Realistic Calculations of Correlated Incompressible Electronic States in GaAs–Al$_x$Ga$_{1-x}$As Heterostructures and Quantum Wells

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Abstract

We perform an exact spherical geometry finite-size diagonalization calculation for the fractional quantum Hall ground state in three different experimentally relevant GaAs-Al$_x$Ga$_{1-x}$As systems: a wide parabolic quantum well, a narrow square quantum well, and a heterostructure. For each system we obtain the Coulomb pseudopotential parameters entering the exact diagonalization calculation by using the realistic subband wave function from a self-consistent electronic structure calculation within the local density approximation (LDA) for a range of electron densities. We compare our realistic LDA pseudopotential parameters with those from widely used simpler model approximations in order to estimate the accuracies of the latter. We also calculate the overlap between the exact numerical ground state and the analytical Laughlin state as well as the excitation gap as a function of density. For the three physical systems we consider the calculated overlap is found to be large in the exper-
imental electron density range. We compare our calculated excitation gap energy to the experimentally obtained activated transport energy gaps after subtracting out the effect of level broadening due to collisions. The agreement between our calculated excitation gaps and the experimental measurements is excellent.
I. BACKGROUND

The fractional quantum Hall effect (FQHE) has been observed in high mobility GaAs-Al$_x$Ga$_{1-x}$As quantum structures at low temperatures and in strong magnetic fields. This effect produces quantized plateaus in the Hall resistivity concurrent with minima in the longitudinal resistivity at special values of the electron density. A well-formed electron correlation driven energy gap separating the ground state from the excited states occurring at these special densities and magnetic fields is the underlying reason for the FQHE phenomenon. The special density and magnetic field needed for the FQHE correspond to a Landau level filling factor $\nu = p/q$ where $q$ is an odd integer in the simplest situation. Laughlin’s theory of the FQHE, valid for filling fractions of the form $\nu = 1/m$, where $m$ is an odd integer, is based on the following two-dimensional (2D) many-body wave function:

$$\psi_m (z_1, \ldots, z_N) = \prod_{i<j} (z_i - z_j)^m \exp \left( -\frac{1}{4} \sum_{j=1}^{N} |z_j|^2 \right)$$

where $z_i = x_i - iy_i$ is the complex representation of the $i^{th}$ electron’s 2D position vector. The Laughlin state describes a droplet of an incompressible correlated 2D electron liquid. At these special values of the filling fraction, the system has an excitation gap that separates the ground state from the excited states. The elementary excitations are fractionally charged anyons. In a single layer 2D system, Laughlin’s theory explains the FQHE at $\nu = 1/m$ and $\nu = 1 - 1/m$, where $m$ is an odd integer. The hierarchy construction extends this theory to filling fractions of the form $\nu = p/q$ where $q$ is an odd integer.

Direct numerical calculations involving the exact diagonalization of a small ($4 \sim 10$) number of interacting 2D electrons has verified the Laughlin theory extremely well. The geometry of choice in most numerical simulations is the translationally invariant, rotationally invariant spherical geometry. Using just a small number of electrons, $N_e$, ($N_e \leq 10$) can yield an accurate picture of the physical system. In this geometry, a magnetic monopole is placed at the center of a sphere of radius $R$, producing a radial magnetic field $B$. By the Dirac quantization condition, the total flux $4\pi R^2 B$ must be an integral multiple, $2S$, ...
of the elemental flux \( \hbar c/e \). From the hierarchy construction a relationship between \( 2S \) and the filling factor \( \nu \) can be found. For \( \nu = 1/3 \), \( 2S = 3(N_e - 1) \). The appropriate unit of length is \( l_c = \sqrt{\hbar c/eB} \). If all of the electrons in the system are placed in the lowest Landau level and the coupling between Landau levels is ignored the resulting many-body problem is exactly soluble. The Hilbert space is of finite dimensions and an exact finite dimensional Hamiltonian matrix can be written down. This matrix can be diagonalized by standard techniques to find the energy eigenvalues and the eigenvectors. It is for this reason that exact finite size diagonalization has become such an important tool for studying the FQHE. In fact such numerical studies have been instrumental in confirming Laughlin’s many-body wave function\(^{14} \)–\(^{16} \).

