Doctoral Thesis

Fractional quantum Hall effect and quantum spin Hall effect in semiconductor heterostructures

Author(s):
Pakrouski, Kiryl

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Fractional quantum Hall effect and quantum spin Hall effect in semiconductor heterostructures

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presented by
KIRYL PAKROUSKI
MSc ETH, ETH Zurich
born on 23.11.1984
citizen of
Republic of Belarus

accepted on the recommendation of
Prof. Dr. Matthias Troyer, examiner
Prof. Dr. Chetan Nayak, co-examiner
Prof. Dr. Werner Wegscheider, co-examiner

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Kiryl Pakrouski

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E-mail kiryl.pakrouski@alumni.ethz.ch
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Abstract

In this thesis we study the topological phases that can arise in the form of the fractional quantum Hall effect (FQHE) and the quantum spin Hall effect (QSHE) in semiconductor heterostructures.

In the first project we study the influence of the "finite width effect" on the $\nu = 5/2$ FQHE state observed in a number of experimental devices. Electron gas located in a quantum well constructed of a semiconductor heterostructure is only approximately two-dimensional: although confined in one dimension it possesses finite width which modifies the effective interaction. We find that the effect can be reliably parametrised by the width of an infinitely deep quantum well. Finite width slightly reduces the gap of the $\nu = 5/2$ state while increasing the overlap with the Moore-Read Pfaffian wavefunction, does not allow however to account for the experimentally observed variance in the energy gap. This indicates the disorder and Landau level mixing may play an important role in real experiment and motivates the studies of the model that includes both finite thickness and Landau level mixing in the following two projects.

In the second project we study the phase diagram of the $\nu = 5/2$ fractional quantum Hall effect in the coordinates of finite width and Landau level mixing strength. The nature of the ground state at $\nu = 5/2$ is known to be sensitive to the changes in the effective electron interaction. Two of the candidate model states that could describe the $\nu = 5/2$ FQHE state, Moore-Read Pfaffian and its particle-hole conjugate, anti-Pfaffian could both be used for implementing topological quantum computing, are however indistinguishable under idealised conditions used in previous studies. In our work we consider the effective interaction that results from simultaneously taking into account the effects of finite thickness and Landau level and subband mixing in GaAs heterostructures perturbatively in $\kappa$, the ratio of Coulomb and cyclotron energies that characterises the significance of Landau level mixing.

We diagonalise the corresponding Hamiltonian exactly in spherical and torus geometries and analyse the ground state according to four criteria: its overlap...
with trial wave functions; the magnitude of energy gaps; the sign of the expectation value of an order parameter for particle-hole symmetry breaking; and the entanglement spectrum.

We find that both Landau level mixing and finite width significantly reduce the energy gap of the \( \nu = 5/2 \) state making it less stable. Comparing several models of finite width we conclude that they are equivalent in terms of the FQHE observables as long as the variance of the electron wavefunction in the confined direction is taken to be the same. Thus we identify a universal quantity that allows to parametrise the finite width effect and convert the models of finite width into each other. Finally, we find that the \( \nu = 5/2 \) state is in the Moore-Read Pfaffian (rather than anti-Pfaffian) universality class for \( \kappa < \kappa_c(w) \), where \( \kappa_c(w) \) is a critical value \( 0.6 \lesssim \kappa_c(w) \lesssim 1 \) that depends on finite width \( w \).

Another fraction where the particle-hole breaking effects may play an important role is the \( \nu = 12/5 \) because its particle-hole conjugate \( \nu = 13/5 \) has never been observed in experiment. In the third project we study the same model that includes realistic finite width and Landau level mixing effects in the second \( (\nu = 12/5, 13/5) \) and lowest \( (\nu = 2/5, 3/5) \) Landau levels. We find that the particle-hole symmetry between the two states in the lowest Landau level remains practically unaffected by Landau level mixing. In contrast, we find significant symmetry breaking in the pair \( 12/5 - 13/5 \) where the energy gap of the \( \nu = 13/5 \) state is strongly suppressed compared to the state at \( \nu = 12/5 \). These findings are in agreement with the experiment and provide a possible explanation for the experimental absence of the \( \nu = 13/5 \) state.

In the fourth project we turn to the topological quantum spin Hall effect that can manifest in InAs/GaSb heterostructures. We derive a general effective \( 4 \times 4 \) low-energy model that respects the symmetry of the host heterostructure interface. We investigate how this model can lead to inverted and non-inverted band structure and how a transition between these can be tuned by changing the applied electric field. Further, we numerically calculate the structure of the Landau levels in this system and find good qualitative agreement with the Landau levels measured in the corresponding experimental samples.
Zusammenfassung

In dieser Arbeit untersuchen wir die topologische Phasen, die in Form des fraktionalen (gebrochenzahligen) Quanten-Hall-Effekts (FQHE) sowie des Quanten-Spin-Hall-Effekts (QSHE) in Halbleiter-Heterostrukturen entstehen können.

Der erste Teil befasst sich mit dem Einfluss des Effekts der endlichen Breite des 2D Elektronengases auf den $\nu = 5/2$ FQHE-Zustand, der in einer Reihe von experimentellen Geräten beobachtet wurde. Elektronengas, das sich in einer aus einer Halbleiter-Heterostruktur aufgebauten Quantentopf befindet, ist nur annähernd zweidimensional: obwohl es in einer Dimension eingeschlossen ist, besitzt es eine endliche Breite ("finite width"), die die effektive Wechselwirkung der Elektronen modifiziert. Wir finden, dass dieser Effekt durch die Breite eines unendlich tiefen Quantentopf zuverlässig parametrisiert werden kann. Die endliche Breite reduziert die Bandlücke des $\nu = 5/2$ Zustandes und steigert gleichzeitig dessen Überlapp mit der Moore-Read Pfaffian Wellenfunktion; erlaubt jedoch nicht, die experimentell beobachtete Varianz in der Bandlücke des $\nu = 5/2$ Zustands zu erklären. Dies deutet an, dass die Unordnung des Materials und Landau-Niveau Vermischung eine wichtige Rolle in realen Experimenten spielen können und motiviert die folgenden zwei Studien in einem Modell, das sowohl endliche Breite als auch Landau-Niveau-Vermischung umfasst.

Im zweiten Projekt untersuchen wir das Phasendiagramm des $\nu = 5/2$ FQHE-Zustandes in den Koordinaten der endlichen Breite und der Landau-Niveau Vermischung. Es ist bekannt, dass die Art des Grundzustandes von $\nu = 5/2$ FQHE von den Details der Wechselwirkung abhängt. Zwei mögliche Modelle, die den $\nu = 5/2$ FQHE-Zustand beschreiben könnten, Moore-Read Pfaffian und sein Teilchen-Loch-Konjugat, Anti-Pfaffian, könnten beide für die Implementierung des topologischen Quantencomputers verwendet werden, sind jedoch nicht unterscheidbar unter idealisierten Bedingungen, die in früheren Studien verwendet wurden. In unserer Arbeit betrachten wir die effektive Wechselwirkung entwickelt in $\kappa$, das Verhältnis von Coulomb- und Zyklotronenergien, die sich aus der gleichzeitigen Berücksichtigung des Effekts der endlichen Breite und der Landau-Niveau und Subband-
Vermischung in GaAs-Heterostrukturen ergibt. Hier, parametrisiert \( \kappa \) den Einfluss der Landau-Niveau und Subband Vermischung.


Wir finden, dass sowohl die Landau-Niveau Vermischung als auch die endliche Breite die Bandlücke des \( \nu = 5/2 \)-Zustandes deutlich reduzieren. Beim Vergleich von mehreren Modellen endlicher Breite schliessen wir, dass sie in Bezug auf die FQHE-Observablen äquivalent sind, solange die Varianz der Elektronenwellenfunktion in der eingeschlossenen Richtung gleich ist. Dadurch identifizieren wir eine universelle Größe, die es erlaubt, den Effekt der endlichen Breite zu parametrisieren und die verschiedene Modelle der endlichen Breite ineinander umzuwandeln. Schliesslich finden wir, dass der \( \nu = 5/2 \)-Zustand in der Moore-Read Pfaffian (eher als Anti-Pfaffian) Universalklasse für \( \kappa < \kappa_c(w) \) ist, wobei \( \kappa_c(w) \) ein kritischer Wert \( 0.6 \lesssim \kappa_c(w) \lesssim 1 \) ist, der von der Breite \( w \) abhängt.

Ein weiterer Bruchteil, bei der die Effekte entstehend durch die Brechung der Teilchen-Loch Symmetrie eine wichtige Rolle spielen könnten, ist \( \nu = 12/5 \), weil ihr Teilchen-Loch-Konjugat \( \nu = 13/5 \) nie im Experiment beobachtet wurde. Im dritten Projekt untersuchen wir das gleiche Modell, das realistische endliche Breite und Landau-Niveau-Vermischungs-Effekte umfasst, im zweiten (\( \nu = 12/5, 13/5 \) und untersten (\( \nu = 2/5, 3/5 \) Landau Niveaus. Wir finden, dass die Teilchen-Loch-Symmetrie zwischen den beiden Zuständen in der untersten Landau-Niveau praktisch von der Landau-Niveau-Vermischung nicht beeinflusst wird. Im Gegensatz dazu finden wir signifikantes Symmetriebrechen im Paar 12/5 – 13/5, wo die Bandlücke des \( \nu = 13/5 \) Zustandes, im Vergleich mit \( \nu = 12/5 \) stark unterdrückt wird. Diese Erkenntnisse stimmen mit dem Experiment überein und liefern eine mögliche Erklärung für die experimentelle Abwesenheit des \( \nu = 13/5 \)-Zustandes.

1 Introduction

At the first sight the task of condensed matter physics - describing the properties of a solid containing \( \approx 10^{23} \) particles that are described by Schrödinger equation appears quite hopeless. In fact, it can be argued that this system cannot be solved by any classical computer in principle since the number of states it would have to operate on would exceed the number of particles in the Universe. The key problem here is the exponential scaling of the number of possible configurations that results from the quantum nature of the particles involved. Fortunately, in many cases the complexity of the problem can be tremendously reduced by introducing several approximations. For example, one can use the Born-Oppenheimer approximation \([6]\) and treat the heavy nuclei of atoms classically. On top of that one can integrate out the irrelevant (in that approximation) degrees of freedom such as the states of core electrons in an atom and arrive at an effective low-energy model for an electron. Density functional theory \([7, 8]\) is a Nobel-Prize-winning method that allows to successfully calculate the approximate band structure (single electron energy levels as a function of wavevector) of a number of materials.

A large part of the modern technology from electronics to drug-design is possible because of the detailed understanding of the electronic properties of materials. Notably, most of the physical phenomena that have been turned into technology are relatively well described by a single-electron picture sketched above.

Many interesting physical effects arise however because of the strong many-body interactions between electrons. Under strong interactions the situation can change qualitatively, which put in a simple language means that 10 strongly-interacting electrons form a state which has nothing to do with the state of just one electron "taken 10 times". This results in such exotic phenomena as insulating behaviour at fractional band filling, particles with fractional anyonic statistics (neither bosons nor fermions), superconductivity manifested at unexpectedly high temperature and the systems that do not thermalise contrary to statistical physics intuition because of the many-body localisation (MBL) effect.

Understanding the interacting systems can potentially allow us to harness new
powerful technologies such as error-free quantum information processing [9] or high-temperature superconductivity. However, the exotic properties of the interacting systems come at a much higher cost of solving them as some of the approximations become invalid.

An important concept that relatively recently emerged in the condensed matter physics is the one of topology. Topological systems in condensed matter context have many facets. One of them is the presence of a non-local order parameter that distinguishes phases of matter. This is opposed to the local order parameter that has long been used in condensed matter physics to characterise different phases. For example, a ferromagnet breaks the rotational symmetry of the spin by having a net magnetisation which has a finite expectation value when measured locally. Landau theory of phase transitions provides a unified picture of phase emergence based on the local symmetry breaking but does not seem to accommodate the topological systems which instead of breaking symmetries may require their presence in order to exist.

Another defining property of the topological systems is that in the low-energy limit they are described by a topological field theory (TQFT). For a field theory "topological" means that the result (measurement probabilities) of such a system's evolution in time solely depends on the topology of the knots or crossovers formed by the world lines of the constituent particles evolving in the (D+time)-dimensional spacetime. The result for such a theory does not depend on any smooth deformations of the world lines (how fast and at what angle the particles move) as long as they do not change the topology of the world lines entangled together, which in turn can be characterised by a knot invariant that maps any combination of "knots" formed by the world lines to a single number. An alternative, more general way to express the above definition is to say that in a topological system all observable properties are invariant under smooth deformations of the space-time manifold [9]. It can be argued that the correlation functions of any local operator in a topological system are precisely zero unless that local operator is unity [9], which has as a direct consequence insensitivity to local noise.

All these properties are somewhat contra-intuitive. One reason why we don't see them so often is that to reach the "low-energy" limit we need to cool system down below the gap which is what actually protects the exotic order of TQFT. The very existence of such systems sounds like a fairy tale but they do seem to exists in experiment. 3/4 of this thesis will be devoted to the fractional quantum Hall effect which is an example of a strongly-interacting topological system. The rest has to do with a non-interacting example - the quantum spin Hall effect. The exotic nature of the abstract TQFT models is established. On the other hand we have experiment that attempts to search for such phases in real world. A major question is: "To what extent the physical state of an experimental system is described by the topological model?". In the present work we attempt to answer
this question by performing numerical simulations under realistic experimental conditions. This approach can also help identify the experimental parameters favourable for observing the topological phases.

The described nature of the topological systems can be of benefit for information processing. Indeed, if we encode information in a non-local way that is completely unaffected by small local perturbations the computational scheme is likely to be more reliable. The computation, the change of the state of the system can then be performed by moving the particles around each other (also referred to as braiding) and thus changing the topology of the world lines.

Topological quantum computation [9, 10] is an approach to the quantum computation that follows this program to construct an error-free computational scheme. As a result, in addition to the qualitatively higher efficiency for some tasks (true for any quantum computer as compared to classical) a topological quantum computer would also operate in a fault-tolerant manner. The information is encoded as a state of the $K$-dimensional degenerate ground-state subspace of a topological system separated from other states by a gap. A change in the state of the subspace corresponds to a transformation that is described by a $K \times K$ matrix. In case such matrices for different transformations do not commute the system is said to have non-Abelian braiding statistics. Although all quantum Hall states are topological only for two of them ($\nu = 5/2$ and $\nu = 12/5$) there exists accumulating evidence of non-Abelian statistics and only one $\nu = 12/5$ is thought to be possibly useful for implementation of universal quantum computation (implements a basis in the space of functions operating on a qubit analogous to the NAND gate of a classical computer).

Fractional quantum Hall effect is the phenomenon observed in a two-dimensional electron gas (2DEG) subject to a perpendicular magnetic field [11]. The kinetic energy of an electron becomes quantized into Landau levels (LL) of the degeneracy given by the number of flux quanta penetrating unit surface as shown in Fig. 1.1. In the simplest approximation the energy difference between the Landau levels is taken to be infinite. In this case the kinetic energy of an electron becomes irrelevant and all what is left in the Hamiltonian is the Coulomb interaction between electrons. Thus the system is inherently strongly interacting, which makes it so interesting. This also explains why an analytical treatment is hard and numerical methods attain crucial importance.

