction potential calculated from a self-consistent electronic structure calculation in the local density approximation. The finite thickness is estimated to make a $\sim$30% correction to the gap in the heterojunction geometry for typical parameters, which accounts for roughly half of the discrepancy between the experiment and theoretical gaps computed for a pure two-dimensional system. Certain model interactions are also considered. It is found that the activation energies behave qualitatively differently depending on whether the interaction is of longer or shorter range than the Coulomb interaction; there are indications that fractional Hall states close to the Fermi sea are destabilized for the latter.

1. Introduction

A fundamental aspect of the phenomenon of the fractional quantum Hall effect (FQHE) [1] is the existence of a gap at certain Landau level fillings in the excitation spectrum for a disorder-free system, which is responsible for properties like fractional charge and the fractionally quantized Hall resistance [2]. An understanding of the physical origin of the gap lies at the heart of the FQHE problem.

The composite-fermion (CF) theory [3–5] gives a simple intuitive explanation for the existence of the gaps. First, electrons capture an even number of vortices to become composite fermions, since this is how they can best screen the repulsive interaction. As a consequence of the phases produced by the vortices, composite fermions experience a reduced effective magnetic field. They form Landau levels (LLs) in the reduced magnetic field, called CF-LLs in order to distinguish them from the Landau levels of electrons. A gap in the excitation spectrum occurs whenever composite fermions fill an integer number of CF-LLs. This provides an excellent description of the phenomenology of the FQHE; in particular, it gives a simple explanation for the observed fractions at $\nu = n/(2pn \pm 1)$, which correspond simply to n filled LLs of composite fermions carrying $2p$ vortices. Thus, an effectively single-particle description of the strongly correlated electron liquid becomes possible in terms of composite fermions. The CF physics was spectacularly confirmed also in tests against exact results known for finite systems from numerical diagonalization studies. The CF wave functions were found to have close to 100% overlap with the exact eigenfunctions, and predicted energies with an accuracy of better than 0.1% for systems of up to 12 particles [4, 6]. A comparison with exact-diagonalization results established that the gaps predicted by the CF theory are accurate to within a few per cent. However, it is only relatively recently that it has become possible

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to make more detailed quantitative comparisons between theory and experiment. The main hurdle was the lack of a suitable method for dealing with large systems of composite fermions. In recent years we have developed a technique [7] that allows us to carry out Monte Carlo calculations on systems containing as many as 60 composite fermions, which are sufficiently large for obtaining reliable information on FQHE states at least up to 6/13. This paper reports on the results of our Monte Carlo calculations for the gaps of various FQHE states, extending our previous work [8] as well as correcting some of the assertions made therein. The main new feature in this work is that we take account of the non-zero thickness of the electron system by determining the effective interaction within the self-consistent local density approximation (LDA). The calculations contain no adjustable parameters; the only inputs are the shape of the confinement potential (heterojunction, square quantum well, or parabolic quantum well) and the electron density.

There is a long history of calculation of gaps in the FQHE, dating back to the work of Laughlin [2]. Accurate estimates for the gap of the FQHE state at $\nu = 1/3$ for a strictly two-dimensional (2D) system, where the interaction between electrons is of 'pure Coulomb' form (as opposed to an 'effective' interaction after non-zero thickness is taken into account), were obtained by Morf and Halperin [9] in a Monte Carlo calculation, using the variational wave functions of Laughlin, and by Haldane and Rezayi [10] from small-system, exact-diagonalization calculations. For lack of accurate wave functions, the gaps of other FQHE states could be estimated initially only from exact-diagonalization calculations [11]. However, as one goes along the sequence $\nu = n/(2n+1)$, it takes larger and larger numbers of particles to get reliable values for the gaps; since the size of Hilbert space increases exponentially with N, the exact-diagonalization studies are of little use for large n. For example, only two systems can be studied at present for 3/7 (with 9 and 12 particles), and no exact diagonalization is possible for 4/9, which requires at least 16 particles. The gaps for the pure Coulomb interaction were computed by Jain and Kamilla [7] for several FQHE states within the framework of the composite-fermion theory, which we believe to provide accurate estimates for an idealized zero-thickness system with no disorder.

It has been well known for quite some time that while the pure Coulomb gaps do give a rough estimate of the magnitude of the experimental gaps, certain quantitatively significant effects present in real experiments must be incorporated for a more detailed comparison. While these do not require any new conceptual input, it is important to ascertain the relative importance of these effects, and to convince ourselves that we are not missing any physics. The aim of this work is to investigate one of these effects, namely the modification in the inter-electron interaction originating from the finite transverse extent of the electron wave function, in as much detail as is possible at the present. Since the early calculations of Zhang and Das Sarma (ZDS) [12] and Yoshioka [13], much of the work dealing with the finite thickness has employed model interaction potentials, e.g. the ZDS potential $e^2/(\lambda^2 + r^2)^{1/2}$, which simulate the effect of non-zero thickness by softening the interaction at short distances. The parameter characterizing the thickness in these potentials must be determined from other considerations. Very recently, Ortalano *et al* [14] carried out a calculation of the gap at 1/3 by feeding into their exact-diagonalization study the interaction that they obtain from a self-consistent LDA calculation. Park and Jain [8] computed the gaps of various other FQHE states using the ZDS model, fixing the thickness parameter λ by requiring that the gap for the 1/3 state agree with that obtained by Ortalano *et al*. This produced an excellent agreement between the theoretical and experimental gaps. However, a comparison with the more realistic Stern–Howard [15, 16] interaction led Morf [17] to conclude that the value of the λ used in this work was too large by approximately a factor of two, and therefore the comparison with experiment was not valid and the agreement fortuitous. To resolve this issue, and also to obtain reliable values for the gaps,

we have computed the gaps directly from the interaction obtained from the self-consistent LDA. It is found that the non-zero thickness makes a 20–50% correction for typical experimental parameters, reducing the discrepancy between pure 2D theory and experiment approximately by half, but the theoretical gaps still significantly overestimate the gaps [18].

There are other effects that will diminish the gaps beyond their values obtained in the present work. One assumption here is that the electronic states are confined to the lowest LL, which is indeed a valid approximation in the limit of sufficiently large magnetic fields, but, at typical experimental fields, Landau level mixing may not be negligible. It is expected that the CF particle and hole excitations will lower their energies by an admixture with higher Landau levels. Previous estimates [19] suggest that it is roughly a 20% effect. The omnipresent disorder, neglected in the present study, is also expected to reduce the gaps. A reliable theoretical treatment of these issues is beyond the scope of the present work.