One direction that research in finite size diagonalization studies of the FQHE has taken is in increasing system size, i.e. increasing the number of electrons in the numerical simulation. In this paper, we take a different approach and place the emphasis on quantitatively improving the model used in describing the electron-electron interaction in the system to make it more realistic with respect to the experimental systems. Historically the first studies of the FQHE used a pure 2D Coulomb potential, and the pure \( 1/r \) Coulomb interaction, where \( r \) is the separation between 2D electrons, is still the most popular model for exact finite size diagonalization studies. It was later pointed out that the finite layer thickness in quantum structures would cause the short range part of the Coulomb interaction to become softened. This could cause the ground state of the system to be no longer incompressible for very thick layers, and the FQHE may eventually be destroyed in thick layers. Zhang and Das Sarma\(^{17} \) and He et al.\(^{18} \) investigated this ‘finite thickness’ phenomena using a simple variant of the Coulomb interaction, namely

\[
V(\vec{r}) = \frac{e^2}{\kappa} \frac{1}{\sqrt{\vec{r}^2 + \lambda^2}}
\]  

(2)

where the length scale \( \lambda \) represents the finite extent of the electron wave function in the \( z \) direction and \( \vec{r} \) is the 2D position vector. Recently the FQHE has been studied using more sophisticated models for the electron-electron interaction\(^{17} \)–\(^{19} \). The most accurate
approximation that one can make in this respect is to do a self-consistent electronic structure
calculation within the framework of the local density approximation (LDA) to describe the
interaction. In this paper we perform such a calculation for a wide parabolic quantum
well (PQW), a narrow square quantum well (SQW), and a heterostructure, and we use
the realistic LDA electronic structure to compute the effective electron-electron interaction
ertering the exact diagonalization study. We use Haldane’s spherical geometry\(^\text{11}\) to do a fully
spin polarized finite size FQHE diagonalization calculation for six electrons, which should be
sufficient for our purpose. The many-body Hamiltonian matrix for the FQHE is constructed
using these LDA-Coulomb matrix elements. Using the Lanczos method, we calculate the
eigenvalues and the eigenvectors of this fairly sparse FQHE Hamiltonian matrix, following
standard techniques. The overlap with the Laughlin \(\nu = 1/3\) state is found by diagonalizing
the Hamiltonian matrix using the pseudopotential parameters appropriate for this state and
then calculating the inner product between this state and the exact numerical ground state
found using the LDA pseudopotential parameters.

The excitation gap is determined by looking at the size of the cusp at the relevant filling
factor. In order to compare this calculated excitation gap to relevant experimental transport
data, we subtract out the level broadening due to collisions, \(\Gamma\). Using \(\mu\), the experimentally
determined value for the mobility, \(\Gamma\) can be determined from

\[
\Gamma = \left( \frac{\hbar}{2\tau_s} \right) = \left( \frac{\hbar e}{2m^*\mu} \right). \tag{3}
\]

However, this equation is not quite correct\(^\text{20}\) for the single particle level broadening if the
scattering is strongly peaked in the forward direction as it is in modulation doped GaAs
structures. We estimate the correct \(\Gamma\) (\textit{i.e.} the single particle broadening) using the transport
data by employing a simple theory\(^\text{21}\) which accounts for this forward scattering correction.
We then take the calculated excitation gap and subtract out \(2\Gamma\) when comparing with
experiment.
II. LOCAL DENSITY APPROXIMATION

We begin with a description of the procedure for a self-consistent electronic structure calculation at zero temperature and in zero magnetic field. We assume that the effective mass and the static dielectric constant do not vary over the width of the quantum well and that interface grading and dielectric mismatch are negligible.

We solve the effective-mass, single-particle effective Schrödinger equation for a particle in a quantum well and Poisson’s equation for the electrostatic potential due to the free electric charge self-consistently. Assuming separability of the planar and perpendicular degrees of freedom, the three dimensional Schrödinger equation reduces to

\[
\left( -\frac{\hbar^2}{2m^*} \frac{d^2}{dz^2} + V_{\text{EFF}}(z) \right) \xi_i(z) = E_i \xi_i(z)
\]  

(4)

where \(\xi_i(z)\) and \(E_i\) are the subband wave functions and energies respectively, and the effective one electron potential energy \(V_{\text{EFF}}(z)\) is given by

\[
V_{\text{EFF}}(z) = V_W(z) + V_H(z) + V_{XC}(z)
\]  

(5)

with \(V_W(z)\) being the quantum well confinement potential, \(V_H(z)\) the self-consistent Hartree potential, and \(V_{XC}(z)\) is the exchange-correlation potential. For the bare confining potential of a quantum well of width \(a\), we take

\[
V_W(z) = \begin{cases} 
  V_0 \theta(|z| - a/2), & \text{for a SQW} \\
  V_0 \theta(|z| - a/2) + \alpha z^2 \theta(a/2 - |z|), & \text{for a PQW} 
\end{cases}
\]  

(6)

with \(V_0\) being the barrier height for a square quantum well and the barrier height above the edge of the parabolic portion for a parabolic quantum well, and \(\alpha\) is the curvature of the parabolic quantum well.