The fractions such as $5/2$ that are used to label a fractional quantum hall state (FQHS) are determined by the ratio of the number of electrons residing on a unit surface to the number of flux quanta penetrating this unit surface (LL degeneracy). The essence of FQHE is that at fractional filling because of the strong interaction electrons form incompressible liquid whose elementary excitations are anyons: they carry a charge of a fraction of electron charge (for example $e/3$ for $\nu = 1/3$) and
Figure 1.1: Schematic representation of the integer quantum Hall effect (IQHE) and the fractional quantum Hall effect (FQHE). In IQHE adding a particle is associated with the cyclotron gap energy between the Landau levels $\hbar \omega_c = eB/mc$, with $e$ electron charge, $B$ magnetic field, $m$ electron mass and $c$ the speed of light. In FQHE the Landau level is only filled partially and the gap is a consequence of strong many-body interaction. The Coulomb energy scale is given by $e^2/\epsilon l_0$.

obey fractional braiding statistics. In contrast to the factor of 1 (bosons) or -1 (fermions) acquired by the wavefunction due to particle exchange in 3 spacial dimensions elementary excitations of the $\nu = 1/3$ FQHS acquire a factor of $e^{i\pi/3}$.

Although very interesting from the fundamental physics point of view [12, 13] (Nobel prize 1998) the FQHE turned out to be a natural host system for topological quantum computation [14, 9] since the elementary excitations for some of the fractions such as $\nu = 5/2, 12/5$ [15, 16]) possess non-Abelian braiding statistics. Other fractions may have this property as well, main suspects being the even-denominator states such as $\nu = 19/8$.

Although some of the properties of FQHE can be captured by a simplified model of ideally two-dimensional electrons interacting by pure Coulomb interaction the experimental situation is different. In this work we will take a step towards a more realistic description of the phenomenon which boils down to considering an effective interaction (instead of $1/r$) in order to include effects most important for the experimental setup.

To capture the physics of FQHE electrons have to be treated quantum-mechanically. The dimension of the Hilbert space that contains all possible configurations of multiple electrons grows exponentially in their number. For most of the numerical physics studies this fact would be a motivation to develop or use one of the approximate methods, where the solution for the non-interacting problem is modified in
some way to account for the weak effect of interactions. However for the FQHE the interactions are strong and such a strategy would not be useful. Here, to obtain the unbiased results we will have to face the exponential scaling problem and employ numerical exact diagonalization for the system sizes that can be reached on a modern supercomputer.

1.1 FQHE problem setup

The fractional quantum Hall experiments considered in this thesis are performed in semiconductor heterostructures manufactured with molecular beam epitaxy (MBE) - a method of growing two-dimensional layers by allowing atoms of selected materials to condense on the two-dimensional surface. Under proper conditions the resulting structure is a single crystal uniform in two dimensions and it’s properties in the third, often referred to as "z-direction", are determined by the sequence of materials used. A sample structure of an FQHE device is shown in Fig. 1.2. Usually such a structure is n-doped leading to the presence of electron density in the conduction band. The density is chosen such that in the z-direction the electrons are in the ground state of the quantum well (GaAs in Fig. 1.2). At low temperatures the quantum number that describes the state in z-direction is "frozen" and the system can be regarded as two-dimensional. It is clear however that the electron wavefunction has finite extent in z-direction (typical quantum well is 30nm long). This "finite thickness" effect modifies the effective interaction between electrons in 2DEG and will be discussed in detail in the chapter 2.3.

Fractional quantum Hall effect occurs when a 2DEG is subject to magnetic field. The characteristic length for the FQHE phenomena is known as magnetic length $l_c = \sqrt{\hbar/eB}$ in SI units system or $l_c = \sqrt{\hbar c/eB}$ in SGS. For a typical experiment this length is about an order of magnitude larger than the distance between the atoms in the lattice of the host material (GaAs). For this reason the presence of such underlying lattice is irrelevant for the fractional quantum Hall effect and will be disregarded in the following. At the same time we would like to note that the case when the two length scales are comparable [17, 18] has been very important for the development of the topological description of solid state systems and is directly related to the 2016 Nobel Prize in Physics. The topological invariant (TKNN) that was identified by Thouless, Kohmoto, Nightingale and den Nijs in Ref. [17] for a periodic system in magnetic field was also shown [19] to be non-zero in a system with no net magnetic field (but still with broken particle-hole symmetry). Eventually, this led to the discovery of a time-reversal invariant model describing topological insulators (quantum spin Hall effect) that are the subject of the last part of this thesis and that are introduced
1.2 Outline

This thesis is organised as follows.

In Chapter 2 we introduce the numerical simulations of the fractional quantum Hall effect and the language used. We discuss several technical details of simulation implementation including the finite thickness effect in both spherical and planar geometries.

Figure 1.2: Typical layout [20] of a FQHE experimental device grown in the MBE group of Prof. Wegscheider at ETH. On the right, the energy of the electrons in the conduction band is shown schematically together with the Fermi level (red solid line).

Generally speaking spin is another degree of freedom in fractional quantum Hall effect. There is however theoretical [21, 22, 23, 24, 25] and experimental [26, 27, 28] evidence for the full spin polarization at the 5/2 and 12/5 filling fractions we are concerned with in this work, although not all the experiments can be clearly interpreted in this sense. We choose to only consider spin-polarized systems in what follows.

All the fractions that we will consider belong to the second Landau level. The general practice is to consider the lowest Landau level to be completely full and inert which then allows one to restrict the Hilbert space to the valence Landau level only. Also all our calculations are performed within a single, valence Landau level although some of them use the effective interaction that includes the effect of transitions between Landau levels - "Landau level mixing effect".

1.2 Outline

This thesis is organised as follows.

In Chapter 2 we introduce the numerical simulations of the fractional quantum Hall effect and the language used. We discuss several technical details of simulation implementation including the finite thickness effect in both spherical and planar geometries.
In Chapter 3 we discuss how the simulation can be efficiently performed on a supercomputer.

The next Chapter 4 presents the results of the FQHE simulation where the finite width effect, specific for each of a number of experimental devices has been taken into account in order to determine the properties of the FQHE $\nu=5/2$ state in each of the devices. Besides, we also compare various models of finite thickness and their difference in terms of FQHE-observables.

In Chapter 5 we introduce the main model [29, 30, 31] that we use for the FQHE simulations onwards. It takes Landau level mixing into account to lowest-order perturbatively in $\kappa$, the ratio of the Coulomb energy scale to the cyclotron gap. It also simultaneously incorporates non-zero width $w$ of the quantum well and sub-band mixing.

The phase diagram of the $\nu=5/2$ FQHE state that results from this model is discussed in Chapter 6 which is to large extent based on Ref. [1]. We find an important property that connects the various finite thickness models as well as identify the universality class of the ground state of the $\nu=5/2$ state in the limit of small $\kappa$.

In Chapter 7 we study the fractional quantum Hall effect at filling factors $\nu=2/5, 3/5, 12/5, 13/5$. We find that the effect of Landau level mixing is profoundly different in the lowest and first excited Landau levels and provide a possible explanation to the absence of the $\nu=13/5$ state in experiment. This part of the thesis is based on Ref. [2].

Finally, in Chapter 8, we switch gears to a topological model that can be understood in terms of a single-particle picture and study the quantum spin Hall phase that arises in the InAs/GaSb heterostructures. Motivated by the observation of unusual Landau level structure in this system we derive the effective low-energy model and show that the untypical pattern observed in the Landau levels is a direct consequence of the inverted band structure in the topological regime. The results of this part appeared in a somewhat more concise form in Ref. [4].
2 FQHE: Basics and implementation

In this chapter we introduce the definitions and the setup of the numerical simulations of the fractional quantum Hall effect.

2.1 Pseudopotentials

The Haldane pseudopotentials \cite{Haldane} (PP) allow to parametrise any isotropic (only function of relative distance between particles) interaction as

\[ H = \sum_{L,L_{tot}} V_L P_{L,L_{tot}}, \tag{2.1} \]

where the pseudopotential \( V_L \) only depends on the relative (angular on the sphere) momentum of two particles

\[ V_L = \langle L | V(r) | L \rangle \tag{2.2} \]

and the operator \( P_{L,L_{tot}} \) projects pairs of electrons on a state with fixed relative and total momenta

\[ P_{L,L_{tot}} = |L, L_{tot}\rangle \langle L, L_{tot}|. \tag{2.3} \]

Within the lowest Landau level pseudopotentials completely specify the real-space interaction. Only pseudopotentials corresponding to the odd total angular momentum are compatible with the fermionic exchange statistics. For bosons, on the other hand, even values are allowed as well.

For filling fractions of the form \( 1/m \) pseudopotentials allow a very concise formulation of the generating Hamiltonian for the corresponding Laughlin state. For example \( \nu = 1/3 \) Laughlin wavefunction is the exact ground state of the "hard-core" Hamiltonian with all pseudopotentials equal to zero and \( V_1 = 1 \).

Mathematically, the problem of electrons interacting with given interaction in a higher Landau level is equivalent to the problem of electrons in the lowest
2.2 Geometries

Landau level (LLL) interacting with modified, effective interaction [11]. We will make extensive use of this property and perform all the numeric calculations in the lowest Landau level.

Pseudopotentials formalism can be generalised for multiparticle interactions [33]. Most important for our purposes will be the 3-body pseudopotentials that will allow us to represent the three-particle interaction in the form of Eq. 2.1.

A few practical facts about the pseudopotentials:

1. If a system is described by a 2-body Hamiltonian and one shifts all the (2-body) pseudopotentials by a constant the FQHE state (incl. overlaps with model wavefunctions and gaps) remains unchanged.

2. The same is valid for a system described by a purely three-body Hamiltonian. Note that all the pseudopotentials (as opposed to a subset of) relevant for a given system size must be shifted by the same amount for the FQHE state to remain unchanged.

3. Whenever one has both 2- and 3-body interactions the basis includes states with all the 3-body pseudopotentials. In case one chooses to put some of the $V_m^{(3)}$ to zero the 3-body states with $L = m$ remain in the Hilbert space and all have equal energy of 0.

2.2 Geometries

Fractional quantum Hall effect is observed in a two-dimensional electron gas. The commonly used for numerical studies in literature two-dimensional surfaces are sphere, disk and torus. Torus and sphere do not have boundaries which is beneficial for examining the bulk properties of the state. The disk geometry in turn is preferable for studying the edge properties. The presence of the edge however reduces already limited size of the bulk and thus worsens the finite-size effects.

The Hamiltonian of an electron in magnetic field is given by

$$H_{LLs} = \frac{1}{2m} \left( p + \frac{eA}{c} \right)^2,$$

(2.4)

where $A$ is a vector potential. This expression is obtained from the classical Hamiltonian of a charged particle in an electro-magnetic field [34] by replacing it’s momentum\(^1\) with the momentum operator [35].

The choice of the geometry also fixes a gauge for the vector potential. However, independently of the gauge choice, the Hamiltonian of an electron in a magnetic

\(^1\)We call momentum the usual momentum of the particle $p$ in the absence of the field. The generalized momentum $P = \partial L / \partial \nu$ is given by $P = p + \frac{eA}{c}$. 

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FQHE: Basics and implementation

Field can be written in the form identical to a harmonic oscillator. This is shown explicitly for the case of Landau gauge in Section 8.3.4. This means that as for the harmonic oscillator the eigenvalues of the Hamiltonian will be equally separated energies $E_n = \hbar \omega_c (n + 1/2)$ (with $\omega_c$ - cyclotron frequency and $n$ - a non-negative integer number) called Landau levels.

Most of the results in this thesis were obtained in spherical geometry and a small portion on a torus.

All the calculations are performed for the constant particle and flux numbers, spin and total momentum (linear for torus, angular for the disk and sphere ($L_z$)).

We give a brief overview of the disk and torus geometries and somewhat more detailed description for the sphere to introduce the notation used throughout.

2.2.1 Disk

Symmetric gauge is used with the vector potential given by

$$A = \frac{B \times r}{2} = \frac{B}{2} (-y, x, 0)$$

Projection of the angular momentum on the $z$ axis $m$ is a suitable quantum number to label one-particle states. These states are located around the circles of radius $\sqrt{2m\ell_c}$, along which the electron "guiding centre" is moving [11]. The cyclotron orbit that determines the energy is of much smaller radius. Quantum number runs from 0 to (generally) infinity. In practice the effective maximum quantum number and the electron density can be fixed by using the confining positive background covering certain number of circular states or([36]) by setting the total momentum to be $M = \frac{N_{el}(N_{el}-1)}{2\nu}$ (to obtain the filling factor $\nu$).

Matrix elements for the full Coulomb and for the short-range potential are written out in Refs. [36, 11]. For the short-range potential data about the 3 lowest states for a number of values of total momentum for the case of 10 electrons can be found in the supplementary materials of the Ref. [37]. For the case of full Coulomb potential rough comparison was done with Ref. [38] and the pure Coulomb potential results of Ref. [39] were reproduced exactly.

Pseudopotentials $V_m$ for the full Coulomb interaction can be found in the book [40] on p.73 and in the Ref. [38] (Eq.7). Matrix elements in terms of the PP coefficients are written out in Eq. 6 in Ref. [38]. In this equation, however, $(m_1+m_2)!$ must be replaced by $(m_1+m_2-m)!$ (otherwise matrix elements grow as $m!$ and the results are apparently wrong). We checked that the corrected formula with the Coulomb PP coefficients calculated up to $V_{83}$ yields the ground state energies in agreement with Ref. [39]. Same formula used with only $V_1$ non-zero (short-range regime) gives results that agree with Ref. [37].
2.2 Geometries

2.2.2 Torus

Torus geometry is obtained when periodic boundary conditions are imposed in both dimensions of a flat rectangle. A free parameter remains the ratio of the rectangle sides which can be tuned to favour some of the phases. To obtain the magnetic field perpendicular to the surface the gauge is fixed to be \( A = B(0, x, 0) \). One-particle states can be labeled by the linear momentum quantum number \( k_y \) and have the shape of stripes in y-direction that are located around \( x = k_y l_c^2 \). These stripes are analogous to the "guiding center" circles in the disk geometry and all have identical energy. Coulomb matrix elements are written out in Ref. [41].

In literature positive background potential is sometimes used to cancel out the \( q = 0 \) term from the Coulomb Fourier image \( 2\pi/q \). Expression for the energy shift due to the positive background can be found in the Ref. [42].

In what follows we will refer to the torus pseudopotentials as "planar".

2.2.3 Sphere

To create uniform radial magnetic field through the surface of a sphere a magnetic monopole of integer strength \( 2Q \), which produces the magnetic flux of \( 2Q\phi_0 \) through the surface of the sphere. One-particle eigenfunctions in this setup are described by the generalised spherical harmonics [11] \( Y_{Q,l,m} \), where \( Q \) is the half-integer quantum number that determines the magnetic flux, and \( l = Q + n \) and \( m = -l..l \) - are familiar quantum numbers that can be associated with angular momentum and its projection on the z axis. Here, the non-negative integer value \( n=0,1,... \) is the Landau level index. For any given calculation we will fix the flux to match the desired filling factor and thus for a given Landau level the only "free" quantum number labelling single-particle states is \( m \).