We also calculate gaps for different kinds of model potentials, some differing from the Coulomb interaction in the short-distance behaviour and others in the long range. The qualitative behaviours give an indication of a relation between the range of the potential and the stability of the CF sea.

The paper is organized as follows. In section 2, we give a brief account of the computational methods, mentioning, in particular, certain modifications in the self-consistent LDA in this work, appropriate for the problem at hand; a summary of the CF wave functions and the Monte Carlo method is also given. Section 3 gives our results for gaps for various densities in three sample geometries: heterojunction, square quantum well, and parabolic quantum well. Section 4 discusses a comparison of our results with experiment, Section 5 contains gaps for several model interactions, and the paper is concluded in section 6.

2. Computational details

For completeness, we provide a brief outline of our computational methods. Readers interested in further details can find them in the literature.

2.1. Self-consistent LDA

Following the standard approach [16, 20], one solves self-consistently the one-dimensional Schrödinger and Poisson equations for the direction perpendicular to the plane of the 2D electron system (taken along the z-axis here):

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}z^2} + V_{eff}(z)\right)\xi(z) = E\xi(z) \tag{1}$$

$$V_{eff}(z) = V_W(z) + V_H(z) + V_{XC}(z) \tag{2}$$

$$\frac{\mathrm{d}^2 V_H(z)}{\mathrm{d}z^2} = -\frac{4\pi e^2}{\epsilon}[\rho(z) - \rho_I(z)] \tag{3}$$

$$\rho(z) = N|\xi(z)|^2. \tag{4}$$

Here, V_H, V_W, and V_{XC} are the Hartree, confinement, and exchange–correlation potentials, and ρ_I is the density of the ionized donor atoms. The exchange–correlation potential is assumed to depend only on the local density, which is usually a quite reasonable approximation.

The equations above have been slightly modified from the ones used at zero magnetic field [14] to suit our present purpose. In the past, it has been assumed that the effective potential was not significantly affected by application of the magnetic field, and the zero-field effective interaction was used for high magnetic fields as well [14]. We make a few changes

from the standard zero-field calculation, which we believe are appropriate when discussing electrons confined to the lowest Landau level. These are as follows:

(i) At zero magnetic field, electrons occupy one or several subbands depending on the density. In our calculations below, we assume that they occupy only one subband. This would clearly be unphysical for sufficiently large densities at zero magnetic field, but is appropriate at large magnetic fields, where only the lowest LL is occupied. This makes no difference at low densities, when the self-consistent solution at zero field also involves only one subband, but the results are affected somewhat at large densities. We have not investigated how much of a quantitative difference this alteration makes at high densities.

(ii) We assume that electrons are fully polarized. This of course is motivated by the fact that we are interested in fully polarized electronic states, which is appropriate for sub-unity filling factors at high magnetic fields.

We further make the following approximations.

(iii) For the exchange–correlation energy we use the form given by Vosko *et al* [21] rather than the more usual one by Hedin and Lundqvist [22], the former being more appropriate for spin-polarized electrons. This does not make appreciable quantitative difference; in fact, leaving out the exchange–correlation corrections entirely is also a rather good approximation for the present problem.

(iv) In heterojunctions, the electron wave function has a small amplitude on the AlGaAs side, with most of the wave function being confined to the GaAs side. A proper treatment will require taking a position-dependent dielectric function as well as a position-dependent mass, and replacing the step function change in these quantities at the interface by a smooth function in order to ensure that the calculations are technically well controlled [20]. In order to avoid these complications, we have assumed that the wave function is entirely confined on one side of the junction; this was found to be an excellent approximation in earlier calculations [20]. Similarly, for the quantum well potential, we have assumed infinite barriers, keeping electrons out of the insulator. This should be a reasonable approximation provided the electron energies are deep in the well.

(v) The depletion charge density in experimental samples is unknown, but often small [23]; we have set it to zero in our calculations. This may not be a good approximation especially when the electron density becomes comparable to the depletion layer charge density. Image charge effects due to a slight mismatch of the dielectric function at the interface have also been neglected.

The above equations are solved by an iterative procedure until convergence is obtained for $\xi(z)$. The effective interaction potential is then given by

$$V_{LDA}(r) = \frac{e^2}{\epsilon}\int \mathrm{d}z_1 \int \mathrm{d}z_2 \, \frac{|\xi(z_1)|^2|\xi(z_2)|^2}{[r^2 + (z_1 - z_2)^2]^{1/2}}. \tag{5}$$

The LDA interaction for the heterojunction geometry is shown in figure 1.

2.2. Composite-fermion wave functions

We compute the energy gaps by evaluating the expectation values of the effective interaction energy $V = \sum_{j<k} V_{LDA}(r_{jk})$ in the composite-fermion wave functions for the ground and excited states:

$$\Delta = \frac{\langle \Phi^{CF-ex}|V|\Phi^{CF-ex}\rangle}{\langle \Phi^{CF-ex}|\Phi^{CF-ex}\rangle} - \frac{\langle \Phi^{CF-gr}|V|\Phi^{CF-gr}\rangle}{\langle \Phi^{CF-gr}|\Phi^{CF-gr}\rangle} \tag{6}$$

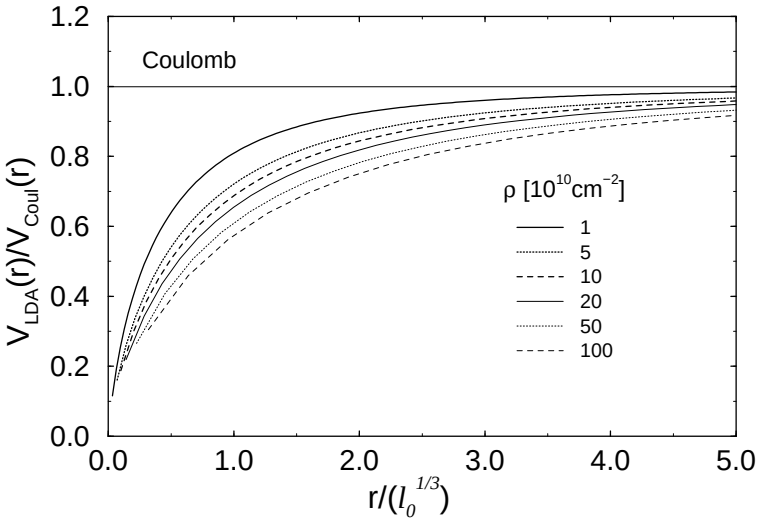

Figure 1. The effective interaction, $V_{LDA}(r)$ for the heterojunction geometry for densities ranging from 1.0×10^{10} cm^{-2} to 1.0×10^{12} cm^{-2}. The interaction is shown in units of the Coulomb interaction and the distance is given in units of the magnetic length at $\nu = 1/3$, $l_0^{1/3}$.

where Φ^{CF-ex} and Φ^{CF-gr} are the CF wave functions for the excited and the ground states, respectively.