Poisson’s equation for the Hartree potential is given by

\[
\frac{d^2V_H(z)}{dz^2} = -\frac{4\pi e^2}{\kappa} (n(z) - n_I(z))
\]  

(7)

where \(\kappa\) is the background dielectric constant for GaAs, \(n(z)\) is the electron density computed from the effective single particle subband wave functions and \(n_I(z)\) is the density of donor
impurities. We do not include $n_I(z)$ explicitly but include it via the boundary conditions in the solution of Poisson’s equation.

The areal density is determined from the subband wave functions by

$$n(z) = 2 \sum_{i}^{imax} N_i |\xi_i(z)|^2$$  \hspace{1cm} (8)

where $N_i$ is the occupancy of the $i$th subband and is given by

$$N_i = \int \frac{kdk}{2\pi} \theta \left( E_F - E_i - \frac{k^2}{2m^*} \right) = \frac{m^*}{2\pi} (E_F - E_i).$$  \hspace{1cm} (9)

The chemical potential $E_F$ is determined by the relation

$$N_s = \int dzn(z) = 2 \sum_{i}^{imax} N_i = \frac{1}{2\pi} \sum_{i}^{imax} 2m^* (E_F - E_i)$$  \hspace{1cm} (10)

where $N_s$ is the total surface density. The above equation is inverted to give $E_F$ and $imax$.

Many-body effects beyond the Hartree approximation are included by means of the density functional theory in the local density approximation (LDA)\textsuperscript{21–23}. A chief concern of density functional theory is the calculation of the exchange-correlation energy functional, $V_{XC}[n]$. This functional of the electron density contains all those interaction parts of the energy functional which in general are unknown. The local density approximation consists of replacing the functional $V_{XC}[n]$ with a function $V_{XC}(n)$ whose value at a given point in space $z_0$, where the density is $n(z_0)$, is determined as though the density was constant and equal to $n(z_0)$ everywhere. The validity of this approximation requires that the variation of the electron density be small over distances of the order of a Fermi wavelength. This condition is in general violated in most semiconductor quasi-2D systems. However, there is considerable evidence that this approximation when used in these systems gives excellent agreement with experiments\textsuperscript{24–28}. For the exchange-correlation potential, we used the parametrization due to Hedin and Lundqvist\textsuperscript{29}:

$$V_{XC}(z) = - \left(1 + 0.7734x \ln(1 + x^{-1})\right) \left(\frac{2}{\pi \beta r_s}\right) Ry^*$$  \hspace{1cm} (11)

where $\beta = (4/9\pi)^{1/3}$, $x = r_s/21$ and
\[ r_s = \left( \frac{4}{3} \pi a^* n(z) \right)^{-1/3} \]  

(12)

with \( a^* \) and \( R_y^* \) being the effective Bohr radius and the effective Rydberg respectively in GaAs.

The self-consistent procedure is to start with an initial guess for the electron density \( n(z) \). The Hartree and exchange-correlation potentials are then computed for this density. The Schrödinger equation is then solved numerically to obtain \( \xi_i \) and \( E_i \). A new density is then computed and compared to the previous \( n(z) \) through

\[ \eta = \frac{\int dz |n_{\text{new}}(z) - n_{\text{old}}(z)|}{\int dz n_{\text{old}}} . \]  

(13)

If \( \eta \) is larger than some specified tolerance, the new density is then mixed with the old density in the form \( n(z) = n_{\text{old}}(z)(1 - f) + n_{\text{new}}(z)f \) where \( f \) is a suitably chosen number between zero and one. This density is used as input to the calculation and the procedure is iterated until \( \eta \) is smaller than the tolerance. That is, convergence is achieved when the previous density and the new density do not vary much.

The above procedure is correct for quantum wells. For a heterostructure\cite{2}, however, this procedure requires modification since \( m^* = m^*(z) \) and \( \kappa = \kappa(z) \). The Schrödinger equation takes the form

\[ \left( -\frac{\hbar^2}{2} \frac{d}{dz} m^*(z) \frac{d}{dz} + V_{\text{EFF}}(z) \right) \xi_i(z) = E_i \xi_i(z) \]  

(14)

with \( V_{\text{EFF}}(z) \) still being given by equation (5) where \( V_W \) is

\[ V_W(z) = V_0 \theta (-z) . \]  

(15)

Poisson’s equation for a position dependent dielectric constant is

\[ \frac{d}{dz} \kappa(z) \frac{dV_H}{dz} = -4\pi e^2 (n(z) - n_I(z)) . \]  

(16)

The remaining pieces of the self-consistent calculation for heterostructures are unchanged from the quantum well case.
The main uncontrolled approximation we are making in applying this LDA procedure to FQHE calculations is the assumption that the applied external magnetic field does not appreciably affect the LDA results. Because the applied magnetic field is in the $z$ direction it is not unreasonable to assume that the single particle Schrödinger equation in the $z$ variable is not substantially modified by the magnetic field. But we assume uncritically that $V_{XC}(z)$ has no explicit magnetic field dependence, which should be a reasonable approximation for subband quantization arising from $z$ confinement.