An unusual property of the sphere is the existence of a "shift" \( S \) - an integer that enters the relation between the number of electrons \( N_e \) and the number of flux quanta \( N_\Phi \). Depending on the universality class of the ground state for a given filling \( \nu \) it will appear on the sphere for

\[
N_\Phi = \nu^{-1} N_e - S. \tag{2.6}
\]

There are two conventions in literature for defining the radius of the sphere. One approach fixes the radius to be \( R = \sqrt{Ql_c} \). With this choice all the finite system sizes corresponding to a given filling factor have due to the "shift" a slightly different electron density. This creates a systematic error in case the finite-size results are used for extrapolations to infinite number of particles.

The radius definition put forward by R. Morf defines \( R = \sqrt{\frac{N_e}{2\nu} l_c} \) and guarantees that at fixed filling all the finite system sizes have the same electron density.
To convert the results obtained with both definitions one can redefine the magnetic length as explained in Ref. [43]. Note that both definitions are only relevant for the extrapolation of energy gaps but lead to the same wavefunctions. We will use Morf’s radius definition for the calculations that involve spherical pseudopotentials and energy gap extrapolation.

Following the common practise most of the calculations will be performed in the sector of total angular momentum projection of 0. States with all possible values of the total angular momentum will be represented in this sector. All valid FQHE ground states are uniform and thus have 0 total angular momentum.

Spherical pseudopotentials for the pure Coulomb interaction in the lowest Landau level are written down in Ref. [44] (Eq. 24).

Consider a pair of electrons on the sphere with the total angular momentum of $L_{\text{tot}}^{(2)}$. As discussed in more detail in Ref. [32] the smaller is the value of $2Q - L_{\text{tot}}^{(2)}$ the smaller is the mean separation between particles. This means that minimal $2Q - L_{\text{tot}}^{(2)}$ corresponds to the "short-range" term on the sphere. Thus $V_{2Q-L_{\text{tot}}^{(2)}}$ is the spherical pseudopotential that corresponds to $V_{L_{\text{tot}}^{(2)}}$ in planar geometry.
2.3 Finite thickness of the 2DEG

In a typical experimental device depicted in Fig. 1.2 electrons are confined in one of the dimensions within a quantum well. When the magnetic field is perpendicular to the resulting 2DEG the electron motion in \( z \)-direction and \( xy \)-plane is decoupled. Thus one can solve the corresponding Schrödinger equations independently. Furthermore, following the commonly accepted approach in literature [45] we neglect the dependence of the \( z \) wavefunction \( \xi(z) \) on the magnetic field.

The strategy for incorporating the finite thickness effect will be as follows. We first consider a one-dimensional problem along the \( z \)-direction and solve for the electron density. Next, based on the density in \( z \)-direction, we find the effective interaction \( V_{\text{eff}} \) between electrons in the \( xy \)-plane. Finally, we exactly solve the problem of electrons restricted to 2 dimensions and interacting with \( V_{\text{eff}} \).

2.3.1 One-dimensional problem

Effective mass approximation, that works quite well for GaAs, allows to parametrize the electron motion in the conduction band by means of piecewise-constant effective electron mass, dielectric constant, conduction band offset and Fermi energy. These parameters are defined by the structure of the sample in the \( z \) direction and particular values for many semiconductor materials can be found in Refs. [46, 47].

The potential landscape for a one-body problem is augmented by the electrostatic potential due to the electron density and electron-electron interactions potential.

To obtain electron density profile \( \xi^2(z) \) in \( z \) direction Poisson and Schrödinger equations have to be solved self-consistently. Potential term can be written as:

\[
V(z) = V_{sc}(z) + \varphi(z) + V_{XC}(z),
\]

with \( V_{sc}(z) \) - confinement potential defined by the semiconductor layout, \( \varphi(z) \) - electrostatic Hartree potential entering Poisson equation and \( V_{XC}(z) \) - exchange-correlation term that takes into account electron interactions. A possible choice for the \( V_{XC}(z) \) is the Hedin and Lundqvist form of the local density approximation (LDA) (eq. 11 in ref.[45]). We note however that in practice the solutions for electron density with and without the exchange-correlation term rarely differ by more than 10 percent and thus it is often justified to neglect the \( V_{XC}(z) \).

The Fermi energy is chosen such that the total electron density matches the sheet density known from the experiment. The density is normally estimated assuming the non-interacting electron gas density of states in \( xy \)-plane [48] and taking into account the number of filled "subbands" in \( z \)-direction. Note that this energy is almost always different from the sheet density of doping that has been
built into the sample. Some of the electrons are trapped by the so-called \( \text{Dx-centers} \) [49] while some others may be trapped by the surface states on the surface of the device. None of them are mobile and thus do not contribute to the measured density. In case the energy level of the surface states is located in the gap of the bulk semiconductor their high density of states can accommodate virtually arbitrary number of electrons which leads to the effect known as "Fermi-level pinning" when the Fermi level becomes "pinned" to the energy of the surface states and thus determines one of the boundary conditions. In turn the \( \text{Dx-centers} \) electrons can be considered to just neutralise the positive doping atoms that released them and can thus be completely eliminated from the problem.

To obtain a self-consistent solution Schrödinger and Poisson equations can be solved every iteration until the convergence is reached [48]. On the other hand the predictor-corrector scheme developed in Ref. [50] allows to estimate the small change in the wavefunction based on the small change in the potential. This way the number of times the Schrödinger equation is solved and the time-to-solution can be reduced significantly. Similar idea is used by the nextNano software [51] that however doesn’t include the exchange-correlation potential.

In our work we use the Schrödinger–Poisson solver developed as a modification of the 1D solver provided by C. May [48] which has been tested to give the results identical to nextNano in the absence of the exchange-correlation term. The result of such calculation is the electron density as a function of \( z \) coordinate \( \xi^2(z) \).

Given the electron density in \( z \)-direction we can obtain the effective interaction in two dimensions as follows

\[
V_{\text{eff}}^{2D}(r_1^{2D} - r_2^{2D}) = \frac{e^2}{\epsilon} \int dz_1 \int dz_2 \frac{|\xi(z_1)|^2 |\xi(z_2)|^2}{\sqrt{r_1^{2D} - r_2^{2D}}^2 + (z_1 - z_2)^2} \tag{2.8}
\]

### 2.3.2 Finite thickness in planar geometry

The results of this section are equations 2.15 and 2.16 that allow to calculate the pseudopotentials in planar geometry for arbitrary Landau level and arbitrary electron density distribution in the \( z \)-direction.

The planar pseudopotentials can be readily calculated in terms of the Fourier transform of the effective interaction which we are going to derive.

**Fourier transform for the 2-body interaction**

\[
V(k) = \frac{1}{2\pi} \int d^2r V(r) e^{-ikr} = \frac{1}{2\pi} \int_0^\infty rdr \int_0^{2\pi} d\Theta V(r) e^{-ikr \cos \Theta}. \tag{2.9}
\]

Note that our \( V(r) = V_{\text{eff}}^{2D}(r_1^{2D} - r_2^{2D}) \) in Eq. 2.8 is a purely real, even function of \( r \). Thus also the Fourier-transform will be real and we can change \( e^{-ikr} = \cos(kr) \)
2.3 Finite thickness of the 2DEG

and remember that the resulting \( \Theta \) integral is equal to the Bessel function (see for instance p.15 in [11])

\[
V(k) = \frac{1}{2\pi} \int_0^\infty r dr V(r) \int_0^{2\pi} d\Theta \cos(kr \cos \Theta) = \int_0^\infty r dr V(r) J_0(kr) \tag{2.10}
\]

Now we insert the expression for \( V(r) \)

\[
V(k) = \int dz_1 \int dz_2 |\xi(z_1)|^2 |\xi(z_2)|^2 \int_0^\infty dr \frac{r J_0(kr)}{\sqrt{(z_1 - z_2)^2 + r^2}} \tag{2.11}
\]

where the integral over \( r \) resembles a standard Bessel integral [52]

\[
\int_0^\infty t^{\nu+1} J_\nu(\alpha t) dt = \frac{\alpha^\nu z^{-\mu}}{2^\mu \Gamma(\mu + 1)} K_{\nu-\mu}(\alpha z) = T, \tag{2.12}
\]

with \( \nu = 0, \mu = -1/2, \alpha = k, z = |z_1 - z_2| \). In our case

\[
K_{1/2}(kz) = \sqrt{\pi/2} e^{-kz} (kz)^{-1/2}, (kz) > 0 \tag{2.13}
\]

and

\[
T = \sqrt{\frac{2}{k\pi}} |z_1 - z_2| K_{1/2}(k|z_1 - z_2|) \tag{2.14}
\]

Finally, the Fourier transform of the effective two-body interaction is given by

\[
V(k) = \frac{e^2}{\epsilon k} \int dz_1 \int dz_2 |\xi(z_1)|^2 |\xi(z_2)|^2 e^{-k|z_1 - z_2|}. \tag{2.15}
\]

Planar pseudopotentials with finite thickness

In terms of the obtained Fourier transform the 2-body pseudopotentials can be calculated as (see for instance Eq. (8.2.9) in [18])

\[
V_m = \int_0^\infty k dk V(k) [L_n(k^2/2)]^2 L_m(k^2) e^{-k^2}, \tag{2.16}
\]

where \( n \) is Landau level index and \( L_n \) - Laguerre polynomials.

If we consider the case of ideal Coulomb with \(|\xi(z)|^2 = \delta(z)\) then the expression 2.16 reduces to

\[
V_m = \int_0^\infty dk [L_n(k^2/2)]^2 L_m(k^2) e^{-k^2}, \tag{2.17}
\]

which in the lowest Landau level (\( n = 0 \)) evaluates to

\[
\frac{1}{2\sqrt{\pi}} \text{Hypergeometric2F1}[1/2, -m, 1, 1] \quad (\text{Mathematica syntax}). \quad \text{Numerical values agree precisely with the values of pseudopotentials for disk geometry and pure Coulomb interaction (see for instance p.73 in Ref. [40])}.
\]
Equations 2.16 and 2.17 are precise for planar geometry, we will refer to them as "planar pseudopotentials". However for various reasons they are sometimes used in the literature for calculations also in spherical geometry. The results have been reported [53] to show no qualitative difference and it was argued planar pseudopotentials might even be better for extrapolating to the infinite system sizes.

To have the commonly used units of $\frac{e^2}{\epsilon l_c}$ for $V_m$ one needs to have dimensionless k in units of $1/l_c$: $k_{\text{real}} = k * (1/l_c)$. This means that in eq. 2.15 z must also be made dimensionless in a way compatible with k. Namely, converted to the units of magnetic length: $z_{\text{real}} = z * l_c$.

**Analytical integration in the lowest Landau level $n = 0$.**

In the lowest Landau level ($n = 0$) the first Laguerre polynomial in eq. 2.16 is just 1. Eq. 2.15 can be substituted into eq. 2.16 and integration over k can be performed analytically leading to the following expression for the pseudopotentials

$$V_m = \frac{e^2}{\epsilon} \int dz_1 \int dz_2 |\xi(z_1)|^2 |\xi(z_2)|^2 \frac{1}{2} \text{HypergeometricU}[1/2, 1/2 - m, |z_1 - z_2|^2/4]$$

(2.18)

, with HypergeometricU - confluent hypergeometric function given here in the Mathematica syntax. In C++ GSL library [54] can be used and the corresponding function has the name gsl_sf_hyperg_U_e(). Note that confluent hypergeometric function has irregularity for $|z_1 - z_2| = 0$. In this case the integral over k reduces however to the integral for ideal Coulomb potential so the value of ideal Coulomb $V_m$ can be substituted instead. In our code this value can be computed with the function PlanarIdealCoulombVmLLL(m) defined in FQHHamiltonian-Sphere.h or by calling GSL function

gsl_sf_hyperg_2F1_e(0.5, -m, 1.0, 1.0, &gslIntegralAtZero)

which give precisely the same result.

For the second and higher Landau levels integral over k can still be done analytically and the result contains then the Hypergeometric function of higher orders ($2F_2$ for SLL, generalised Hypergeometric function in general case). These are not currently implemented in BOOST or GSL. Therefore, currently, for all LL other than the lowest one both integrals are done numerically.

We performed a test to compare analytical integration in the LLL against numerical integration. For the case of 2000 grid points in k-space it was found that the pseudopotentials agree with 8 to 16 digits precision which allows one to expect adequate integration precision for the higher LL case where only numerical integration can be done.
2.3 Finite thickness of the 2DEG

Figure 2.1: Experimental device structures used to reproduce the results of Ref. [45].

2.3.3 Planar finite thickness: reproducing published results

Comparison to Ref. [45]

To test the presented framework we reproduce the results of Ref. [45] by first, calculating self-consistently the electron density profile in \( z \)-direction given the experimental sample parameters and then calculating the corresponding pseudopotentials.

Unfortunately, many details of the simulations performed in Ref. [45] (dielectric constant, magnetic field, effective mass) are not given or can only be extracted from the experimental paper referenced in Ref. [45] with some limited precision which in turn limits the precision of the agreement expected. We used the following parameters: \( \epsilon = 13.18, m_{\text{eff}} = 0.067 \) of bare electron mass that were considered to be constant over the whole \( z \) domain. Magnetic field used for the parabolic quantum well (PQW) was taken to be 6.25 Tesla. The structure simulated is shown in the Fig. 2.1 with the maximal depth of both wells of 0.276eV. Fig. 2.2
Figure 2.2: Density profiles (shown in arbitrary units) for different total sheet densities of 4.9, 6.0, 7.3 and 8.5 (10^{10} \text{cm}^{-2}) calculated self-consistently to reproduce the results of Ref. [45]

shows the density profiles obtained for the PWQ with sheet densities of 4.9, 6.0, 7.3 and 8.5 (10^{10} \text{cm}^{-2}). The results are in very good qualitative agreement with Fig. 2a of Ref. [55] which is referenced by Ref. [45] for experimental details.

Pseudopotentials evaluated for the sheet density equal to 4.9E10(1/cm^2) agree with the values quoted in Ref. [45] up to 4 digits. Similar agreement was also observed for the square quantum well.

2.3.4 Finite thickness for spherical geometry

In this section we derive the two-body spherical pseudopotentials including the finite thickness effect.