We use the spherical geometry in this work, which considers N electrons on the surface of a sphere, moving under the influence of a strong radial magnetic field. Fully spin-polarized electrons and a complete lack of disorder are assumed. The flux through the surface of the sphere is defined to be $2Q\phi_0$, where $\phi_0 = hc/e$ is the flux quantum and $2Q =$ integer. The single-particle eigenstates are the monopole harmonics [24], denoted by $Y_{Q,n,m}(\Omega)$, where $n = 0, 1, \ldots$ is the LL index, $m = -Q - n, -Q - n + 1, \ldots, Q + n$ labels the $2Q + 2n + 1$ degenerate states in the nth LL, and Ω represents the angular coordinates θ and ϕ.

According to the CF theory [3], the problem of interacting electrons at Q is equivalent to that of weakly interacting composite fermions at effective monopole strength $q = Q - p(N-1)$. The many-body CF states can be constructed from the following 'single-CF' wave functions [7]:

$$Y^{CF}_{q,n,m}(\Omega_j) = \tilde{Y}_{q,n,m}(\Omega_j)\prod_k{}'(u_j v_k - v_j u_k)^p \tag{7}$$

$$\tilde{Y}_{q,n,m}(\Omega_j) = N_{qnm}(-1)^{q+n-m}\frac{(2S+1)!}{(2S+n+1)!}u_j^{q+m}v_j^{q-m} \times \sum_{s=0}^{n}(-1)^s\binom{n}{s}\binom{2q+n}{q+n-m-s}u_j^s v_j^{n-s}\mathcal{U}_j^s\mathcal{V}_j^{n-s} \tag{8}$$

$$N^2_{qnm} = \frac{(2q+2n+1)}{4\pi}\frac{(q+n-m)!(q+n+m)!}{n!(2q+n)!} \tag{9}$$

$$\mathcal{U}_j = p\sum_k{}'\frac{v_k}{u_j v_k - v_j u_k} + \frac{\partial}{\partial u_j} \tag{10}$$

$$\mathcal{V}_j = p\sum_k{}'\frac{-u_k}{u_j v_k - v_j u_k} + \frac{\partial}{\partial v_j}. \tag{11}$$

Here the prime denotes the condition $k \neq j$, p is an integer, $S = q + p(N-1)/2$, and the spinor coordinates are defined as [25]

$$u_j \equiv \cos(\theta_j/2)\exp(-\mathrm{i}\phi_j/2) \qquad v_j \equiv \sin(\theta_j/2)\exp(\mathrm{i}\phi_j/2).$$

The binomial coefficient $\binom{\alpha}{\beta}$ is to be set to zero if $\beta > \alpha$ or $\beta < 0$. The subscript n in $Y^{CF}_{q,n,m}$ labels the CF-LL index. Note that the wave function of the jth composite fermion involves the coordinates of *all* electrons. In the form written above, the CF wave function is fully confined to the lowest electronic LL.

The wave functions for the system of many composite fermions are the same as the corresponding wave functions of non-interacting electrons at q, but with $Y_{q,n,m}$ replaced by $Y^{CF}_{q,n,m}$. The incompressible ground state consists of an integer number of filled LLs of composite fermions. The excited states are constructed by promoting one composite fermion from the topmost occupied CF-LL to the lowest unoccupied CF-LL, which creates a CF particle–hole pair. We are interested in the energy of this excitation in limit where the distance between the CF particle and the CF hole is very large, so we consider the excited state in which they are on the opposite poles of the sphere. Prior to an extrapolation of our results to the limit of $N \to \infty$, we correct for the interaction between the CF particle and the CF hole, which amounts to a subtraction of $-(2p+1)^{-2}/2\epsilon\sqrt{Q}l_0$, the interaction energy for two point-like particles of charges $e/(2p+1)$ and $-e/(2p+1)$ at a distance $2R$, where $R = \sqrt{Q}l_0$ is the radius of the sphere. We also correct for a finite-size deviation of the density from its thermodynamic value, by multiplying by a factor $\sqrt{(\rho/\rho_N)} = \sqrt{(2Q\nu/N)}$, where ρ is the thermodynamic density and ρ_N is the density of the N-particle system.

We emphasize here that both the ground- and excited-state wave functions above *contain no adjustable parameters*; they are completely determined by symmetry in the restricted Hilbert space of the CF wave functions. Also, since the wave functions constructed here are strictly within the lowest *electronic* LL, their energies will provide strict variational bounds. Of course, there is no variational theorem for the energy *difference*, but the CF wave functions are known to be extremely accurate; they produce gaps with an accuracy of a few per cent for a given interaction potential, at least for 1/3, 2/5, and 3/7, for which exact results are known for finite systems. For these fractions, any error in the gaps will owe its origin mainly to various approximations in our calculation of the effective interaction; insofar as finite-width effects are concerned, we expect our gap calculations to be reliable at the level of 20% [14].

An unusual feature of the composite-fermion wave functions is that they are independent of the actual form of the interaction, since they have no parameters to adjust. While this may seem objectionable at first sight, it captures the fact that the *actual* wave functions (as obtained, say, in exact-diagonalization studies) are also largely insensitive to the form of the interaction. This rigidity against perturbations can be understood physically by analogy to the integer QHE. The electron wave functions at integer filling factors are quite independent of the interaction provided that it is small compared to the cyclotron gap (i.e., LL mixing is negligible). In the CF theory, this would imply that the interaction dependence of the wave function is negligible so long as the residual interaction between the composite fermions is weak compared to the CF cyclotron gap. For the $n/(2n+1)$ states with large n, the CF cyclotron gap may not necessarily be large compared to the inter-CF interactions, and the actual wave functions may have some dependence on the form of the interaction. While the actual wave functions are not known for these states, it may be possible to investigate the issue in a variational approach by incorporating some variational degree of freedom which allows mixing between *CF*-LLs to determine the extent to which the CF wave function is perturbed. We will, however, continue to work with the unperturbed composite-fermion wave functions here, with the caveat that the results may not be completely reliable at large n (we suspect though, that the intrinsic error in

the CF wave function may still be small compared to the uncertainty arising from Monte Carlo methods and from various approximations involved in evaluation of the effective interaction).