III. PSEUDOPOTENTIALS

The basic ingredients entering the finite size FQHE diagonalization study are the Coulomb pseudopotential parameters, $V_m$, introduced by Haldane. Once all the $V_m$’s are known, the FQHE Hamiltonian is completely defined. The pseudopotential parameters are the energies of pairs of particles with relative angular momentum $m$. They are given by

$$V_m = \int_{0}^{\infty} q dq \tilde{V}(q) \left( L_n \left( \frac{q^2}{2} \right) \right)^2 L_m \left( q^2 \right) \exp \left( -q^2 \right)$$

where $\tilde{V}(q)$ is the Fourier transform of the electron interaction potential, $V(r)$, and $n$ is the Landau level index. For small (large) $m$, $V_m$ describes the short (long) range part of the interaction. If the electrons are fully spin-polarized, then only $V_m$ with odd $m$ are relevant. For the density as determined from an LDA calculation, where $|\xi(z)|^2$ represents the density profile in the $z$ direction, the relevant equation for $\tilde{V}(q)$ is given by

$$\tilde{V}(q) = \frac{2\pi e^2}{\kappa q} \int dz_1 \int dz_2 |\xi(z_1)|^2 |\xi(z_2)|^2 \exp(-q|z_1 - z_2|).$$

Various approximations to the electron wave function in Eq. (18) give rise to different pseudopotential parameters $V_m$.

The simplest approximation that one can make is to take the electron-electron interaction to be a pure 2D Coulomb interaction. In this case,
\[ V(q) = \frac{2\pi e^2}{\kappa q}. \]  \hspace{1cm} (19)

In order to take into account the effect of finite layer thickness in a quasi-2D electron system, a useful and simple approximation for the electron-electron interaction is the finite-\( \lambda \) model

\[ V(\vec{r}) = \frac{e^2}{\kappa} \frac{1}{(r^2 + \lambda^2)^{1/2}} \]  \hspace{1cm} (20)

where \( \lambda \) is the effective half-width of the electron layer in the \( z \) direction and \( \vec{r} \) is the 2D position vector. In momentum space,

\[ \tilde{V}(q) = \frac{2\pi e^2}{\kappa} \frac{\exp(-q\lambda)}{q}. \]  \hspace{1cm} (21)

For an infinite barrier square quantum well of width \( d \),

\[ \tilde{V}(q) = \frac{2\pi e^2}{\kappa q} \frac{1}{(qd)^2 + 4\pi^2} \left( 3qd + \frac{8\pi^2}{qd} - \frac{32\pi^4}{(qd)^2((qd)^2 + 4\pi^2)} \right). \]  \hspace{1cm} (22)

For a heterostructure, the Fang-Howard variational result is

\[ \tilde{V}(q) = \frac{2\pi e^2}{\kappa_{avg} q} \left( \frac{1}{16} \left( 1 + \kappa_{rel} \right) \left( 1 + \frac{q}{b} \right)^{-3} \left( 8 + \frac{9q}{b} + \frac{3q^2}{b^2} \right) \right) \]  \hspace{1cm} (23)

with \( \kappa_{avg} = (\kappa_{sc} + \kappa_{ins})/2 \) being the average dielectric constant and \( \kappa_{rel} = \kappa_{ins}/\kappa_{sc} \) being the relative dielectric constant of the insulating and semiconductor materials and \( b = 3/z_0 \) where \( z_0 \) is the average extent of the electron wave function in the \( z \) direction. In terms of the density, \( b \) is given by

\[ b = \left( 48\pi m^* e^2 N^*/\kappa_{sc} \hbar^2 \right)^{1/3} \]  \hspace{1cm} (24)

where

\[ N^* = N_d + \frac{11}{32} N_s \]  \hspace{1cm} (25)

with \( N_d \) being the depletion charge density in GaAs and \( N_s \) is the 2D electron density in the layer.
A major focus of our work is to determine how accurate these approximate models are when used in a FQHE calculation. In particular, pseudopotential parameters for these simple model approximations will be compared to those calculated using the self-consistent LDA calculation.