There are two ways to approach the problem. One starting point can be the effective two-dimensional interaction Eq. 2.8. It is already "softened" after the 3rd dimension has been integrated out and now in spherical geometry we would allow both vectors $r_1^{2D}$ and $r_2^{2D}$ to live on the surface of the sphere of radius $R$. Integrat-
2.3 Finite thickness of the 2DEG

ing out the third dimension according to Eq. 2.8 is closest to the experiment where
the experimental sample is actually planar and the finite-thickness-dimension is
perpendicular to it. Most of the results in this section will be related to the choice
discussed and as well the "spherical finite thickness pseudopotentials" will refer to
this case throughout the text. The effective interaction can be written in this case
in the form

\[ V_{\text{eff}} = \frac{e^2}{\epsilon} \int dz_1 \int dz_2 \frac{|\xi(z_1)|^2|\xi(z_2)|^2}{\sqrt{2R} \sqrt{a(z_1, z_2) - \cos \gamma}}, \quad (2.19) \]

with real coefficient

\[ a(z_1, z_2) = 1 + \frac{(z_1 - z_2)^2}{2R^2} \geq 1 \quad (2.20) \]

Alternatively, one could consider an interaction \(1/|r_1 - r_2|\) where the two
vectors live within a spherical shell spanning from radius \(R - \Delta/2\) to \(R + \Delta/2\),
where \(R\) is the radius determined by the number of electrons and fluxes and \(\Delta\) is
the finite thickness. In this case we denote \(|r_1| = R + z_1\) and \(|r_2| = R + z_2\) and
the effective interaction given by

\[ V_{\text{shell}}^{\text{eff}} = \frac{e^2}{\epsilon} \int dz_1 \int dz_2 \frac{|\xi(z_1)|^2|\xi(z_2)|^2}{\sqrt{B(z_1, z_2) \sqrt{a(z_1, z_2) - \cos \gamma}}}, \quad (2.21) \]

with real coefficients

\[ a_{\text{shell}}^{\text{eff}}(z_1, z_2) = \frac{2R^2 + 2R(z_1 + z_2) + z_1^2 + z_2^2}{2(R + z_1)(R + z_2)} \geq 1 \quad (2.22) \]

and

\[ B_{\text{shell}}^{\text{eff}}(z_1, z_2) = 2(R + z_1)(R + z_2) > 0. \quad (2.23) \]

In both cases the dependence on the spherical coordinates is only through a
function of the angle between the two vectors

\[ f(\cos \gamma) = \frac{1}{\sqrt{a - \cos \gamma}}. \quad (2.24) \]

Note that the pure Coulomb interaction is a special case with \(a = 1\).

Such a function can be expanded in the complete, orthogonal basis of Legendre
polynomials

\[ f(x) = \sum_{l=0}^{\infty} A_l P_l(x), \quad (2.25) \]

with the expansion coefficients given by

\[ A_l = \frac{2l + 1}{2} \int_{-1}^{1} f(x) P_l(x). \quad (2.26) \]
For each \( l \) the integration over \( z_1 \) and \( z_2 \) can be performed numerically and we define
\[
\tilde{A}_l = \frac{1}{\sqrt{2R}} \int dz_1 \int dz_2 |\xi(z_1)|^2 |\xi(z_2)|^2 A_l(z_1, z_2).
\] (2.27)

For the case of pure Coulomb all \( \tilde{A}_l = 1/R \).

Legendre polynomials are related to the (generalised) spherical harmonics as follows
\[
P_l(\cos \gamma) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_{0lm}^* (\theta_1, \phi_1) Y_{0lm} (\theta_2, \phi_2).
\] (2.28)

Thus the 2-body interaction can finally be written as
\[
V_{\text{eff}}(r_1, r_2) = \frac{e^2}{\epsilon} \sum_{l=0}^{\infty} \frac{A_l}{2l+1} \sum_{m=-l}^{l} Y_{0lm}^*(r_1) Y_{0lm}(r_2).
\] (2.29)

Now, remembering that the basis states on the sphere are generalised spherical harmonics
\[
|l_n, m_1, l_n, m_2\rangle = Y_{Ql_n, m_1} (r_1) Y_{Ql_n, m_2} (r_2),
\] (2.30)

the calculation of the matrix elements \( \langle l_n, m_1, l_n, m_2 | V_{\text{eff}} | l_n, m_3, l_n, m_4 \rangle \) reduces to the known integrals of their products properties of which are listed in detail in Ref. [11].

Finally, in terms of the Clebsh-Gordan coefficients the matrix elements are given by
\[
\langle l_n, m_1, l_n, m_2 | V_{\text{eff}} | l_n, m_3, l_n, m_4 \rangle =
\]
\[
e^{-2l_n} \sum_{m=0}^{l_n} (-1)^{m_3-m} \langle l_n, m_1; l, m | l_n, m_3 \rangle (\langle l_n, Q; l, 0 | l_n, Q \rangle)^2 \langle l_n, m_2; l, -m | l_n, m_4 \rangle
\]
\[
\] (2.31)

and the spherical pseudopotentials that include finite thickness by
\[
V_L = \frac{e^2}{\epsilon} \sum_{l_n} \sum_{m_1=-l_n}^{l_n} \langle l_n, m_1; l_n, -m_1 | 2l_n - L, 0 \rangle \langle l_n, m_3; l_n, -m_3 | 2l_n - L, 0 \rangle *
\]
\[
\sum_{l=[m_3-m_1]}^{2l_n} \tilde{A}_l (-1)^{l-m_3+m_1} (\langle l_n, Q; l, 0 | l_n, Q \rangle)^2 (\langle l_n, m_1; l, m_3 - m_1 | l_n, m_3 \rangle)^2.
\] (2.32)

Note that the pseudopotential \( V_L \) corresponds to the total angular momentum of a pair of electrons of \( 2l_n - L \) and the flux penetrating the spherical surface is \( 2Q\phi_0 \).
2.3 Finite thickness of the 2DEG

2.3.5 Reproducing published results in spherical geometry

In this section we reproduce and extend to higher system sizes the results of Ref. [43] that quotes the energy gaps of various FQHE states including $\nu = 5/2$ calculated with both ideal Coulomb and finite thickness pseudopotentials in spherical geometry.

First, we reproduced the results of Ref. [43] for pure Coulomb interaction up to the precision with which data can be read off the plots. Our results for the quasiparticle-quasihole and exciton energies agree with the lowest Landau level Figs. 2 and 3 of Ref. [43] for all shown system sizes. As an example of our data in the second Landau level we show in Fig. 2.3 the exciton energies we obtained for pure Coulomb interaction at $\nu = 5/2$, our plot appears identical to the Fig. 13 of Ref. [43].

![Figure 2.3: Exciton energies for pure Coulomb interaction as a function of the inverse system size (number of electrons)](image)

In Fig. 2.4 we compare the quasiparticle-quasihole energy gap calculated with different models of finite thickness. The data obtained with spherical pseudopotentials (blue and red datapoints) reproduces the data shown in Fig. 14 of Ref. [43]. Compared to Ref. [43] we have however one higher system size (18 electrons) for the finite thickness data (red data points, compare to the lowest line in Fig. 14 of Ref. [43]). The additional data point shifts the extrapolated value to higher values...
Figure 2.4: Quasiparticle/quasihole energies calculated for the electron density in \( z \)-direction of the "Gaussian" form \( \xi(z) \sim e^{-\frac{(z-\alpha w)^2}{4w^2}} \) (Eq. 20 in Ref. [43]) with the width parameter \( w/l_0 = 1.17 \). For the spherical pseudopotentials the finite thickness in \( z \)-direction was integrated out according to Eq. 2.19. The results for Eq. 2.21 (not shown) differ by not more than 1-2 percent. Pure Coulomb interaction was assumed for the background energy and energy gap corrections. The sse value quantifies the error of the linear fit.

which we discuss in some more detail in Section 6.9 and caption of Fig. 6.15.

We observe that independently of the model used finite thickness reduces the energy gap albeit by smaller amount than concluded in Ref. [43] where the finite thickness data for \( N_e = 18 \) was not available. Overall we conclude that using spherical or planar pseudopotentials leads to qualitatively the same results.
The FQHE Hamiltonian within a certain Landau level written in the second quantisation form reads:

\[
H = \sum_{m_1,m_2,m_3,m_4} a_{m_1}^\dagger a_{m_2}^\dagger a_{m_3} a_{m_4} \langle m_1,m_2|V|m_3,m_4\rangle + \\
\sum_{m_1,m_2,m_3,m_4,m_5,m_6} a_{m_1}^\dagger a_{m_2}^\dagger a_{m_3}^\dagger a_{m_5} a_{m_6} a_{m_4} \langle m_1,m_2,m_3|V|m_4,m_5,m_6\rangle,
\]

(3.1)

where \(m\) is the quantum number labelling one-particle orbitals and \(a_{m_i}^\dagger\) is the operator that creates an electron in the \(m_i\)th state. The 2- and 3-body matrix elements \(\langle m_1,m_2|V|m_3,m_4\rangle\) and \(\langle m_1,m_2,m_3|V|m_4,m_5,m_6\rangle\) can be readily computed for a given set of pseudo potentials.

We diagonalise this Hamiltonian numerically and calculate 1-2 lowest eigenvalues for typically 8-24 electrons. Following information can be extracted from the eigenvector:

- overlap with a model wave function to see how well it describes the exact state.
- entanglement entropy and entanglement spectrum of the 2 parts of the system which turned out to be extremely useful for locating a phase transition and for phase characterisation.
- pair correlation function

Eigenvalues can be used to estimate the gap energy. Normally the gap is calculated for a set of system sizes and is then extrapolated in \((1/N_e)\) to the infinite system.

### 3.1 Algorithms and codes

Lowest eigenvalues and eigenvectors are computed using the Lanczos algorithm [56] implemented in the ALPS project [57]. This eigensolver is templated on the Hamiltonian class defining the matrix-vector multiplication function.
multiply(const VectorT& w, VectorT& v)

that takes a vector $w$ multiplies it by the Hamiltonian matrix and returns the result in the vector $v$. This function represents the most important part of the code from the computational perspective. To obtain the lowest eigenvalues, Lanczos performs multiple calls (typically 400-600) of the multiply function.

### 3.1.1 Parallelisation approach

Parallelisation is performed by means of MPI+OMP for dividing the workload. In addition to that, each node fills up the available memory by independently precomputing a fraction of (or all) matrix elements it needs.

We need to perform calculations for multiple system sizes. For some of them the matrix representation of the Hamiltonian can be completely stored in memory which leads to a very significant speedup. For the biggest systems the Hilbert space is so large that only a few vectors fit into the node memory and the matrix cannot be precomputed. In our code, the amount of memory per node that is used to store matrix elements is a parameter. The strategy is to get the maximum possible speedup by using all the available memory for precomputing the matrix elements.

When the program starts with $N$ MPI tasks, every task performs identical Lanczos and other lightweight operations. MKL Lapack calls of Lanczos are parallelised over all cpus available on a node by means of OMP but typically constitute a negligible fraction of the cpu time. The heaviest part of the code - the multiply() function - is parallelised as follows. When the Hamiltonian class is initialised, the Hilbert space is divided equally between the nodes, defining the indices $\text{MPIstartInd}$ and $\text{MPIstopInd}$ that mark the first and the last basis states that will be processed by a certain MPI task. After that for a predefined number of basis states, matrix elements are precomputed ($\text{precomputedMEL}$) and stored in memory such that these matrix elements use up the allowed amount of memory. The parallelised multiply() function is sketched below:

```cpp
multiply(const VectorT& w, VectorT& v){
VectorT lV

// ======================= part that uses precomputed mel begin
#pragma omp parallel for
for( i=\text{MPIstartInd}; i<=\text{MPIstartInd+numOfBasisStatesPrecomp}; ++i){
  tmp = 0;
  melIndex = index where the matrix elements that belong to state $i$ begin
  for(# of matrix elements that belong to state $i$)
```
tmp += precomputedMEL[melIndex] * w[ precomputedIndeces[melIndex] ];
    melIndex++;
}
1V[i-MPIstartInd] += tmp;
} // basis i
// ======================= part that uses precomputed mel end

// ======================= on-the-fly part begin
#pragma omp parallel for schedule(dynamic,1)
for( i=MPIstartInd+numOfBasisStatesPrecomp; i<=MPIstopInd; ++i){
    tmp = 0;
    state = index2State(i);
    for( all terms term of the Hamiltonian applicable to state ){
        (weight, newState) = term(state);
        tmp += weight * w[ state2index(newState) ];
    }
    1V[i-MPIstartInd] += tmp;
}
// ======================= on-the-fly part end
MPI_Allgatherv(&1V[0],1V.size(),MPI_DOUBLE,&v[0],rc,dis,MPI_DOUBLE, MPI_COMM_WORLD);
}

Each of the nodes computes the part of the vector \( v \) for its assigned range of basis states in the \( 1V \) vector. In the very end the full vector \( v \) is assembled using a single collective MPI call. As a result each node has the full vector \( v \) and the Lanczos iteration can continue.

Although quite simple this parallelisation approach allows to perform the computationally heaviest operations locally and gives a quite good scaling as discussed in the next section.

### 3.1.2 Parallelism and scaling

Scaling analysis was performed on the cpu partition of the Piz Daint machine at CSCS.

We analyse the scaling behaviour for the system of 14 electrons at 38 orbitals. This corresponds to the filling fraction 12/5 and the shift equal to -2. Hilbert space dimension in this case is 115195490 = 1.15 * 10^8, which corresponds to the vector \( (w \text{ or } v) \) size of 879Mb. We use full 3-body Hamiltonian that arises when Landau level mixing is included. The experience of the previous projects shows that this is
3.1 Algorithms and codes

Figure 3.1: Strong scaling for the target system size where the matrix has linear dimension $115195490 = 1.15 \times 10^8$

the maximum system size that is meaningful to use for our purposes where 3-body Hamiltonian has to be diagonalised for a number of various parameters.

We let the Lanczos perform 20 iterations (10 for eigenvalues calculation and 10 for eigenvectors) and use the time elapsed for the strong scaling analysis. We exclude the initialisation time since it will become negligible in the production runs where 800 iterations are typically performed. MPI_Wtime() is used for time measurements. The corresponding timings in seconds are shown in the table.

<table>
<thead>
<tr>
<th>14 nodes</th>
<th>28 nodes</th>
<th>56 nodes</th>
<th>112 nodes</th>
<th>224 nodes</th>
<th>448 nodes</th>
<th>896 nodes</th>
</tr>
</thead>
<tbody>
<tr>
<td>6931.1</td>
<td>3457.5</td>
<td>1709.7</td>
<td>851.2</td>
<td>420.7</td>
<td>204.1</td>
<td>97.12</td>
</tr>
</tbody>
</table>

On each node we use 20000Mb of memory to precompute the matrix elements.
When running on 14 nodes (112 cpus) this corresponds to approximately 1.35% of the total number of matrix elements. For 448 and 896 nodes this is 43.5% and 86% respectively (note that the percentage varies slightly between MPI tasks). This is the key for the scaling behaviour we observe in Fig. 3.1: precomputed part of the matrix can be processed much faster. The communication overhead due to the increase of the cpu count is compensated by the reduction of the number of matrix elements we have to calculate on-the-fly.
4 FQHE: Experimental devices and finite width effect

In this chapter we study the fractional quantum Hall effect in the experimental devices grown in the group of Prof. Wegscheider at ETH.

For each device we first perform a one-dimensional self-consistent calculation to obtain the electron density profile in \( z \)-direction. Based on this profile for each device we calculate the pseudopotentials that include the device-specific finite thickness effects as described in Section 2.3. Finally, we perform the exact diagonalisation of finite systems and study the influence finite thickness of the 2DEG has on the parameters of the fractional quantum Hall state at \( \nu = 5/2 \).

4.1 Experimental devices

In Table 4.1 we summarise the information about the devices we considered. This information along with the precise layout of each device was supplied by Christian Reichl from the group of Prof. Wegscheider. All the devices are intended for the \( \nu = 5/2 \) fractional quantum Hall experiments and for all of them the \( \nu = 5/2 \) FQHE gap has been measured experimentally.

4.2 Model profiles of the electron wavefunction in \( z \)-direction

Several model profiles for the electron wavefunction in the confined dimension have been suggested in literature. Their use is motivated by the possibility to easily parametrise the electron density in \( z \)-direction and to avoid the self-consistent calculation.