2.3. The Monte Carlo method

The Monte Carlo method employed in our work is quite standard. Unfortunately, it is not possible to use in our problem certain clever time-saving techniques for updating fermion Slater determinants [26], since moving a single particle alters all elements of the determinant, due to the strongly correlated nature of the problem (remember, the wave function of each composite fermion depends also on the positions of all other composite fermions). Therefore, we must compute the full Slater determinant at each step, which takes $O(N^3)$ operations rather than $O(N^2)$. However, we are able to improve on the accuracy by moving all particles at each step. We note that the ground- and excited-state energies must be evaluated extremely accurately in order to get a reasonable estimate for the gap, which is an O(1) quantity. We also utilize the fact that the ratio of the gap to a reference gap (say, for the pure Coulomb interaction) has much smaller variance than the gap itself from one Monte Carlo run to another. A typical calculation of the energy gap requires 10^7 Monte Carlo steps, taking up to 200 hours of computer time on a 500 MHz workstation.

Since there are no edges in the geometry being studied, we expect the gap to have a linear dependence on N^{-1} to leading order, which is also borne out by our results. Therefore, we obtain the thermodynamic limit by a linear fit to the finite-system gaps. The error is determined by the standard least-squares method.

3. Results

The only inputs in our calculations are the electron density and the sample geometry. We have computed the gaps for a range of densities (from 1.0×10^{10} cm^{-2} to 1.0×10^{12} cm^{-2}) and for three sample geometries most popular in experiments: heterojunction, square quantum well (SQW), and parabolic quantum well (PQW). All results have been obtained by an extrapolation of the finite-system results to the limit $N^{-1} \to 0$, as shown for the case of $\nu = 2/5$ in figure 2;

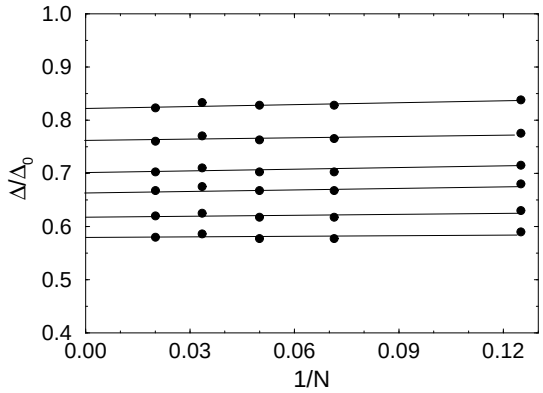

Figure 2. Extrapolation of the activation gap at $\nu = 2/5$ to the thermodynamic ($N^{-1} \to 0$) limit for the heterojunction geometry for densities (starting from top) of 1.0×10^{10} cm^{-2}, 3.0×10^{10} cm^{-2}, 1.0×10^{11} cm^{-2}, 2.0×10^{11} cm^{-2}, 5.0×10^{11} cm^{-2}, and 1.0×10^{12} cm^{-2}. The Monte Carlo uncertainty is smaller than the symbol size and the solid line is the best straight-line fit. Systems of up to 50 composite fermions.

systems of up to 50 particles were considered for the extrapolation. Figures 3, 4, and 5 show the gaps as a function of density for several sample geometries. Since the ratios Δ/Δ_0 are determined quite accurately, as seen in figure 2, the uncertainty in Δ comes almost entirely from Δ_0, for which we use values given in reference [7]. For a typical sample density of 2×10^{11} cm^{-2}, the 1/3 gap is reduced roughly by 30% in a heterojunction, by 30% in a square quantum well of width 300 Å, and by 50% in a parabolic quantum well. As expected, the gaps approach their Coulomb values at small densities in the heterojunction geometry, and also at small QW widths in the quantum well geometries.

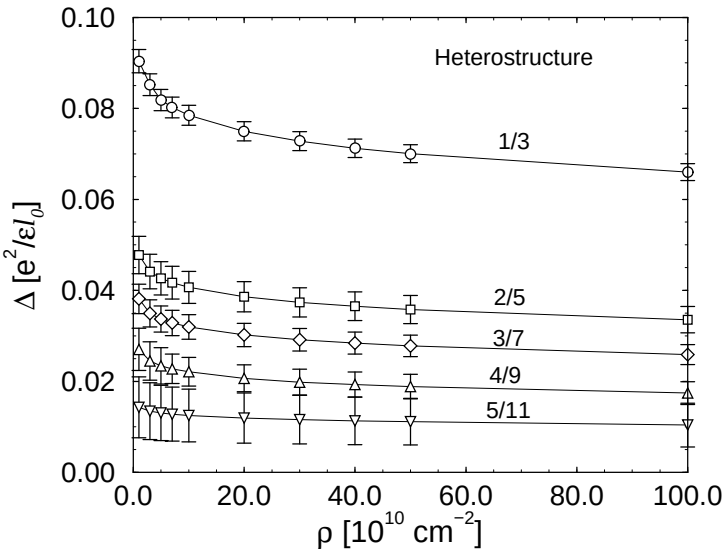

Figure 3. The CF predictions for the gaps in the heterojunction geometry as a function of the density (ρ) ranging from 1.0×10^{10} cm^{-2} to 1.0×10^{12} cm^{-2}, for FQHE states at 1/3, 2/5, 3/7, 4/9, and 5/11, with the filling factors indicated in the figure. The gaps are expressed in $e^2/\epsilon l_0$ where ϵ is the dielectric constant of the background material ($\epsilon \approx 13$ for GaAs) and l_0 is the magnetic length.

A similar calculation for the gap was carried out by Ortalano *et al* for $\nu = 1/3$, who obtain a bigger gap reduction, for reasons that are not known at the moment. The pseudopotentials from our effective interaction are in agreement with theirs, provided the Bohr radius is set equal to the magnetic length. The gaps reported in reference [14] were for a six-particle system whereas we have determined the thermodynamic limit, which may account for part of the discrepancy; also, the result of reference [14] was obtained from an exact diagonalization of the Hamiltonian as opposed to our calculations which employ the CF wave functions, but this ought not to cause more than a few per cent difference.