The eigenstates of a many-body Hamiltonian are unchanged if the Hamiltonian (or the potential in the Hamiltonian) is shifted by a constant amount. This suggests that differences of the $V_m$ would be a useful quantity to look at. The f-parameters are defined in terms of the pseudopotential parameters by

$$f_m = \frac{V_3 - V_m}{V_1 - V_3}. \quad (26)$$

$f_1 = -1$ and $f_3 = 0$ for any pair potential. The Laughlin $\nu = 1/3$ state is the exact nondegenerate ground state for a hard core model Hamiltonian. In terms of pseudopotential parameters, the hard core model is given by $\{V_1, V_3, V_5, \ldots\} = \{V_1, 0, 0, \ldots\}$ and its f-parameters are $\{f_1, f_3, f_5, \ldots\} = \{-1, 0, 0, \ldots\}$. A large deviation from these values implies that the system is not well represented by the hard core model and consequently the ground state of the system may not be incompressible. Our goal in this paper is to investigate the ground state incompressibility in increasingly more realistic approximations for the Coulomb pseudopotentials.

IV. PARABOLIC QUANTUM WELL

In this section we show the results obtained for a wide parabolic quantum well. A PQW is constructed by grading the Al concentration in such a way as to give the conduction band edge a parabolic shape. As the areal electron density in the well is increased, the half width at half maximum of the density, $\lambda$, increases. Shayegan et al., reported that the FQHE excitation gap decreases dramatically when $\lambda/l_c \approx 3.5$ to 5. This would indicate that the FQHE is becoming weakened and that the ground state of the system is no longer incompressible.
From the physical parameters given in Shayegan et al., we take $V_0 = 276$ mev, $\alpha = 5.33 \times 10^{-5}$ mev$/\text{Å}^2$, and $a = 3000\text{Å}$. The LDA pseudopotential parameters were calculated using these values for several densities. In Fig. 1, we show our calculated LDA $V_m$ for LDA for the experimentally determined carrier densities of Shayegan et al. compared with the $V_m$ for a pure Coulomb interaction. In Fig. 2, $V_m$ for two relevant approximate models, the infinite well model and the finite-$\lambda$ model, are shown. For $m$ greater than approximately 12, $V_m$ for the different models agree well with the LDA pseudopotentials. For small $m$ the pure Coulomb and the infinite well model seem to overestimate $V_m$, while the finite-$\lambda$ model underestimates $V_m$. In Figs. 3 and 4 we show the corresponding f-parameters for these pseudopotential parameters. The f-parameters in the finite-$\lambda$ model rise more rapidly with increasing density than the f-parameters for LDA and the other models. This would give the appearance that for large densities the ground state would no longer be incompressible in the finite-$\lambda$ model, as has been concluded in the literature.

Using the LDA pseudopotential parameters, we studied the $\nu = \frac{1}{3}$ FQHE state employing the finite size exact diagonalization technique. Figs. 5 and 6 show the calculated overlap with the Laughlin $\nu = \frac{1}{3}$ state, and the calculated bare excitation gap, $\Delta$, and the gap minus the level broadening, $\Delta - 2\Gamma$, as a function of electron density. Also shown is the gap as measured experimentally by Shayegan et al. The agreement between the experimental results and our calculation is very good. For a pure Coulomb interaction, $\Delta \approx 14.2$ K and $\Delta - 2\Gamma \approx 11.4$ K and using the finite-$\lambda$ model, $\Delta \approx 2.9$ K to 1.4 K and $\Delta - 2\Gamma \approx 0.1$ K to 0.0 K. The overlap of the LDA result with the Laughlin state is found to be quite large for all densities. This is to be contrasted with the finite-$\lambda$ model where the overlap is $\approx 0.8$ to 0.4 for the given range of densities. For a pure Coulomb interaction the overlap with the Laughlin state is also quite large.

We also studied the subband dependence of the PQW results in an artificial model calculation which bears no resemblance to reality. Pseudopotential parameters were calculated assuming that (a) only the lowest subband was occupied, (b) only the first excited subband was occupied, and (c) only the second excited subband was occupied. We then performed
a FQHE calculation using the parameters for (a)-(c). The difference between these results and our full LDA results was quite small (less than 1%) for the overlap with the Laughlin \( \nu = 1/3 \) state. The differences for the gap were larger (as much as 30%).