Having at our disposal the precise wavefunction calculated self-consistently for experimental devices we ask how well model wavefunctions describe the actual
4.2 Model profiles of the electron wavefunction in z-direction

Table 4.1: Devices. Spacer and quantum well (QW) lengths are given in Angstrom; electron density ($n_e$) in $10^{11} \text{cm}^{-2}$; electron mobility in $10^6 \text{cm}^2/\text{V} \cdot \text{s}$ and B is the magnetic field in Tesla at which the $\nu = 5/2$ FQH state was observed experimentally. The layout corresponding to the DS-QW type of doping is shown in Fig. 4.1.

<table>
<thead>
<tr>
<th>id</th>
<th>spacer</th>
<th>QW</th>
<th>doping</th>
<th>$n_e$</th>
<th>mobility</th>
<th>gap, mK</th>
<th>B,T</th>
<th>$l_e10^8, m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>D1110728B</td>
<td>750</td>
<td>300</td>
<td>DS-QW</td>
<td>2.81</td>
<td>23.21</td>
<td>47.98</td>
<td>5.05</td>
<td>1.143</td>
</tr>
<tr>
<td>D110922B</td>
<td>750</td>
<td>300</td>
<td>DS-QW</td>
<td>3.24</td>
<td>15.15</td>
<td>17.7</td>
<td>4.84</td>
<td>1.167</td>
</tr>
<tr>
<td>D120427C</td>
<td>1000</td>
<td>300</td>
<td>DS-QW</td>
<td>2.15</td>
<td>22.42</td>
<td>138.5</td>
<td>3.47</td>
<td>1.379</td>
</tr>
<tr>
<td>D120622A</td>
<td>1000</td>
<td>270</td>
<td>DS-QW</td>
<td>2.196</td>
<td>24.09</td>
<td>58.44</td>
<td>3.82</td>
<td>1.314</td>
</tr>
<tr>
<td>D120724A</td>
<td>800</td>
<td>300</td>
<td>DS-QW</td>
<td>2.591</td>
<td>19.8</td>
<td>50.68</td>
<td>4.43</td>
<td>1.22</td>
</tr>
<tr>
<td>D111114D</td>
<td>750</td>
<td>300</td>
<td>DS-QW</td>
<td>3.133</td>
<td>16.6</td>
<td>19.40</td>
<td>5.24</td>
<td>1.218</td>
</tr>
<tr>
<td>D120113C</td>
<td>1000</td>
<td>270</td>
<td>DS-trench</td>
<td>2.354</td>
<td>20.22</td>
<td>32.84</td>
<td>4.27</td>
<td>1.243</td>
</tr>
</tbody>
</table>

distribution of electrons.

We consider three model profiles. Two of them (Gaussian and $z$-Gaussian) have been found to be the most suitable for the description of experimental devices by an extensive publication [43]. The third model represents the ground state of a particle in an infinitely deep quantum well. The expressions for the three models read

$\triangleright$ Cos: $c_1 \ast \cos(c_2 \ast (z - c_3))$,

$\triangleright$ Gaussian: $A \ast \exp(-\frac{(z-B)^2}{(4w)^2})$,

$\triangleright$ $z$-Gaussian: $d_1 \ast (z - d_2) \ast \exp(-\frac{(z-d_2)^2}{(9w^2d_3^2)})$,

where $c_1, c_2, c_3, A, B, w, d_1, d_2, d_3$ are constant parameters.

These parameters can be adjusted to fit the wavefunction obtained self-consistently for an experimental sample.

In Fig. 4.2 we show such best fits along with the self-consistent electron wavefunction for the device D120113C (experimental doping quantity assumed). For this particular case cosine function represents the best fit out of the three model profiles considered.

Although the density plots give some idea about the quality of the fit we are actually interested in the extent to which this density difference effects the properties of the FQHE state. To evaluate this we first use Eq. 2.16 to calculate the pseudopotentials corresponding to each of the density profiles shown in Fig. 4.2. Next, we perform exact diagonalization for each of the density profiles and consider the
**Figure 4.1:** Experimental device layout [20] corresponding to the DS-QW type of structure. The main quantum well that hosts the 2DEG is the region 6 and is composed of GaAs. Doping (regions 3 and 9) is placed on both sides of the quantum well. The cap layer (region 1) is composed of GaAs and is intended to prevent the Al in the following region 2 (AlGaAs) from oxidation. Two small auxiliary quantum wells are placed in regions 4 and 8 between the doping and the main quantum well. The expected conduction band structure is shown schematically on the right.
4.2 Model profiles of the electron wavefunction in z-direction

self-consistent density as a reference. The diagonalization is performed for $\nu = 5/2$ and the system sizes of 10 and 14 electrons at the shift (see Eq. 2.6) corresponding to the Moore-Read Pfaffian model wavefunction. The result of the diagonalisation is the ground state wavefunction corresponding to each of the z-direction density profiles.

Finally, we compare how much the properties of these ground states differ from the reference ground state obtained for the self-consistent density. The most important observables here are the energy gap - the difference between the two lowest energy eigenstates and the Pfaffian overlap - the overlap between the ground state wavefunction and the model Pfaffian wavefunction.

We summarise the results for $N_e = 14$ in Table 4.2, the results for 10 electrons (not shown) are in good agreement with these.

As could be anticipated from Fig. 4.2 the minimum distortion of the ground state is achieved when the cosine model profile in z-direction is used. We note however that all three model profiles lead to quite small errors compared to the self-consistent case.
Table 4.2: Difference between various density profiles with the self-consistent profile as a reference. $\delta PP_{max}$ - is the maximum (over allowed angular momenta $L$) relative difference in the pseudopotentials (Eq. 2.16). $\delta Overlap$ - is relative difference for the Pfaffian overlap and $\delta \Delta$ is the relative difference for the energy gap max("roton" gap at $L = 4$ and quasiparticle-quasihole gap).

<table>
<thead>
<tr>
<th>Observable</th>
<th>Cos</th>
<th>Gaussian</th>
<th>z-Gaussian</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\delta PP_{max}$</td>
<td>0.09%</td>
<td>1.14%</td>
<td>1.45%</td>
</tr>
<tr>
<td>$\delta Overlap$</td>
<td>0.05%</td>
<td>0.55%</td>
<td>0.65%</td>
</tr>
<tr>
<td>$\delta \Delta$</td>
<td>0.24%</td>
<td>3.1%</td>
<td>3.8%</td>
</tr>
</tbody>
</table>

The self-consistent calculation takes the material parameters as input. Even for the well-studied materials such as GaAs their values variate depending on the source. The conduction band offset - the difference between the energy of conduction band in GaAs and AlGaAs controls the depth of the quantum well and could potentially effect the FQHE ground state the most compared to other material parameters.

In the Table 4.3 we present the error in pseudopotentials, energy gap and Pfaffian overlap that arises from the uncertainty in the conduction band offsets. This time a self-consistent calculation was performed 4 times for the 4 possible values of the conduction band offset available in the literature: Ref. [58] and minimal, recommended and maximal values from ref. [46] and the maximum difference between the four cases was considered.

Table 4.3: Maximal relative difference for different choices of the conduction band offsets. The data is presented for $N_e = 10$, $\nu = 5/2$ and the shift corresponding to the Moore-Read Pfaffian.

<table>
<thead>
<tr>
<th>Observable</th>
<th>maximal relative difference over 4 cases</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\delta PP$</td>
<td>0.03%</td>
</tr>
<tr>
<td>$\delta \Delta$</td>
<td>0.06%</td>
</tr>
<tr>
<td>$\delta Overlap$</td>
<td>0.06%</td>
</tr>
</tbody>
</table>

We see that the choice of the conduction band offsets changes the parameters of the FQHE state only negligibly compared to the errors introduced by using model density profiles.

We conclude with two points. First, any of the three model profiles can be safely
4.3 Results for the experimental samples

We study the properties of the $\nu = 5/2$ fractional quantum Hall states for the devices listed in Table 4.1. Our workflow for each of the device is as follows:

- solve 1D Schrödinger-Poisson equations $\rightarrow$ el. density in the 3rd dimension
- calculate effective interaction (pseudopotentials) in the equivalent 2D system
- calculate FQHE properties (gap, overlap,..)

An important property of the FQHS ground state is the energy gap. In Fig. 4.3 we show the quasiparticle-quasihole gap extrapolation for a few selected devices (compare to Fig. 14 in Ref. [43]). We use one additional higher system size (18el) for the finite thickness cases which was not available in Ref. [43]. Presence of this higher system size results in higher extrapolated energy gap than reported in
The results for all the devices are summarized in Table 4.4. Besides the energy gap we also present the overlap between the actual ground state for each device and the model Moore-Read Pfaffian wavefunction for the system with 18 electrons (Pf. overlap column in Table 4.4). We note that realistic finite thickness brings the state closer to the non-Abelian phase as the overlap for the experimental devices is always higher than for the pure Coulomb case.

Table 4.4: Gap energies and model wavefunction overlaps for a number of 5/2 experimental samples

<table>
<thead>
<tr>
<th>κ</th>
<th>Δ experiment, K</th>
<th>Δ q.p.-q.h., $\frac{e^2}{4\pi\epsilon_0 l_0}$</th>
<th>Δ q.p.-q.h., K</th>
<th>Pf. overlap</th>
</tr>
</thead>
<tbody>
<tr>
<td>pure Coulomb</td>
<td>0</td>
<td>0.02473</td>
<td>-</td>
<td>0.676542</td>
</tr>
<tr>
<td>D110728B</td>
<td>1.12</td>
<td>0.0458</td>
<td>0.02346</td>
<td>2.652</td>
</tr>
<tr>
<td>D110922B</td>
<td>1.15</td>
<td>0.0175</td>
<td>0.02352</td>
<td>2.603</td>
</tr>
<tr>
<td>D120427C</td>
<td>1.35</td>
<td>0.1371</td>
<td>0.0239</td>
<td>2.240</td>
</tr>
<tr>
<td>D120622A</td>
<td>1.29</td>
<td>0.0525</td>
<td>0.02294</td>
<td>2.256</td>
</tr>
<tr>
<td>D120724A</td>
<td>1.20</td>
<td>0.0492</td>
<td>0.02364</td>
<td>2.503</td>
</tr>
<tr>
<td>D111114D</td>
<td>1.10</td>
<td>0.0186</td>
<td>0.02343</td>
<td>2.698</td>
</tr>
</tbody>
</table>

Comparing the theoretical prediction for the energy gaps ($\Delta$ q.p.-q.h., K column in Table 4.4) with experimentally measured ($\Delta$ experiment, K column in Table 4.4) we observe that the experimentally measured gaps are about an order of magnitude smaller than the gaps obtained from an infinite system size extrapolation. Similar result is obtained (not shown) in case the so-called exciton gap energy is used instead of the quasiparticle-quasihole. This discrepancy is not new. A detailed review in Ref. [43] compared the experimental and theoretical results and concluded that the disorder broadening on the order of $2K$ is probably responsible for the observed difference.

Thus disorder present in experiment and absent in our model is one of the important ingredients that has to be understood in order to connect the experimental gap measurements with theory.

Another important approximation in our theory so far is the absence of Landau level mixing which is equivalent to assuming an infinite energy difference between Landau levels or in other words infinite magnetic field. One way to quantify the importance of Landau level mixing is by evaluating the ratio of the two relevant energy scales: the many-body gap energy unit (Coulomb energy scale $\frac{e^2}{4\pi\epsilon_0 l_0}$) and the cyclotron energy ($\hbar w_c$ - energy difference between Landau levels). We will
4.4 Conclusions

denote this ratio $\kappa$ and its value for the considered devices is shown in the second column of Table 4.4. We observe that the two energy scales are comparable for a typical experiment and thus Landau level mixing can potentially have significant impact.

We will devote Chapters 6 and 7 to a detailed study of the interplay between the Landau level mixing and finite thickness effects for the $\nu = 5/2$ and $\nu = 12/5$ FQH states. We will find that Landau level mixing indeed significantly reduces the energy gap for the $\nu = 5/2$ state and is responsible for the qualitative changes to the ground state.

Another important finding of Chapter 6 (see Fig. 6.15 in Section 6.9) is that within our model of finite thickness (no disorder, no roughness of quantum well boundaries etc) the only parameter of the electron density in the confined dimension that matters for the FQHE physics is the variance of the electron wavefunction in $z$-direction.

4.4 Conclusions

The results can be summarised as follows.

Parametrisation of the electron wavefunction in the confined dimension with a model profile leads to insignificant changes (order of 3 percent) in the predicted FQHE properties compared to the wavefunction calculated self-consistently. Thus any profile can be used as long as it’s parameters are optimised to match the self-consistent wavefunction. The uncertainty in the material parameters of the host structure does not affect the FQHE physics.

Finite thickness effect in experimental devices slightly reduces the energy gap of the $\nu = 5/2$ state but increases the overlap with the model Pfaffian wavefunction. Landau level mixing is the effect that may have significant impact on the properties of the $\nu = 5/2$ state for a typical experiment.
5

FQHE: Model

We introduce an effective Hamiltonian for spin-polarized electrons confined to the $N^{th}$ Landau level that incorporates the effects of finite width, Landau level and subband mixing, derived for GaAs heterostructures. This Hamiltonian will be used in Chapters 6 and 7.

The Hamiltonian we will use was derived in Ref. [29] and similar results were obtained in Refs. [30, 31]. In this Chapter we will explain the idea and strategy of the calculation [29] and the details can be found in the original publication.

Fig. 5.1 illustrates the key steps of the derivation. Starting from a bare Coulomb interaction $\frac{1}{r}$ one first introduces the finite thickness effects through integrating out the dimension perpendicular to the 2DEG. This leads to a modified interaction in two dimensions which however remains two-body and thus preserves particle-hole symmetry. As a next step the virtual transitions to higher quantum well subbands and other Landau levels are integrated out to the leading order in the parameter $\kappa = \frac{e^2/(\epsilon_0\hbar c)}{\hbar \omega_c} \approx 2.52/\sqrt{B[T]}$, which is the ratio of the Coulomb and cyclotron energies. The result is a further renormalised two-body interaction and the emergence of the particle-hole symmetry breaking three-body terms.

The resulting effective interaction is represented in terms of the two- and three-body pseudopotentials introduced in Section 2.1.

5.1 Finite width

Pseudopotentials can be derived in both the spherical and planar geometries. Because the planar pseudopotentials do not depend on the system size it is more convenient to compute the pseudopotentials that include effects of finite thickness and Landau level mixing in the planar geometry. The spherical pseudopotentials extrapolate to the planar pseudopotentials in the limit of a sphere of infinite radius, i.e., the thermodynamic limit (see Section 6.12). Further, it has been demonstrated
Finite thickness

\[ V_{\text{eff}}(r^2_D) = \frac{e^2}{\varepsilon} \int dz_1 \int dz_2 \frac{\psi_\xi(z_1) \psi_\xi(z_2)}{\sqrt{(z_1 - z_2)^2 + r^2_D}} \]

Figure 5.1: Schematic representation of the steps that lead to constructing the effective Hamiltonian that includes simultaneously the effects of Landau level mixing and finite thickness.

that using planar pseudopotentials in the spherical geometry does not lead to qualitative differences compared with using spherical pseudopotentials (see for example Ref. [59]).