4. Comparison with experiment

Figure 6 shows a comparison of our results for the heterojunction geometry with experiment for two densities [27]. The finite thickness reduces the gaps from their pure Coulomb values bringing them into better agreement with experiment. Figures 7 and 5 compare our theoretical gaps with experimental gaps in square [28] and parabolic [29] quantum wells. Here, again the gaps are reduced from their pure Coulomb values, but a substantial deviation still remains between theory and experiment.

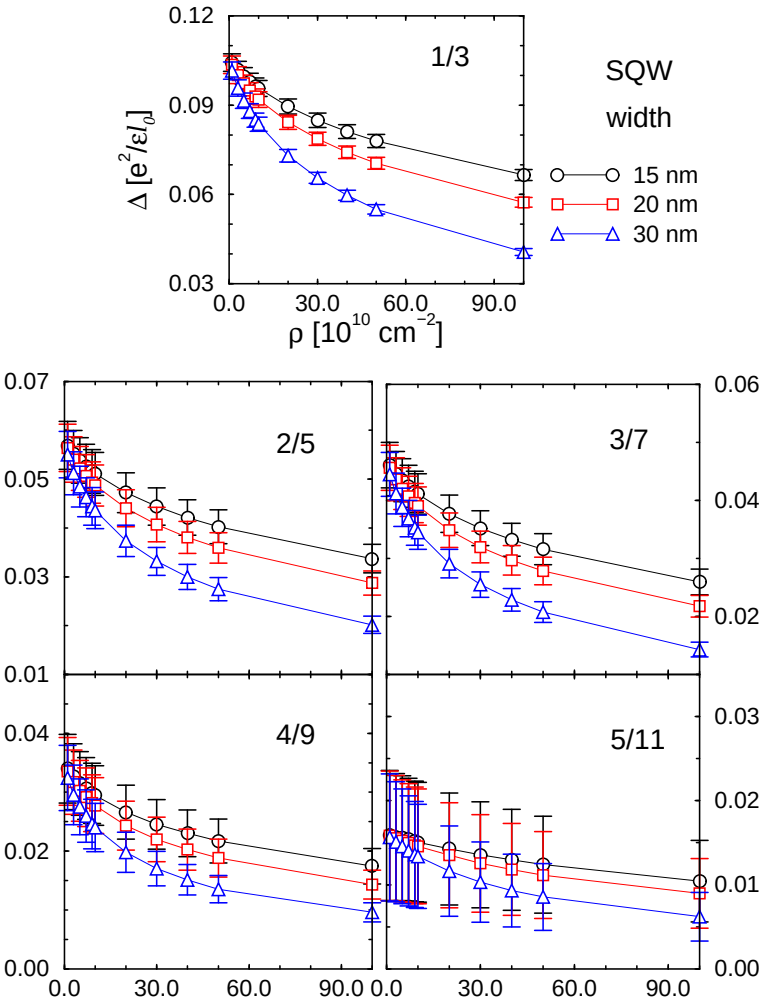

Figure 4. The CF predictions for the gaps in the square-quantum-well (SQW) geometry for densities ranging from 1.0×10^{10} cm^{-2} to 1.0×10^{12} cm^{-2} for quantum well widths of 150 Å, 200 Å, and 300 Å. The filling factors are shown in the figure. The labels for the axes are shown only for 1/3 for convenience.

There are many possible sources that can cause disagreement between our theoretical gaps and the experimental gaps. There are approximations involved in our determination of the effective interaction, which may lead to a 20% uncertainty in the theoretical gap values [14]. Then there are effects left out in the theory, namely Landau level mixing and disorder. Landau level mixing is likely to be most significant in the hole-type samples (the square quantum well here [28]), due to the relatively small cyclotron energy of holes. The disorder is most relevant perhaps in parabolic quantum wells, due to alloy disorder, which leads to relatively low mobilities; the strong suppression of the PQW gaps relative to the computed values indicates that disorder can be rather important quantitatively. In view of this discussion, the comparisons of our results with heterojunction gaps are most meaningful. One message that one can take from these comparisons is that Landau level mixing and disorder also make a sizable correction to the excitation gaps in typical experiments. As mentioned earlier, for 5/11 and 6/13, the

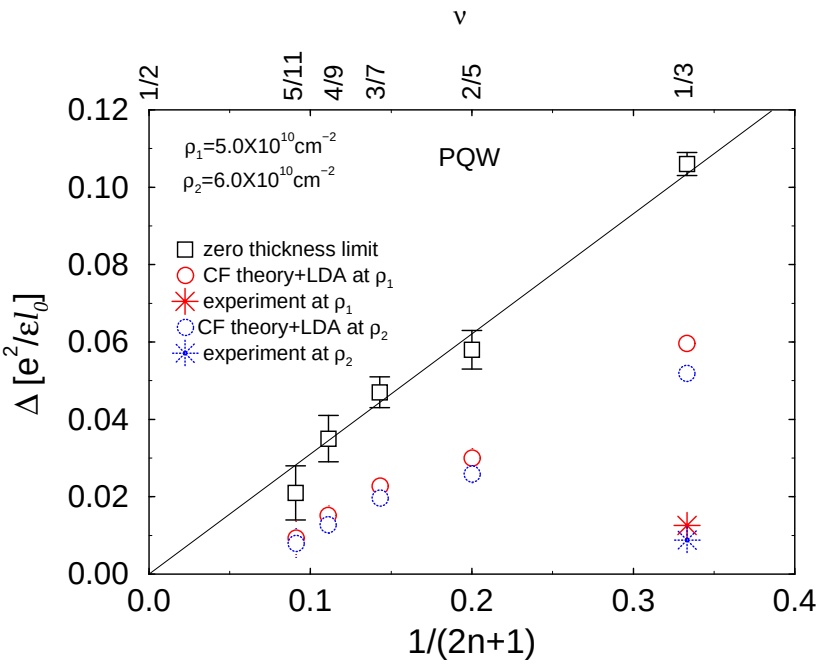

Figure 5. The CF predictions for the gaps in the parabolic-quantum-well (PQW) geometry for two densities 5.0×10^{10} cm^{-2} and 6.0×10^{10} cm^{-2} as a function of filling factor (top axis). The squares are for pure Coulomb interaction, circles for the LDA interaction, and stars are the experimental results taken from Shayegan *et al* [29]. The experimental PQW is 3000 Å wide, with curvature $\alpha = 5.33 \times 10^{-5}$ meV Å^{-2} and barrier height from the bottom $V_0 = 276$ meV. We have set the barrier height to infinity in our LDA calculations.

intrinsic errors in the 'unperturbed' CF wave functions, not yet quantified, may also be partly responsible for the deviations between theory and experiment.