## V. HETEROSTRUCTURE

For the LDA calculation, we took the physical parameters to be those appropriate for a typical GaAs-Al\(_x\)Ga\(_{1-x}\)As heterostructure: \( V_0 = 276 \) mev, \( \kappa_{sc} = 12.8 \), \( \kappa_{ins} = 12.1 \), \( m^*_{sc} = 0.068 \) \( m_0 \), and \( m^*_{ins} = 0.088 \) \( m_0 \). In Fig. 4 we show the pseudopotential parameters for electron densities between \( 1 \times 10^{10} \) to \( 3 \times 10^{11} \) cm\(^{-2} \). From Fig. 8 it is clear that the approximate variational model\(^{25}\) is fairly reliable when compared to the LDA pseudopotentials especially for large densities. Figs. 4 and 10 show the corresponding f-parameters. These parameters are fairly constant for all densities greater than \( \approx 1 \times 10^{11} \) cm\(^{-2} \). For smaller densities, the f-parameters deviate more strongly from the hard core model f-parameters.

The overlap with the Laughlin state as a function of density is shown in Fig. 11. As expected it is quite large, especially for the larger densities. The finite-\( \lambda \) model also gives a large overlap with the Laughlin state, \( \approx 0.9 \) to 0.99 for this range of densities. The disagreement between the LDA results and the finite-\( \lambda \) model is larger for smaller densities.

Figure 12 shows calculated gaps \( \Delta \) and \( \Delta - 2\Gamma \) as a function of density. The agreement between our ‘subtracted’ gap and the experimental measurement\(^5\) of Willet et al. is very good. For comparison, a pure Coulomb interaction gives \( \Delta \approx 14.2 \) K and \( \Delta - 2\Gamma \approx 13.8 \) K, while the finite-\( \lambda \) model gives \( \Delta \approx 12.8 \) K to 5.7 K and \( \Delta - 2\Gamma \approx 12.7 \) K to 5.3 K.

## VI. SQUARE QUANTUM WELL

We consider a typical narrow SQW with a width 139\( \AA \) and \( V_0 = 276 \) mev, for a typical range of densities, \( N_S = 1 \times 10^{10} \) to \( 5 \times 10^{11} \) cm\(^{-2} \). The LDA pseudopotentials are shown in Fig. 13. For this well and this range of densities the calculated \( V_m \) show very little density variation. The pseudopotential parameters for the other models are shown in Fig. 14. As
in the PQW case, the infinite well model overestimates the $V_m$ while the finite-$\lambda$ model underestimates the $V_m$. However, for all $m$ greater than 4, the $V_m$ for all of the models are approximately equal. The f-parameters are shown in Figs. 15 and 16. These parameters for the LDA model are almost constant for the given range of densities and they are close to being equal in all of the models. These parameters do not rise above one for any of the models. Since the $V_m$s remain small for all $m$, it is reasonable to assume that the ground state should be incompressible over this range of densities in a square quantum well.

The overlap of the exact numerical wave function with the $\nu = 1/3$ Laughlin state is shown in Fig. 17. It also shows almost no variation with density and it is very close to the overlap computed using either the pure Coulomb or the finite-$\lambda$ model.

The gap, as shown in Fig. 18, shows almost no variation with density. It is very close to the pure Coulomb value, $\Delta \approx 14.2$ K. Using the finite-$\lambda$ model, $\Delta \approx 13.8$ K for this range of densities. Thus, for a square quantum well, all of the approximations for the pseudopotential should work well in FQHE calculations.

VII. EVEN DENOMINATOR FQHE : $\nu = 5/2$

The first unambiguous observation of an even denominator filling factor in a single layer system was made by Willet et al. Magnetotransport experiments carried out in a high mobility GaAs-AlGaAs heterostructure showed a plateau in the Hall resistivity concurrent with a deep minima in the longitudinal resistivity corresponding to a filling factor of $5/2$. Tilted field experiments on the $5/2$ state have shown that it is rapidly destroyed by increasing the Zeeman energy which indicates that the spin degree of freedom may be important in understanding this state.

In analogy with the Laughlin state for odd denominator filling factors, Haldane and Rezayi have proposed a ‘hollow core’ model wave function that may describe the physics of the $\nu = 5/2$ state. This spin-singlet wave function represents an incompressible state for $\nu = 1/2$. However this hollow-core wave function requires a substantially reduced short
range repulsion between the electrons relative to a pure 2D Coulomb interaction.