Finite-width can be modelled in various ways however as we discuss in detail in Section 6.9 the FQHE results of all the models can be converted into each other since the only parameter that determines the properties of an FQHE state is the variance of the wavefunction in \( z \)-direction. Thus, we focus on only one parametrisation of finite thickness modelling the electron distribution in \( z \)-direction as a ground state of an infinitely deep square quantum well of width \( w \).

In the absence of Landau level and subband mixing the planar two-body pseudopotentials can be calculated using Eq. 2.16, where the finite width enters through the Fourier transform of the effective interaction (Eq. 2.15) as \( \xi(z) \) - the electron wave function in the \( z \)-direction. For a realistic experimental system, \( \xi(z) \) can be determined from solving the Schrödinger and Poisson equations
self-consistently. Here, we parametrise the finite width through \( w \) - the width of an infinitely deep square quantum well, hence, for the \( s \)th subband we have \( \xi(z) = \sqrt{2/w} \sin((s + 1)\pi z/w) \).

### 5.2 Landau level mixing

Finite width causes a ‘softening’ of the Coulomb interaction at short distances and the Coulomb interaction can now cause virtual electron excitations to higher subbands (excited states of the Schrödinger equation in the perpendicular to the 2DEG direction) in addition to higher Landau levels.

Importantly, the energy difference between the quantum well subbands is comparable to the energy difference between the Landau levels since the energy of an electron in Landau level \( n \) and in subband number \( s \) is given by \( E_n \equiv \hbar \omega_c [(n + 1/2) + (\pi^2/2w^2)(s + 1)^2] \) [29], where \( w \) is the width of the infinitely deep quantum well that we use to model finite thickness. Thus it is important to treat both effects on equal footing.

Hence, Landau level and subband mixing are taken into account perturbatively to first order in \( \kappa \) through the terms that are generated by virtual excitations of electrons to the \( N = 2, 3, \ldots \) Landau levels and higher quantum well subbands or of holes to the \( N = 0 \) Landau level (here the second Landau level \( N = 1 \) is the Landau level of interest). As noted in Ref. [29], virtual excitations into all unoccupied Landau levels are taken into account in this perturbative scheme producing a controlled model that is exact in the \( \kappa \rightarrow 0 \) limit.

Generally speaking, while the virtual transitions are integrated out the resulting effective action is frequency dependent which is equivalent to a retarded interaction. The frequency dependence enters the effective action through expressions of the type \( i(\omega_i - \omega_k) - (E_n - \mu) \). The transition to the Hamiltonian description in Ref. [29] is made by neglecting \( i(\omega_i - \omega_k) \) or in other words assuming that all the energies \( \omega_{i,k} \) in the system (\( \omega_i \) are energies of an electron in the LL of interest) are negligible compared to the (multiple of the cyclotron frequency) energy difference between the Landau level of interest and the Landau level virtual transition into which is considered \( (E_n - \mu) \).

The resulting effective Hamiltonian has the form:

\[
H(w/\ell_0, \kappa, N) = \sum_m V^{(2)}_m(w/\ell_0, \kappa) \sum_{i<j} \hat{P}_{ij}(m) + \frac{1}{3!} \sum_m V^{(3)}_m(w/\ell_0, \kappa) \sum_{i<j<k} \hat{P}_{ijk}(m) \tag{5.1}
\]

where \( \hat{P}_{ij}(m) \) and \( \hat{P}_{ijk}(m) \) are projection operators that project, respectively, the...
5.3 Qualitative picture

The pure Coulomb interaction is repulsive and is known to generate incompressible electron liquid. The model above starts off from the pure Coulomb at $\kappa = 0$ but what can be expected at finite $\kappa$?

Some intuition for the gaps under the modified effective interaction can be gained if we consider the corrections to the two-body pseudopotentials at $\kappa \neq 0$. For illustration purposes let’s consider the two-body pseudopotentials at $w = 3\ell_0, n = 1$ at $\kappa = 0$ and $\kappa = 0.1$ listed in the table 5.1.

---

1The precise values used (that have 2 more precision digits compared to Ref. [29]) are given in the file pseudopotentials.txt that can be found in the supplementary materials of Ref. [1].

2More generally, at $k^\text{th}$-order in $\kappa$, $k + 2$-body interactions are generated.
Table 5.1: The two-body planar pseudopotentials for the second Landau level (relevant for $\nu = 5/2, 12/5$) for $w = 3l_0$ and $\kappa = 0; 0.1$. The pseudopotentials corrections are taken from Ref. [29].

<table>
<thead>
<tr>
<th></th>
<th>$\kappa = 0$</th>
<th>$\kappa = 0.1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_1$</td>
<td>0.3829</td>
<td>0.3829 - 0.1*0.1617</td>
</tr>
<tr>
<td>$V_3$</td>
<td>0.2942</td>
<td>0.2942 - 0.1*0.087</td>
</tr>
<tr>
<td>$V_5$</td>
<td>0.2263</td>
<td>0.2263 - 0.1*0.0473</td>
</tr>
<tr>
<td>$V_7$</td>
<td>0.1906</td>
<td>0.1906 - 0.1*0.0273</td>
</tr>
<tr>
<td>$V_9$</td>
<td>0.1677</td>
<td>0.1677 - 0.1*0.0176</td>
</tr>
</tbody>
</table>

At $\kappa = 0$ all the two-body pseudopotentials are positive and thus give positive energy to the pairs of electrons in the states with a certain total angular momentum. As a result the electrons repel and one could anticipate a many-body gap. For non-zero $\kappa$ all the corrections to the pseudopotentials are negative. Therefore the energy of electrons repulsion is decreased and one could also expect the decrease of the many-body gap.

If one would further increase $\kappa$, for certain values, the negative correction would become comparable to the bare pseudopotentials making the system similar to non-interacting. Further increase of $\kappa$ would change the sign of all the pseudopotentials and make the electrons attract. Of course, we should remember that the corrections derived perturbatively to first order in $\kappa$ only give physical results for small values of $\kappa$.

The picture presented above would be valid if the two-body terms of the Hamiltonian prevail over the three-body ones and the magnitude of the two-body pseudopotentials is the only parameter that determines the many-body gap. The results in the following chapters will allow us to compare this simplified prediction with the exact diagonalization results.

We also note that in general both electron excitations to higher and hole excitations to lower Landau levels are integrated out in the scheme leading to the effective Hamiltonian. However, for the special case when the lowest Landau level is considered (for instance in case of $\nu = 2/5, 3/5$), no hole excitations are possible and as noted in Ref. [29] not all the diagrams contribute to the renormalisation of the effective interaction. Thus it is justified to expect that the exact results for the FQHE states in the lowest and higher Landau levels may differ significantly.
The Phase Diagram of the $\nu = 5/2$ Fractional Quantum Hall Effect: Effects of Landau Level Mixing and Non-Zero Width

Interesting non-Abelian states, e.g., the Moore-Read Pfaffian and the anti-Pfaffian, offer candidate descriptions of the $\nu = 5/2$ fractional quantum Hall state. But the significant controversy surrounding the nature of the $\nu = 5/2$ state has been hampered by the fact that the competition between these and other states is affected by small parameter changes. To study the phase diagram of the $\nu = 5/2$ state we numerically diagonalize a comprehensive effective Hamiltonian describing the fractional quantum Hall effect (FQHE) of electrons under realistic conditions in GaAs semiconductors. The effective Hamiltonian takes Landau level mixing into account to lowest-order perturbatively in $\kappa$, the ratio of the Coulomb energy scale to the cyclotron gap. We also incorporate non-zero width $w$ of the quantum well and sub-band mixing. We find the ground state in both the torus and spherical geometries as a function of $\kappa$ and $w$. To sort out the non-trivial competition between candidate ground states we analyze the following 4 criteria: its overlap with trial wave functions; the magnitude of energy gaps; the sign of the expectation value of an order parameter for particle-hole symmetry breaking; and the entanglement spectrum. We conclude that the ground state is in the universality class of the Moore-Read Pfaffian state, rather than the anti-Pfaffian, for $\kappa < \kappa_c(w)$, where $\kappa_c(w)$ is a $w$-dependent critical value $0.6 \lesssim \kappa_c(w) \lesssim 1$. We observe that both Landau level mixing and non-zero width suppress the excitation gap, but Landau level mixing has a larger effect in this regard. Our findings have important implications for the identification of non-Abelian fractional quantum Hall states.

Results presented in this chapter were published in Ref. [1]. The calculations in torus geometry were performed by Thierry Jolicoeur. The order parameter calculations on the sphere were done by Michael R. Peterson with whom we also cross-checked many other results in spherical geometry for the smaller system sizes. All other calculations were performed by the author of the thesis.
6.1 Introduction

The $\nu = 5/2$ fractional quantum Hall state is well-established: it has a robust energy gap and has been observed in a large number of different GaAs samples [61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83], yet its underlying quantum order remains mysterious. Although there is strong evidence that the ground state is spin-polarized [26] with a fractional quasiparticle effective charge of $e/4$ [71, 73, 84, 85], there are some experiments that remain difficult to interpret in this light [86, 87]. Perhaps the most interesting hypothesized property of this state – non-Abelian quasiparticle braiding [88, 89, 90, 91, 92, 93, 94, 95] – is controversial. There are experiments consistent with non-Abelian quasiparticles [84, 96, 97, 98] but also some experiments that are not [99, 100].

Theoretical guidance can play an important role in identifying the state. Exact diagonalization [21, 101, 102, 103, 104, 23, 105, 106] and density-matrix renormalization group [107, 22] studies of simplified model Hamiltonians show that non-Abelian states, such as the Moore-Read (MR) Pfaffian state [15] and the anti-Pfaffian (aPf) state [108, 109] are viable ground states, but transitions to other ground states can occur as a result of small changes in Hamiltonian parameters [101, 102, 103, 105]. Since the details of the Hamiltonian matter (unlike in the case of states in the lowest Landau level, such as the $\nu = 1/3$ state), it is important to analyze Hamiltonians that model realistic experimentally-relevant systems and include effects such as Landau level mixing and the finite-width of the quantum well. Moreover, only a particle-hole symmetry-breaking effect, such as Landau level mixing, can split the degeneracy between the MR Pfaffian and aPf states [110, 111].

The exact diagonalization study of Ref. [105] found the ground state for the half-filled $N = 1$ Landau level for systems with up to $N_{\Phi} = 2N_{e} - S = 33$ magnetic flux quanta in the spherical geometry using an effective Hamiltonian [112] that included Landau level mixing with virtual excitations to the $N = 0$ and $N > 1$ Landau levels integrated out perturbatively to lowest-order in

$$\kappa = \left(\frac{e^2}{\epsilon\ell_0}\right)/\hbar \omega_c \propto 1/\sqrt{B}$$  \hspace{1cm} (6.1)

($\ell_0 = \sqrt{\hbar c/eB}$ is the magnetic length, $\epsilon$ is the dielectric constant of the host semiconductor, $\omega_c = eB/mc$ is the cyclotron frequency, and $S$ is a topological quantum number called the shift [113]). The ground state at the MR Pfaffian shift of $S = 3$ was found to have larger overlap with the MR Pfaffian wave function than the ground state at the aPf shift of $S = -1$ had with the aPf wave function indicating, naively, that the ground state was in the MR Pfaffian universality class. Two caveats are that: 1) Ref. [105] used two-body pseudopotentials [112]
The Phase Diagram of the $\nu = 5/2$ Fractional Quantum Hall Effect: Effects of Landau Level Mixing and Non-Zero Width

with a subtle normal-ordering error that was corrected later [29, 30, 31] and 2) These results only took account of the finite width of the quantum well via a scaling of the pseudopotentials. Meanwhile, an exact diagonalization study [23] of a truncated Hamiltonian for a few Landau levels found larger overlap with the aPf wave function on the torus. (Similar ideas were used in Ref. [114].) Ref. [23] used a truncated Hamiltonian approximation in hopes that it would capture the correct physics at intermediate values of $\kappa$, even though it is uncontrolled, i.e., it is not exact in any limit, unlike the Hamiltonians of Refs. [112, 29, 30, 31] which are exact in the $\kappa \to 0$ limit. Moreover, the overlap between a ground state and a trial wave function may reflect short-distance non-universal details of that particular trial wave function, rather than its universality class. Indeed, such an overlap vanishes in the thermodynamic limit.

In this work, we solve an effective Hamiltonian (defined in Chapter 5) that incorporates both Landau level-mixing and finite quantum well width. We then analyze the resulting ground states and low-lying excited states by several criteria. We begin by describing a qualitative picture in Sec. 6.2. In Sec. 6.3 we compute the overlaps in the spherical geometry between the ground states at $S = 3$ and $S = -1$ with, respectively, the MR Pfaffian and the aPf wave functions, and on the torus using the hexagonal unit cell where the MR Pfaffian and aPf occur at the same flux and are orthogonal for an odd number of electrons. We corroborate our overlap findings in Sec. 6.4 by calculating the entanglement spectrum. In Sec. 6.5 we compare the energy gaps in the spherical geometry at $S = 3$ and $S = -1$ and provide estimates of the excitation gaps in the thermodynamic limit that take into account Landau level mixing and finite width. In Sec. 6.6 we introduce an operator that is odd under a particle-hole transformation and, therefore, can be used as an order parameter distinguishing between the MR Pfaffian and aPf states. We compute this order parameter in the ground state of our Hamiltonian on the torus and sphere. According to all of these criteria, our central finding is that there is a $\kappa_c(\omega)$ such that the ground state for $0 < \kappa < \kappa_c(\omega)$ is in the universality class of the MR Pfaffian. We find that $\kappa_c(0) \approx 0.6$, monotonically increasing to $\kappa_c(4\ell_0) \approx 1$.

A phase transition occurs at $\kappa = \kappa_c(\omega)$, identified by the collapse of both the energy gap and the overlap with the MR Pfaffian wave function, as well as a sharp peak in the bipartite entanglement entropy. For $\omega < 1.5\ell_0$, there appears to be a second phase transition at slightly larger $\kappa$. The intermediate phase between the two transitions may be a different fractional quantum Hall state, such as the aPf or a strong pairing phase [115], but the gap is too small for us to say anything definitive at these system sizes. We culminate our findings in a phase diagram.
6.2 Qualitative Picture

Geometries

We note that while we work in the spherical geometry, we utilize planar geometry pseudopotentials. It has been argued that these more accurately represent the thermodynamic limit [103]. Furthermore we extrapolate several of our results to the thermodynamic limit and find that the choice of pseudopotentials is not crucial (See Section 6.12).

In our calculations on the sphere, \( N_e \) 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 centre (\( N_\Phi/2 \) is an integer or half-integer by Dirac's quantization condition). Total angular momentum \( L \) is a good quantum number, and any fractional quantum Hall state will be uniform and incompressible with \( L = 0 \) [60, 11]. For half-filling we have \( N_\Phi = 2N_e - S \); the filling factor in the \( N = 1 \) Landau level is given by \( \nu = \lim_{N_e \to \infty} N_e/N_\Phi \). As noted above, the MR Pfaffian has \( S = 3 \) while the aPf has \( S = -1 \) which can be seen by particle-hole transforming the MR Pfaffian.

We also consider the torus geometry. The torus is a two-dimensional plane with periodic boundary conditions with pseudomomentum \( K \) in a Brillouin zone that can be either rectangular or hexagonal. On the torus there is no shift, and \( N_\Phi = 2N_e \), which makes a direct comparison between MR Pfaffian and aPf states more straightforward.