An extrapolation of the experimental gaps suggests that they might vanish at a finite n. Certainly, any finite amount of disorder will cause such a behaviour. However, it is an interesting question whether the gaps will vanish at a finite n even in the absence of disorder. There is no fundamental reason that this could not happen. In our computations, while the Coulomb gaps extrapolate to zero at $\nu = 1/2$, within numerical uncertainty, the non-zero thickness gaps appear to vanish at a finite n (along the sequence $\nu = n/(2n + 1)$), at least for a straight-line fit through them. This is clearest for relatively large gap reductions, e.g. in the heterostructure or the parabolic-quantum-well systems. These results might indeed be indicating an intrinsic absence of FQHE for n larger than a critical value, even for an ideal situation with no Landau level mixing and no disorder. This does not imply, however, that the composite-fermion theory becomes invalid here, but only that composite fermions do not show the integer QHE (IQHE), presumably because the residual inter-CF interactions become increasingly significant as the gap decreases, finally destroying the gap altogether. (We note that for small magnetic fields, the electron system also does not exhibit the IQHE; a better starting point here is the Fermi sea, with the magnetic field treated as a perturbation, rather than a filled Landau level state.) This kind of breakdown of the FQHE, if one actually occurs, will be due to a short-range modification in the inter-electron interaction due to non-zero thickness, to be distinguished from another possibility, discussed in the following section, which has to do with the *long-range* behaviour of the interaction [30].

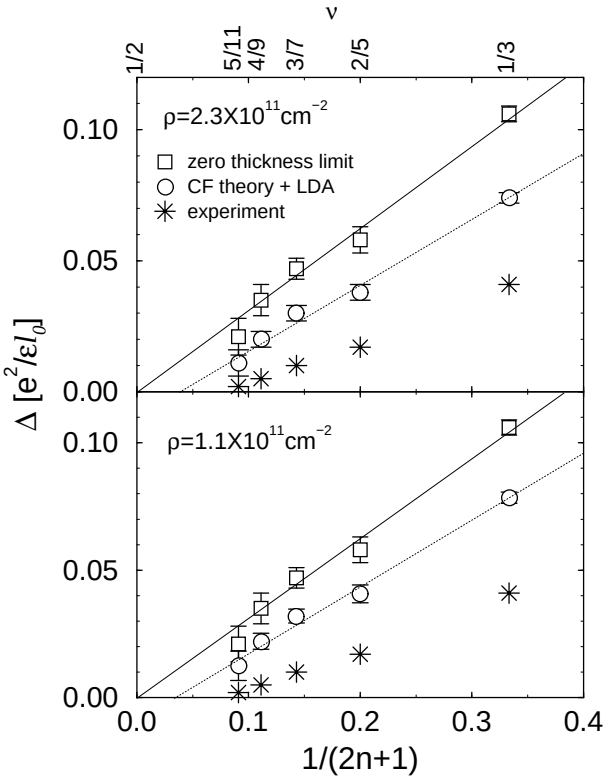

Figure 6. Comparison of the theoretical and the experimental gaps for the heterojunction geometry for two different densities shown in the figures. The squares are for pure Coulomb interaction, circles for the LDA interaction, and stars are taken from the experiment of Du *et al* [27].

The activation gaps can be equated to an effective cyclotron energy to define an effective mass for the composite fermions [30]:

$$\Delta = \hbar \frac{eB^*}{m^* c} = \frac{\hbar^2}{m^* l_0^2} \frac{1}{(2n+1)} \tag{12}$$

where we have used the fact that the effective field for composite fermions is given by $B^* = B/(2n+1)$ at $\nu = n/(2n+1)$. On the other hand, since the gaps are determined entirely by the Coulomb interaction (the only energy in the lowest LL constrained problem), they must be proportional to e^2/l_0, implying that $m^* \sim \sqrt{B}$. This would suggest that the gaps, measured in units of $e^2/\epsilon l_0$, are proportional to $(2n+1)^{-1}$, consistent with the behaviour found in our calculations for the Coulomb interaction. However, for the realistic gaps, the effective mass has some filling factor dependence. Figure 8 shows the effective mass determined from our theoretical gaps, along with the effective mass deduced from an analysis of the resistance oscillations at small B^* in terms of Shubnikov–de Haas oscillations of ordinary fermions [31, 32]. The experimental effective mass is seen to increase with n [32, 33]; our results suggest that part of the increase may be caused by the short-distance softening of the Coulomb interaction due to non-zero sample thickness. A logarithmic divergence of the mass predicted by the Chern–Simons approach [30] has a different physical origin; it is governed by the long-distance behaviour of the interaction.

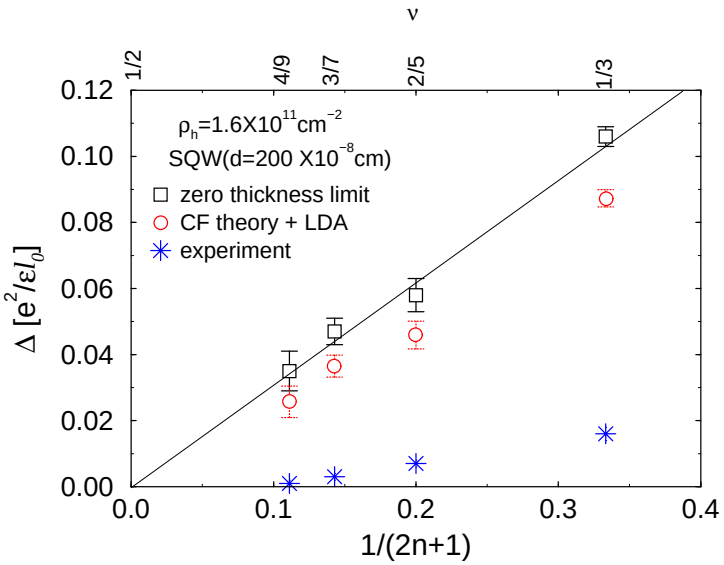

Figure 7. Comparison of the theoretical and the experimental gaps for the square-quantum-well geometry. The squares are for pure Coulomb interaction, circles for the LDA interaction, and stars are taken from Manoharan *et al* [28].