From the physical parameters for the heterostructure of Willet et al.\(^7\) we calculate the LDA pseudopotential parameters for the first Landau level \((n = 1)\). These parameters are shown in Table 1 and in Fig. 19. Figure 19 also shows the effect on the pseudopotential parameters for the variational model when the electron density is varied by 20% and also the effect of varying the relative dielectric constant, \(\kappa_{\text{ins}}/\kappa_{\text{sc}}\) from 0 to 1.5. Our reason for varying the system parameters (i.e. electron density and background dielectric constants) is to check whether such parameter modifications could produce an incompressible hollow core state at \(\nu = 5/2\). Assuming that the lowest Landau level is completely filled and inert, we perform a finite size diagonalization calculation for a system of eight electrons in the spherical geometry. Shown in Fig. 20 is the excitation spectrum as a function of total angular momentum \(L\) for total spin \(S\) equal to 4. We find that the ground state is in the \(L = 0 \ S = 4\) sector. The ground state energy for \(L = 0 \ S = 4\) is however close to the energies found for the other \(L = 0\) sectors. The overlap of our wave function from the finite size diagonalization calculation with the hollow core model is quite small \((5 \times 10^{-3})\) indicating that this model is not a good candidate for the 5/2 state. At this stage, therefore, we conclude, in agreement with earlier investigations\(^3\) of this issue, that the 5/2 FQHE phenomenon as observed in ref. 7 remains unexplained theoretically, and in particular, the hollow core model proposed in ref. 32 is not quantitatively consistent with the system parameters of the experimental sample in ref. 7.

**VIII. CONCLUSION**

In summary, we have obtained realistic Coulomb pseudopotential parameters for FQHE calculations in 2D GaAs–Al\(_x\)Ga\(_{1-x}\)As quantum structures using a self-consistent LDA electronic subband structure results. We compare the LDA pseudopotential parameters with those from a number of simpler model approximations (e.g. the pure 2D Coulomb model, the finite-\(\lambda\) model, the infinite well model, and the variational model) to estimate the quantita-
tive accuracy of the simpler models for various systems and different electron densities. Our most realistic calculations yield FQH excitation gaps which, when corrected for the level broadening effect, are in excellent quantitative agreement with the experimentally determined activation gaps as obtained from transport data. For the $\nu = 5/2$ FQHE observed in ref. [7] our calculations show that the hollow core model of ref. [32] is quantitatively inconsistent with the LDA Coulomb pseudopotentials for the experimental sample parameters of ref. [7]. Our calculated realistic Coulomb pseudopotentials for various systems should enable future FQHE finite size exact diagonalization calculations to be quantitatively more realistic.

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FIGURES

FIG. 1. Pseudopotential parameters in units of $e^2/\kappa l_c$ for a pure Coulomb interaction (short lines) and for the LDA calculation (long lines) for a PQW. The electron densities are: $4.9, 6.0, 7.3, 8.5 \times 10^{10}\text{cm}^{-2}$.

FIG. 2. Pseudopotential parameters in units of $e^2/\kappa l_c$ for the finite-$\lambda$ model (short lines) and the infinite well model (long lines) for a PQW. The electron densities are the same as in Fig. 1.

FIG. 3. $f$-parameters as a function of electron density for the LDA pseudopotential parameters for a PQW for odd $m$.

FIG. 4. $f$-parameters as a function of electron density for the finite-$\lambda$ model (dashed lines) and the infinite well model (solid lines) for a PQW for odd $m$.

FIG. 5. Overlap between the Laughlin $\nu = 1/3$ state and the exact numerical ground state found using the LDA pseudopotential parameters for a PQW.

FIG. 6. The excitation gap (dashed line), the ‘subtracted gap’ (solid line), and the experimental measurement of Shayegan et al. (*) for a PQW.

FIG. 7. Pseudopotential parameters in units of $e^2/\kappa l_c$ for the pure Coulomb (short lines) and the LDA results (long lines) for a heterostructure. The electron densities are $0.1, 0.5, 1.0, 2.0, 3.0 \times 10^{11}\text{cm}^{-2}$.

FIG. 8. Pseudopotential parameters in units of $e^2/\kappa l_c$ for a heterostructure for the variational model (long lines) and the finite-$\lambda$ model (short lines). The electron densities are the same as in Fig. 7.

FIG. 9. $f$-parameters as a function of electron density for the LDA pseudopotential parameters for a heterostructure for odd $m$. 

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FIG. 10. f-parameters as a function of electron density for the the variational model (solid lines) and the finite-λ model (dashed lines) for a heterostructure for odd \( m \).

FIG. 11. Overlap between the Laughlin \( \nu = 1/3 \) state and the exact numerical ground state found using the LDA pseudopotential parameters for a heterostructure.

FIG. 12. The excitation gap (dashed line), the ‘subtracted’ gap (solid line), and the experimental measurement\(^\text{\textregistered}\) of Willet \textit{et al.} (*) for a heterostructure.

FIG. 13. Pseudopotential parameters in units of \( e^2/\kappa l_c \) for the pure Coulomb interaction (short lines) and the LDA results (long lines) for a SQW. The electron densities are 0.1, 0.5, 1.0, 5.0 \( \times 10^{11} \text{cm}^{-2} \).