6.2 Qualitative Picture

There is very strong evidence that the ground state of Eq. (5.1) is in the MR/aPf universality class for \( \kappa = 0 \) and that finite thickness increases the stability of this ground state [21, 101, 102, 103]. This is true using the torus or spherical geometry. A remaining question, and the one we answer here, is what happens under the influence of a particle-hole symmetry breaking effect like Landau level mixing, i.e., is the ground state in the MR or aPf universality class or neither universality class?

On the torus, at \( \kappa = 0 \), the ground state is doubly degenerate in the thermodynamic limit (over and above the 6-fold topological degeneracy on the torus). One of these states is in the MR Pfaffian universality class and the other is in the aPf universality class; their degeneracy is guaranteed by particle-hole symmetry. On the sphere, the former occurs at \( S = 3 \) and the latter at \( S = -1 \). As \( \kappa \) is increased, the two-body terms are modified and three-body terms are generated. The former cannot break the symmetry between the MR and aPf states since they preserve particle-hole symmetry.

To understand the effect of the latter qualitatively, we consider their effect
to lowest-order in perturbation theory, i.e., we compute the expectation value of
\[ H_{3\text{body}} = \sum_m V_m^{(3)}(w/\ell_0, \kappa) \sum_{i<j<k} \hat{P}_{ijk}(m) \]
in the two ground states on the sphere. As may be seen from Fig. 6.1, the energy of the \( S = 3 \) state (MR) is lowered more
than that of the \( S = -1 \) state (aPf).

![Graph](image)

**Figure 6.1:** Expectation value of the three-body terms in the Hamiltonian \( \langle \Psi_{gs} | H_{3\text{body}} | \Psi_{gs} \rangle \) in the \( S = 3 \) (MR) and \( S = -1 \) (aPf) ground states obtained at \( \kappa = 0 \) and \( w/\ell_0 = 0 \) in the system with \( N_\Phi = 33 \) in the spherical geometry. Here \( H_{3\text{body}} \) is the second term in Eq. (5.1) and introduces \( \kappa \) dependence. This is the lowest-order perturbative contribution to the energies of these states. The energy of the \( S = 3 \) (MR) state is lowered more.

The preceding calculation was done at \( N_\Phi = 33 \). To check whether this conclusion is likely to hold in the thermodynamic limit, we repeat it for different system sizes and consider the extrapolation to \( N_e = \infty \). In Fig. 6.2, we plot the expectation value per particle of the three-body terms of \( H(w/\ell_0 = 0, \kappa = 0.1, 1) \) given
in Eq. (5.1) evaluated in the Coulomb ground state for systems with \( N_\Phi = 13 \) to \( N_\Phi = 37 \). A linear fit in the inverse number of particles/holes provides an estimate for the thermodynamic limit. We observe that the energy at \( S = 3 \) is lowered more
than at \( S = -1 \) for all available system sizes as well as in the thermodynamic limit.
6.2 Qualitative Picture

Figure 6.2: The expectation value of the three-body terms in the Hamiltonian $\langle \psi_{gs}|H_{3\text{body}}|\psi_{gs}\rangle$ per particle at various system sizes. This is the leading contribution to the energy difference between these states computed perturbatively in $H_{3\text{body}}$. $N_p$ is the number of electrons for $S = 3$ and number of holes for $S = -1$. The energy difference between the extrapolated values is $0.00018 \, e^2/\epsilon \ell_0 = 0.12 \kappa |V_3^{(3)}|$. 

This is in agreement with our conclusions drawn in previous paragraph and in Fig. 6.1. Thus, from this result, we expect the MR state to be the ground state for small $\kappa$. We verify this expectation by exact diagonalization in the sections that follow.

The manner in which the three-body terms favor the MR state is subtle. The lowest angular momentum term, $V_3^{(3)}(w/\ell_0, \kappa)$, has vanishing expectation value in the MR trial wave function and small but negative expectation value in the aPF trial wave function and, therefore, one might expect the aPF state to have lower energy if $V_3^{(3)}(w/\ell_0, \kappa)$ dominates over higher angular momenta. However, as may be seen from the top panel of Fig. 6.3, the energy contributions of the $V_m^{(3)}(w/\ell_0, \kappa)$ for $m = 5$ and 6 are generally larger and will dominate (we have chosen $w/\ell_0 = 0$ and $\kappa = 0.2$ for illustrative purposes). Of course, the MR wave
Figure 6.3: Top Panel: Expectation value of the three-body terms in the MR and aPf trial wavefunctions as a function of angular momentum $m$, i.e., $\langle \Psi_{\text{trial}} | H_{3\text{body}}(m) | \Psi_{\text{trial}} \rangle$ where $H_{3\text{body}}(m) = V^{(3)}_m(w/\ell_0, \kappa) \sum_{i<j<k} \hat{P}_{ijk}(m)$, and $\Psi_{\text{trial}} = \Psi_{\text{MR}}$ or $\Psi_{\text{aPf}}$. Bottom Panel: Expectation value of the three-body terms for the $S = 3$ and $S = -1$ ideal Coulomb ground states as a function of angular momentum $m$. 

$N_{\Phi} = 33$, $w/\ell_0 = 0$, $\kappa = 0.2$
6.3 Wave Function Overlap

According to the argument of the previous section, the ground state is in the MR universality class for small $\kappa$. We now corroborate the arguments of the previous section using wave function overlap.

The MR wave function takes the following form on the sphere:

$$
\Psi_{\text{MR}} = \text{Pf} \left( \frac{1}{u_iv_j - v_iu_j} \right) \prod_{i>j} (u_iv_j - v_iu_j)^2 \tag{6.2}
$$

where $(u_i, v_i) = (e^{-i\phi_i/2} \cos \theta_i, e^{i\phi_i/2} \sin \theta_i)$ are the spherical coordinates of the $i$th particle. Here Pf denotes the Pfaffian, i.e., the square root of the determinant of an antisymmetric matrix. On the torus, this wave function takes the form:

$$
\Psi_{\text{MR}} = \text{Pf} \left( \frac{\partial_a(z_i - z_j)}{\partial_1(z_i - z_j)} \right) \prod_{i>j} (\partial_1(z_i - z_j))^2 \Phi_c.m.(\sum_i z_i) \tag{6.3}
$$

Here, $\partial_1(z)$ and $\partial_a(z)$, $a = 2, 3, 4$ are the Jacobi theta functions and $\Phi_c.m.(\sum_i z_i)$ is the center-of-mass wave function. $z_i$ is a complex planar coordinate of the $i$th particle. The aPf wave functions on the sphere and torus are obtained by taking the particle-hole conjugates of these wave functions.
Figure 6.4: Energy gap (energy difference between the two lowest states) and model wave function overlap ($N_\Phi = 33$ system) at the MR Pfaffian ($N_e = 18$) and aPf ($N_e = 16$) shifts. Note that for small $\kappa$ both the gap and overlaps are higher for the MR Pfaffian than they are for the aPf.

Fig. 6.4 shows the numerical wave function overlaps between the ground state at $S = 3$ and $S = -1$ for $N_\Phi = 33$ and, respectively, the MR and aPf wave functions on the sphere as a function of $\kappa$ for $w/\ell_0 = 0, 1, 2,$ and $3$. An overlap of unity or zero means the exact ground state of Eq. (5.1) is either identical to or completely different from the trial MR or aPf wave function. We remind that an overlap is not a universal quantity of a ground state that can be extrapolated to the thermodynamic limit since, unless it is unity for all $N_e$, it will vanish as the number of particles goes to infinity. The overlap between the ground state of Eq. (5.1) and both the MR and aPf wave functions are reasonably large for small $\kappa$. 

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6.3 Wave Function Overlap

and drop dramatically at larger $\kappa$, falling to zero somewhere in the range $0.7 - 1.0$, with larger $\kappa$ occurring for larger widths. Importantly, the overlap with the MR state is consistently larger. Although not shown here, smaller system results are consistent with the $N_B = 33$ results. This is an indication that the ground state is likely to be in the same universality class as the MR state for small $\kappa$. But, as we cautioned above, it is possible that the aPf's smaller overlaps are merely expressing the fact that non-universal short-distance physics is not well-captured by this wave function.

On the torus, the MR and aPf states occur at precisely the same flux. With a rectangular unit cell the MR and aPf states are 3-fold degenerate (after factoring out the 2-fold center-of-mass degeneracy) with each zero-energy state existing at $K = (0, N_0/2), (N_0/2, 0)$, and $(N_0/2, N_0/2)$ where $N_0$ is the greatest common divisor of $N_e$ and $N_B$. $K_x$ and $K_y$ are in units of $2\pi \hbar/a$ and $2\pi \hbar/b$ where $b/a$ is the aspect ratio of the rectangular unit cell. Generically, in this geometry, the MR and aPf are not orthogonal rendering ambiguous the use of overlaps. However, in the hexagonal unit cell containing an odd number of electrons, the MR and aPf states are orthogonal and both have $K = (0,0)$. At $\kappa = 0$ the Coulomb ground state is a doublet at $K = (0,0)$ (provided $N_e \neq 6n + 1$) and we find that for nonzero $\kappa$ this doublet is split in such a way that each member has a nonzero overlap with either MR or aPf state, as described by Papic et al. [116]. The lowest-lying state has nonzero overlap only with the MR state.

The top panel of Fig. 6.5 shows the overlap between the MR state and the ground state for the hexagonal unit cell as a function of $\kappa$ and $w/\ell_0$ for $N_e = 15$. The overlap is relatively large, dropping to zero at a critical $\kappa$ in the range $0.6 - 1$, with larger values occurring for larger widths. Meanwhile, on the torus the first excited state has a similarly large overlap with the aPf wave function, essentially mirroring the overlap between the ground state and the MR wave function. The overall shape of the overlap is very similar to that on the sphere, shown in the bottom panel of Fig. 6.5, further corroborating previous results and, as we show below, these conclusions are supported by criteria that do not depend on any particular trial wave functions.

Our results for $S = -1$ on the sphere and for the first excited state on the torus are a bit surprising. If the ground state at $S = 3$ is firmly in the MR universality class, then the ground state at $S = -1$ should have 8 quasiholes on the $S = 3$ ground state. Instead, it has high overlap with the aPf state. Similarly, the first excited state on the torus should look like an exciton on the MR ground state but, instead, it has high overlap with the aPf ground state. If the ground state is in the universality class of the MR state, then the energy gap to a state with high overlap with the aPf should be extensive in system size. What we observe can thus only happen in small systems. For larger system sizes, the $S = -1$ ground state

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Figure 6.5: The overlap between the ground state and the MR wave function as a function of \( \kappa \), for \( w/\ell_0 = 0, 1, 2, 3, \) and 4. \( w/\ell_0 = 0 \) is the left-most curve and \( w/\ell_0 = 4 \) is the right-most. Top panel is on the torus for \( N_e = 15 \) and hexagonal unit cell, bottom panel for the sphere with \( N_\phi = 29 \) with \( S = 3 \) \((N_e = 16)\).

on the sphere and the first excited state on the torus must look, respectively, like the \( S = 3 \) ground state on the sphere or the torus with excitations on top. It is possible, in principle, to correctly identify the ground state in the thermodynamic limit without correctly identifying the precise ordering of excited states. The latter can change without the gap closing. That appears to be what is occurring in our case. The finite-size extrapolation shown in Figs. 6.2 and 6.18 show that the corrections that we include favor the MR Pfaffian ground state. (Similarly, the exciton gap shows scaling with system size.) However, the first excited state does not scale as simply with system size. This is presumably an indication that there are level crossings among the excited states that occur on the way to the thermodynamic limit and these prevent us from correctly identifying the precise ordering of the excited states. Such a scenario must occur in the present case since
the anti-Pfaffian state cannot be the first excited state at large-$N_e$. While we have not shown that this occurs in our model, we see no evidence for gap closure as $N_e$ is increased, supporting our identification of the correct ground state.

6.4 Entanglement Spectrum

We have called the $S = 3$ and $S = -1$ ground states the MR state and the aPf state, respectively, due to their large overlaps with the corresponding trial wave functions (Eq. (6.2), and its particle-hole conjugate). However, the overlap with trial wave functions is not universal and vanishes in the thermodynamic limit. Therefore, we now identify these states by a universal criterion, the entanglement spectrum.

In the spherical geometry, we divide the system in two pieces A and B [117, 118, 119, 120, 121], and obtain the reduced density matrix for one half by tracing out the degrees of freedom of the remaining half. The eigenvalues $\rho_n$ of the density matrix are interpreted as energies, $\rho_n \equiv e^{-\xi_n/2}$ [122]. If we make a cut in orbital space, then the entanglement spectrum for a state in the MR universality class should have negative slope for the entanglement energies as a function of the $z$-component of the angular momentum $L^A_z$ in sector A, for example, as discussed in Ref. [122].

A state in the MR Pfaffian universality class displays the following structure in the entanglement spectra: the spectra is essentially divided into two pieces by a "gap" with the low-lying states corresponding to the conformal field theory (CFT) describing the MR edge states. Starting from the "root" configuration of the MR states one can define $\Delta L^A_z = (L^A_z)_{\text{root}} - L^A_z$ where $(L^A_z)_{\text{root}}$ is the $z$-component of angular momentum of the "root" configuration, cf. Ref. [122]. The slope of the "energy" spectra, i.e., whether $\Delta L^A_z$ is positive or negative as a function of $L^A_z$, expresses the chirality of the edge modes of the CFT. In our convention, a state in the MR universality class has an entanglement spectra with a negative slope. Thus, the entanglement spectrum for a state in the aPf universality class has a positive slope corresponding to edge modes with opposite chirality.

Fig. 6.6 shows that the entanglement spectrum at $S = 3$ for $\kappa = 0.1$ and $w/\ell_0 = 1$ has negative slope, similar to that of the entanglement spectrum for the MR trial wave function, Eq. (6.2). Meanwhile the entanglement spectrum at $S = -1$ has positive slope, similar to that of the aPf trial wave function (the particle-hole conjugate of Eq. (6.2)). We therefore find that both the entanglement spectrum and overlaps allow us to identify the $S = 3$ and $S = -1$ ground states as the MR state and the aPf state, respectively. The phase transition at $\kappa \approx 0.6 - 1.0$ is also observed in the entanglement spectra, as shown in Fig. 6.7 and discussed
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Figure 6.6: The entanglement spectrum for the MR Pfaffian (blue) and aPf (red) on the sphere at $S = 3$ and $S = -1$, respectively, are shown in the top panel. The MR state has a negative slope (discussed more in the text) while the aPf has a positive slope. The middle and lower panel show the entanglement spectrum for the exact ground state at $S = 3$ and $S = -1$, respectively, for $\kappa = 0.1$ and $w/\ell_0 = 1$. At $S = 3$, the low-lying states show the same slope and level structure as the MR state and at $S = -1$ they show the same slope and level structure as the aPf state. Both systems are at $N_\Phi = 29$ and were partitioned to have 15 orbitals in each hemisphere (this corresponds to the partition of $P[0|0]$ in Li and Haldane’s notation [122]).

Further in Sec. 6.7. As $\kappa$ increases, the structure of the low-lying states first changes chirality and then changes completely and no longer resembles the MR or aPf entanglement spectra.