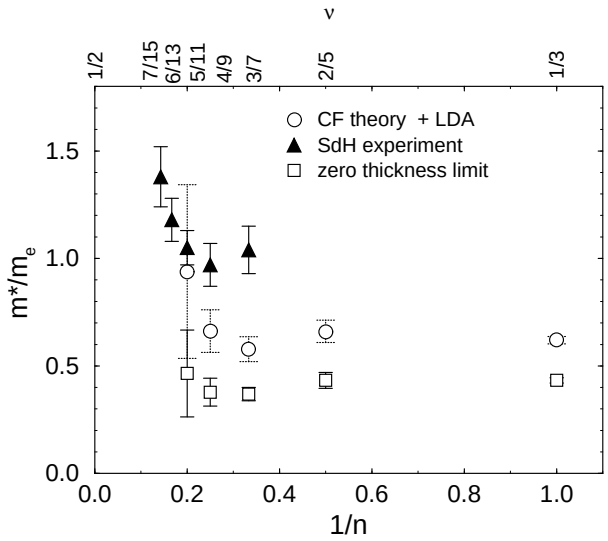

Figure 8. The mass of the composite fermion (m^*) in units of the mass of the electron in vacuum (m_e) as a function of the filling factor for a heterojunction sample with density 2.3×10^{11} cm^{-2}. Both the mass computed from the theoretical gaps in figure 6 (circles for the realistic calculation, squares for zero transverse thickness) and that deduced from an analysis of the SdH experiment (triangles, from Du *et al* [32]) are shown.

5. Model interactions

Model interactions have been used in the past to study finite-thickness effects. There are other reasons for investigating how the gaps behave for various types of interaction. First,

certain analytical approaches find some forms of interaction more tractable, and our Monte Carlo results provide a test for their validity [34]. Second, the Chern–Simons field theoretical formulation of composite fermions finds that the CF Fermi sea behaves qualitatively differently depending on whether the interaction is of shorter or longer range than the Coulomb one [30]; there are infrared singularities in the self-energy for the former, indicating a divergent effective mass for composite fermions; for Coulomb interaction, a logarithmic behaviour is predicted, whereas no divergence occurs for interactions that are of longer range than the Coulomb one. It is plausible that some indication of this physics may be seen away from the CF sea, in the FQHE regime. Finally, it may also be possible to actually change the form of the interaction, e.g., by fabricating the 2D electron gas close to a parallel conducting plane. Motivated by these considerations, we have computed the gaps for various kinds of repulsive interaction: $1/r^2$; logarithmic ($\ln 1/r$), Gaussian ($\exp(-r^2/2)$), Yukawa ($\exp(-r)/r$), and ZDS ($e^2/\sqrt{(r^2+\lambda^2)}$).

The finite-size extrapolations for the gaps are shown in figure 9 for the r^{-2}-interaction. Figure 10 depicts the gaps for various potentials; the Coulomb results are included here for reference. The longer-range potentials (e.g. logarithmic) have a qualitatively different behaviour from the shorter-range potentials. In fact, there is an indication that for the latter, the gaps may vanish at a *finite* n, which we believe is related to the infrared divergences predicted by the Chern–Simons approach [30]. As stressed earlier, we are working with wave functions which are independent of the form of the interaction, which raises the question of the relevancy of our study to the issue of stability of the CF sea; here, due to the lack of a gap to excitations, the wave functions, at least in their long-distance behaviour, will necessarily be highly susceptible to changes in the interaction. We must remember, however, that the CF wave functions are expected to be accurate so long as the gap is not too small, which is the case for the CF states with only a few filled CF-LLs. Therefore, we believe that the trends seen in our study are meaningful.

Figure 11 shows the gaps for the ZDS potential as a function of λ. The gaps for fixed values of λ/l_0 are shown in figure 12 and the effective masses derived from them in figure 13.

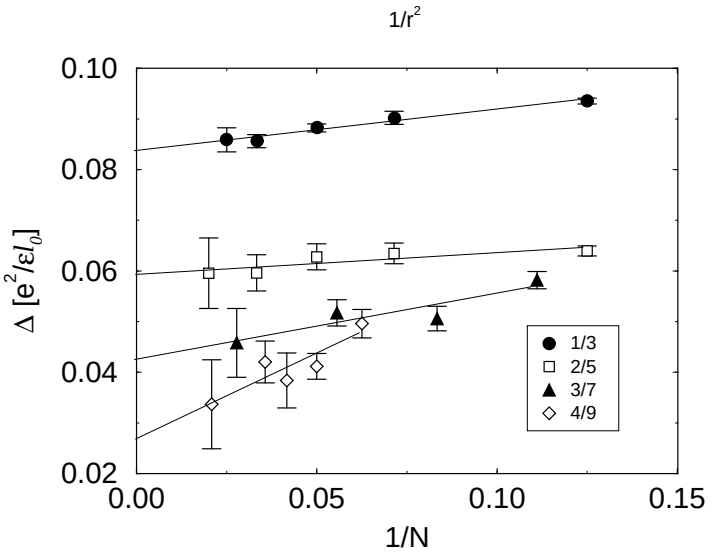

Figure 9. Estimation of the thermodynamic limit of the gap from the finite-system results for the r^{-2}-interaction for 1/3, 2/5, 3/7, and 4/9.