FIG. 14. Pseudopotential parameters in units of \( e^2/\kappa l_c \) for the finite-λ model (short lines) and the infinite well model (long lines) for a SQW. The electron densities are the same as in Fig. 13.

FIG. 15. f-parameters as a function of electron density for the LDA pseudopotential parameters for a SQW for odd \( m \).

FIG. 16. f-parameters as a function of electron density for the finite-λ model (dashed lines) and the infinite well model (solid lines) for a SQW for odd \( m \).

FIG. 17. Overlap between the Laughlin \( \nu = 1/3 \) state and the exact numerical ground state found using the LDA pseudopotential parameters for a SQW.

FIG. 18. The excitation gap as a function of electron density for a SQW.

FIG. 19. LDA pseudopotential parameters in units of \( e^2/\kappa l_c \) for the heterostructure of Willet \textit{et al.} (long lines) for the \( \nu = 5/2 \) FQHE. Also shown are the pseudopotential parameters for the variational model (short lines) assuming a twenty percent variation in the electron density and separately assuming \( \kappa_{rel} \) is between 0 and 1.5.
FIG. 20. The excitation spectrum for $S = 4$ for an eight particle calculation using the LDA pseudopotential parameters for the heterostructure of Willet et al.\textsuperscript{[22]}
TABLES

TABLE I. The LDA pseudopotential parameters in units of $e^2/\kappa l_c$ for the heterostructure of Willet et al. 

| Parameter | Value |
|-----------|-------|
| $e^2/\kappa l_c$ | 0.123 |

...
| m | $V_m$       |
|---|------------|
| 0 | 0.47665957508 |
| 1 | 0.37332084804 |
| 2 | 0.35230370587 |
| 3 | 0.2884405415  |
| 4 | 0.24996235081 |
| 5 | 0.22361694066 |
| 6 | 0.20414646380 |
| 7 | 0.18900642725 |
| 8 | 0.17679961714 |
| 9 | 0.16668746764 |
| 10| 0.15813248355 |
| 11| 0.15077224603 |
| 12| 0.14435235363 |
| 13| 0.13868828532 |
| 14| 0.13364252111 |
| 15| 0.12911019556 |
| 16| 0.12500975822 |
| 17| 0.12127670242 |
| 18| 0.11785925293 |
| 19| 0.11471532800 |
| 20| 0.11181031734 |
$V_m$ for PQW of Shayegan
$V_m$ Das Sarma & Mason and Zhang & Das Sarma

For PQW (Shayegan)

- Das Sarma & Mason

Zhang & Das Sarma

-1 0 1 2 3 4 5 6 7 8 9 10 11

$m$
$f_m$ for PQW of Shayegan

Electron Density $x10^{10}$ (cm$^{-2}$)
$f_m$ for DS&M and Z&DS(dotted) for PQW
Overlap with Laughlin $1/3$ state for PQW.
Gap for PQW of Shayegan

![Graph showing the relationship between gap (K) and electron density (x10^10 cm^-2).]
$V_m$ for GaAs/AlGaAs Heterostructure
$V_m$ AFS and Zhang & Das Sarma

For Heterostructure

Ando-Fowler-Stern

Zhang & Das Sarma
$f_m$ for GaAs/AlGaAs Heterostructure

![Plot of $f_m$ vs. Electron Density $x10^{11}$ (cm$^{-2}$)](plot.png)
$f_m$ for AFS and Z&DS (dotted) for Heterostructure
Overlap with Laughlin $1/3$ state for Heterostructure
Gap for GaAs/AlGaAs Heterostructure

Graph showing the gap (K) versus electron density (x10^{11} cm^{-2}).
$V_m$ for SQW

- Pure Coulomb
- LDA $n_x = 1d10 - 5d11$
$f_m$ for DS&M and Z&DS (dotted) for SQW

Electron Density x $10^{11}$ (cm$^{-2}$)

$-2.0$ $-1.0$ $0.0$ $1.0$

$-2.0$ $-1.0$ $0.0$ $1.0$
Overlap with Laughlin 1/3 state for SQW

![Graph showing the overlap with Laughlin 1/3 state for SQW. The x-axis represents Electron Density x10^{11} (cm^{-2}), and the y-axis represents Overlap. The graph shows a horizontal line at an overlap value of 0.99.](image-url)
Gap for Square QW

![Graph showing the relationship between Gap (K) and Electron Density (x10^{11} cm^{-2}). The graph is a horizontal line indicating a constant gap value across different electron densities.](attachment:image.png)
$V_m$ for Willet et al. and from AFS  \( n=1 \)
Spectrum at $\nu=5/2$ for Willet et al. $S=4$