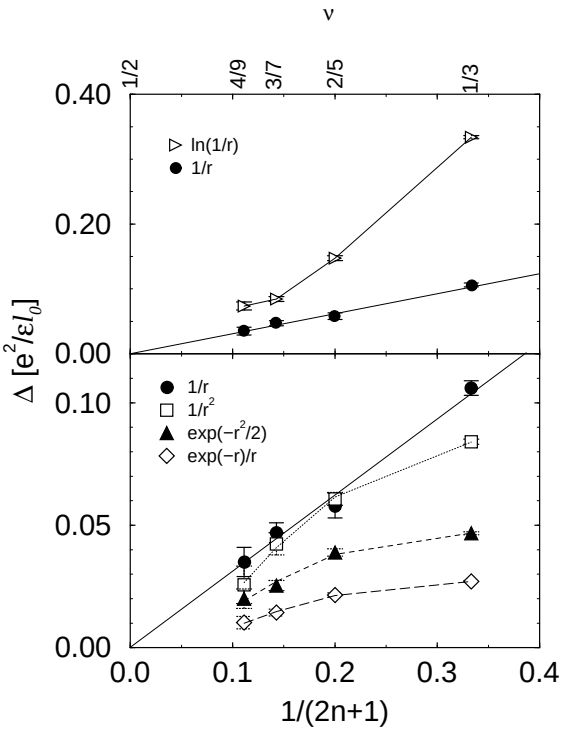

Figure 10. The activation gaps at 1/3, 2/5, 3/7, and 4/9 for several model interactions. The pure Coulomb gaps are also shown for reference. All distances are quoted in units of the magnetic length, l_0.

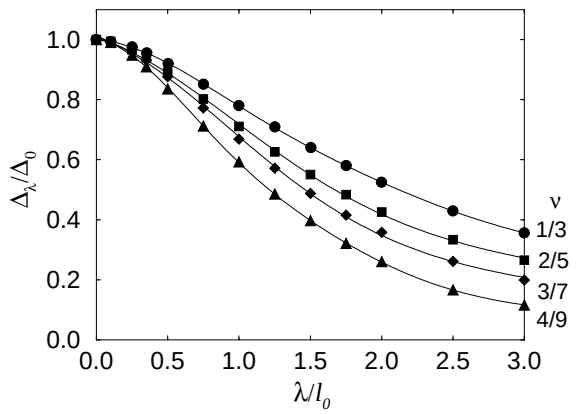

Figure 11. The activation gaps at 1/3, 2/5, 3/7, and 4/9 for the Zhang–Das Sarma potential, $e^2/(r^2+\lambda^2)^{1/2}$, plotted as a function of the parameter λ. Δ_0 is the gap for pure Coulomb interaction.

(Note that λ/l_0 is kept fixed here rather than λ; however, since the magnetic length does not change appreciably in the range of filling factors considered, the results are qualitatively independent of which of the two is taken as constant.) These figures demonstrate that for the

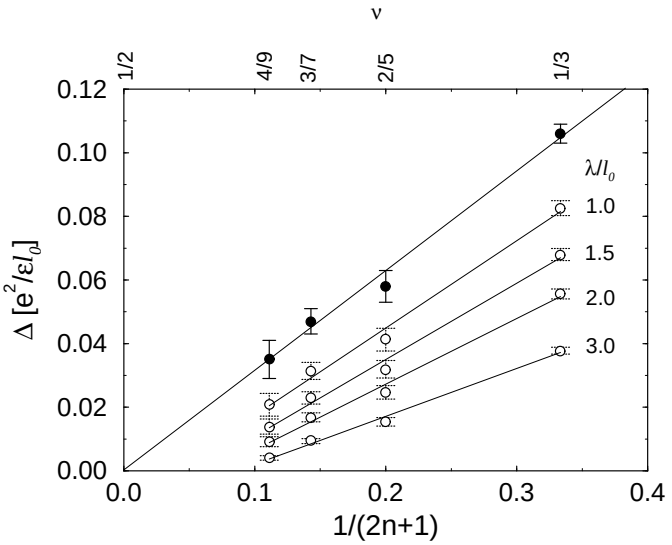

Figure 12. The activation gaps for several values of λ/l_0 as functions of the filling factor for the Zhang–Das Sarma potential. The solid line is the best straight-line fit through the gaps.

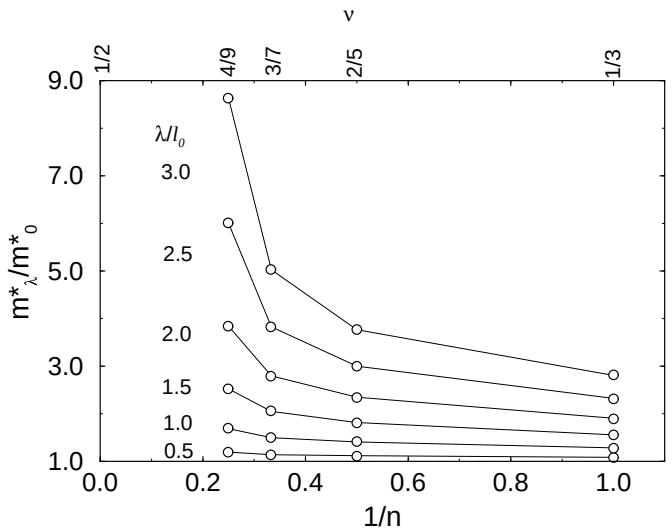

Figure 13. The ratio of the CF effective mass for the ZDS interaction (obtained from the gaps in figure 12) to the effective mass for the Coulomb interaction for several values of λ/l_0.

ZDS potential also, similarly to the case for the more realistic potentials, a straight-line fit through the gaps has a negative intercept, and the effective mass increases as the half-filled Landau level is approached. The overall qualitative behaviour is quite similar to that found in the more sophisticated LDA calculation; a comparison of the two figures shows that the appropriate value for λ for the samples in the experiments of Du *et al* [27] is $\lambda/l_0 \approx 1$, as also argued by Morf [17].

6. Conclusions

We have carried out the most comprehensive study to date of the effect of non-zero transverse width on activation gaps for the FQHE states. The effective interaction between electrons has been computed by means of the density functional theory in the LDA, which is then used to determine the gaps for CF states with up to five filled CF-LLs (corresponding to FQHE at 1/3, 2/5, 3/7, 4/9, and 5/11). Several different geometries are considered, and the theoretical results are compared to experiment. It is concluded that for typical experimental parameters, the non-zero thickness reduces the gaps by 30%, which does not fully account for the observed gaps. This underscores the quantitative importance of effects left out in our study.

We have also considered a number of model interactions, and discovered a qualitative difference depending on whether the interaction is of longer or shorter range than the Coulomb one. We find that the gaps for the FQHE states decrease faster for the latter, as the CF sea is approached, which is consistent with expectations based on the Chern–Simons formulation of the composite-fermion sea [30], according to which the infrared behaviour of the CF sea exhibits singularities for interactions of shorter range than the Coulomb one but is well behaved for interactions of longer range than the Coulomb one.

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