We adopt the definition of the “topological gap” for the Pfaffian-like phase introduced in [122] with $\Delta L_z^A = 0$, thus defining it as difference between the single universal level at $L_z^A = 64$ and the lowest generic level at the same $L_z^A$ (see Fig. 6.7).
6.5 Energy Gaps

In addition we track the difference between the lowest two levels at $L_z^A = 56$, which is the symmetry point between the MR Pfaffian and aPf spectra (see the Top Panel of Fig. 6.6) and also appears to be the lowest-$L_z^A$ "universal" level after the first phase transition ($\kappa \approx 0.66$).

In Fig. 6.8 we show the topological gap in the Pfaffian-like phase for different widths along with the $L_z^A = 56$ gap at $w/\ell_0 = 0$. We observe that the topological gap remains relatively robust to the variations of finite thickness and Landau level mixing strength for small $\kappa$. For each width there exists a critical value of $\kappa$, that can be approximately inferred from the MR Pfaffian overlap, where the topological gap vanishes. We see that the $L_z^A = 56$ gap displays a sharp jump simultaneous with the vanishing of the MR Pfaffian topological gap at $w = 0$. This may indicate a topological phase transition where the new state is also topological but has opposite chirality. We further discuss this state in the Section 6.7. With increasing Landau level mixing strength the $L_z^A = 56$ gap is suppressed until a different phase appears around $\kappa = 0.73$.

We also studied the dependence of the MR Pfaffian topological gap on the system size for $N_\Phi$ up to 29 (not shown). System size dependence is similar to the one presented in [122] with the smaller systems developing large finite-size effects for higher $\kappa$. Reasonable extrapolation to the thermodynamic limit was therefore only possible for $\kappa \leq 0.45$ where we see that the extrapolated topological gap remains finite and relatively robust to the variation of the Landau level mixing strength.

6.5 Energy Gaps

We now turn to the energy gap and show that the gap collapses as $\kappa$ is increased, mirroring the collapse of the wave function overlap, thereby justifying the claim that the latter signals the onset of a phase transition. There are several different energy gaps in a fractional quantum Hall system, with different experimental manifestations. The simplest gap, which we will simply call the “energy gap” is the difference in energy between the two lowest eigenvalues of the Hamiltonian, for fixed particle number. This gap must become small (i.e., vanishing in the thermodynamic limit) at a phase transition. Hence, it is the appropriate quantity to compute when looking for a phase transition. However, the energy gap may not be relevant to transport experiments, which are insensitive to the gap to neutral excitations. The transport gap is typically deduced in one of two ways, which we discuss in Section 6.10. For reasons that are explained there, we primarily use the so-called ‘exciton gap’ to estimate the transport gap. As shown in Fig. 6.15
Figure 6.7: Entanglement spectrum for \( N_\Phi = 29 \) at \( \kappa = 0.2, 0.53, 0.66, \) and 0.73. The entanglement spectra at \( \kappa = 0.2 \) and 0.53 are shown in blue to emphasize their consistency with a ground state in the universality class of the MR Pfaffian. At \( \kappa = 0.66 \) we show the entanglement spectra between the two entanglement entropy peaks in the lower panel of Fig. 6.13. It is colored red to indicate that its low-lying level structure has some similarity to states in the aPf universality class although the entanglement gap is too small to allow for any definitive statements. At \( \kappa = 0.73 \) the entanglement spectra completely changes to that of the unknown phase to the right of the second entanglement entropy peak in Fig. 6.13. We also indicate the definition of the “topological gap” for \( \kappa = 0.2, 0.53, \) and 0.66 as described in the text.

In Section 6.10, the various different ways of computing the transport gap are broadly consistent though there are quantitative differences. In Section 6.10, we also establish the connection to previous important work [43] that estimated the transport gap in the spherical geometry with \( S = 3 \) including finite thickness but
6.5 Energy Gaps

Figure 6.8: Topological gap, the difference between the universal and lowest generic level at \( L^A_z = 64 \), is calculated in spherical geometry at \( S = 3 \) for the system with \( N_\Phi = 29 \). Note that qualitatively the behaviour and collapse of the topological gap is similar to the collapse of the overlaps shown in Fig. 6.5. We also show the topological gap at \( L^A_z = 56 \) (black filled circles) in the region of parameter space where the entanglement spectrum qualitatively changes and has the same chirality as the aPf state (cf. the \( \kappa = 0.66 \) panel in Fig. 6.7).

The dependence of the energy gap on \( \kappa \) and \( w/\ell_0 \) is shown in Fig. 6.4. The gaps at \( S = 3 \) and \( S = -1 \) both decrease monotonically with \( \kappa \) and collapse to zero at approximately the same value of \( \kappa \), coinciding with the vanishing of the overlaps (\( \kappa \sim 0.7 - 1.0 \), depending on the width, with larger widths corresponding to larger critical \( \kappa \)’s). This supports the conclusion that the decrease of the overlap signals the approach to a phase transition, rather than just a failure of the trial wave functions.

Moreover, the energy gap is larger at \( S = 3 \) than at \( S = -1 \) for most Landau level mixing strengths. If the true ground state of the system were at \( S = 3 \), then we would expect that, in the thermodynamic limit, there would be no gap at \( S = -1 \) since this would be a state with 8 charge \( e/4 \) quasiholes, leading to
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gapless excitations. The reduction of the gap at $S = -1$ relative to the gap at $S = 3$ is consistent with this, but the fact that it is not zero indicates that we may not be seeing the asymptotic behaviour of the system. For instance, while the aPf ground state must have higher energy than the MR ground state (assuming that the latter is the ground state) by an extensive energy difference, it may still have lower energy than the MR state with 8 quasiholes at these system sizes. There are numerical indications that the size of the quasiholes is on the order of many magnetic lengths. Therefore they may strongly overlap at these system sizes, thereby leading to a finite gap for finite size systems [123]. Hence, the extrapolation to the thermodynamic limit might be a much more delicate procedure then previously appreciated and, in fact, could point to a potential reason for the long-noticed discrepancy between calculated energy gaps and experimentally measured gaps [62, 63, 64, 65, 66, 67, 68, 69, 70, 72, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83].

To provide qualitative guidance to the experiment and to connect to the previous gap estimates in the literature we show in Fig. 6.9 our estimates of the exciton gap extrapolated to the infinite system size. Our results show that Landau level mixing and finite-thickness have a non-trivial interplay in the second Landau level. Landau level mixing reduces the energy gaps more significantly than finite-thickness alone. But we find that both effects, taken together, produce a further reduction. This is in direct contrast to what has been found in the lowest Landau levels [124, 125] where both effects were not found to be additive.

Our results show that Landau level mixing lowers energy gaps, thereby bringing theoretical estimates closer to experimental measurements [62, 63, 64, 65, 66, 67, 68, 69, 70, 72, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83] of the transport gap. Furthermore, the strong suppression of the gap as a function of the Landau level mixing strength that we observe is in good qualitative agreement with the experimental findings presented in Fig. 4 of Ref. [126]. There, four different experiments are analysed following the idea originally suggested in [127] and a similar trend for the dependence of the intrinsic (disorder-corrected) gap on the $\kappa$ parameter is found. Based on the experimental evidence the authors come to the conclusion that “the $\nu = 5/2$ FQHS should not develop for $\kappa > \kappa_{th}$”. This is in agreement with our findings that gaps and trial wavefunction overlaps vanish beyond some critical $\kappa$ mixing strength that we cannot predict precisely due to the fact that our effective Hamiltonian is, strictly speaking, only valid for small $\kappa$.

In Section 6.9 we demonstrate that width of an infinitely deep quantum well $w$ provides a reasonable parameterization for the finite-width effect. In order to compare with experiment one should find the variance of the electron wave function in the direction perpendicular to the two-dimensional electron gas in the specific heterostructure (for instance by means of a coupled Schrödinger-Poisson solver in 1D (see also Section 2.3)). Infinite quantum well width $w$ leading to the same
6.5 Energy Gaps

Figure 6.9: Color map of extrapolated exciton gap at $S = 3$ versus both well width and $\kappa$. The contours show specific values of the extrapolated exciton gap. Note that the extrapolation becomes less reliable when approaching the phase transition. The black circles show the transition border determined by the first peak in the entanglement entropy for $N_\varphi = 29$ on the sphere (discussed in Sec. 6.7). We do not extrapolate the exciton gap after the phase transition (white area). The top x-axis is the magnetic field for GaAs samples.

The variance should be taken. Note that the width $w$ is given in Fig. 6.9 in units of magnetic length and therefore depends on magnetic field since $\ell_0 \approx 25\text{nm}/\sqrt{B[T]}$, where $B[T]$ is the magnetic field in Tesla.
6.6 Particle-Hole Symmetry-Breaking Order Parameter

States in the MR and aPf universality classes cannot be invariant under particle-hole symmetry. Indeed, under a particle-hole transformation, a state in the MR universality class is transformed into a state in the aPf universality class [108, 109]. Thus, if we consider an operator \( \phi \) that is odd under a particle-hole transformation, then \( \langle \phi \rangle \equiv \langle \Psi_{\text{trial}} | \phi | \Psi_{\text{trial}} \rangle \) must have one sign in any state in the MR universality class and the opposite sign in any state in the aPf universality class, assuming that \( \langle \phi \rangle \) vanishes only in states that are symmetric under particle-hole symmetry (i.e., excluding, through a judicious choice of \( \phi \), the possibility that \( \langle \phi \rangle \) vanishes ‘accidentally’). We choose the order parameter to be built from the operator that is conjugate to the variable \( \kappa \) that controls the particle-hole symmetry breaking. This operator is \( H_{3\text{body}} = \sum_m V^{(3)}_m(w/\ell_0, \kappa) \sum_{i<j<k} \hat{P}_{ijk}(m) \). Note that \( \kappa \) can be pulled out of this expression completely since \( H_{3\text{body}} \) is linear in \( \kappa \), hence, we can write \( H_{3\text{body}} = \kappa H'_{3\text{body}} = \kappa \sum_m V^{(3)}_m(w/\ell_0, 1) \sum_{i<j<k} \hat{P}_{ijk}(m) \). The order parameter is then taken to be

\[
\phi \equiv \frac{1}{2} (H'_{3\text{body}} - H'_{3\text{body}}) \tag{6.4}
\]

where the overline denotes particle-hole conjugation.

To demonstrate this definition, let us consider a model that interpolates adiabatically between the pure Coulomb Hamiltonian and the Hamiltonians whose ground states are in the MR and aPf universality classes. That is, \((1 - \alpha)H(0,0,1) + \alpha H_3\) or \((1 - \alpha)H(0,0,1) + \alpha H_3^\prime\) where \(H_3 = \sum_{i<j<k} \hat{P}_{ijk}(m = 3)\) is the Hamiltonian that generates the MR wave function as an exact zero-energy ground state and \(H_3^\prime\) is its particle-hole conjugate and generates the aPf wave function. For this model, we take the order parameter to be \((H_3 - H_3^\prime)/2\) since \(H_3\) is the operator that breaks the particle hole symmetry by increasing the variable \( \alpha \). The expectation value of this operator has sign \( \langle \Psi_{\text{MR}} | \phi | \Psi_{\text{MR}} \rangle < 0 \) and \( \langle \Psi_{\text{aPf}} | \phi | \Psi_{\text{aPf}} \rangle > 0 \), and changes sign in the expected manner, as shown in Section 6.11. Therefore, we expect the above definition of \( \phi \) (Eq. (6.4) for the Landau level mixing Hamiltonian) will show similar behaviour and \( \langle \phi \rangle \) will be negative (positive) for an eigenstate in the MR (aPf) universality class.

We first examine this operator in the system in which it is most straightforward. Recall that on the torus the MR and aPf states occur at the same flux. Here \( \langle \phi \rangle \) is particularly useful in determining the universality class of the ground state of Eq. (5.1). The expectation of \( \phi \) in the ground state is the most important quantity but we will focus on the lowest and first excited eigenstates on the torus with a hexagonal unit cell containing an odd number of electrons as a function of \( \kappa \) for
Figure 6.10: The expectation value of a particle-hole anti-symmetric order parameter $\phi$ for the ground state and first excited state of Eq. (5.1) on the torus using the hexagonal unit cell for $N_\Phi = 18$, 22, and 30 as a function of $\kappa$ for $w/\ell_0 = 0$. The ground state is consistent with the MR state and has $\langle \phi \rangle < 0$ (filled symbols) while the first excited state is consistent with the aPf state with $\langle \phi \rangle > 0$ (open symbols).

$w/\ell_0 = 0$. In Fig. 6.10, we show the expectation value of $\phi$ in the ground and first excited states for $N_\Phi = 18$, 22, and 30. These results clearly show that the ground state breaks particle-hole symmetry in the same way as the MR state and $\langle \phi \rangle < 0$. Moreover, the expectation value of $\phi$ in the first excited states is positive and, therefore, breaks particle-hole symmetry in the same way as the aPf state.

In Fig. 6.10 it is observed that $\langle \phi \rangle \not= 0$ for $\kappa = 0$. The hexagonal unit cell has an exact degeneracy for $\kappa = 0$ for an odd number of electrons in the unit cell as
Figure 6.11: The expectation value of the particle-hole anti-symmetric order parameter for the ground state of Eq. (5.1) in the spherical geometry at the particle-hole symmetric shift $N_\Phi = 2N_e - 1$ for $N_\Phi = 13, 15, 17, 19, 21$ and 23 as a function of $\kappa$ for $w/\ell_0 = 0 - 4$. Note the $y$-axis is not the same scale for each system size.
Figure 6.12: The total energies relative to the ground state energy on the torus using the hexagonal unit cell for $N_\Phi = 18$, 22, and 30 as a function of $\kappa$ for $w/\ell_0 = 0$. Similar to Fig. 6.10, a state with $\langle \phi \rangle < 0$ has a filled symbol while a state with $\langle \phi \rangle > 0$ has an open symbol. The right panel shows the 6 lowest eigenstates. We have zoomed in on the lowest two eigenstates in the left panel. While many of the higher energy excitations look like they belong to the MR universality class according to $\langle \phi \rangle$, the first excited state looks like an aPf ground state rather than an excitation above a MR ground state, unlike the other low-lying excited states. Note that the energy scale is much larger in the right panel, so the ground and first excited states are not resolvable there.

discussed above in Sec. 6.3. At $\kappa = 0$ there is a basis in which one of the degenerate states has positive $\langle \phi \rangle$ and the other state has a negative value. This basis evolves smoothly into the $\kappa > 0$ eigenstates. However, we could just as easily take the symmetric and anti-symmetric combinations of these two degenerate states, and these combinations would respect the particle-hole symmetry and have vanishing
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$\langle \phi \rangle$. For an even number of electrons per unit cell, where the degeneracy is not exact at $\kappa = 0$, the energy splitting between the symmetric and anti-symmetric combination is non-zero due to tunnelling in a finite sized system, and the ground state at $\kappa = 0$ is the symmetric combination, with $\langle \phi \rangle = 0$.

Next we consider $\langle \phi \rangle$ in the spherical geometry. Here we fix $N_\Phi = 2N_e - 1$ to be at the particle-hole symmetric point since the shift $S$ explicitly breaks particle-hole symmetry and we want to observe this symmetry breaking due to Landau level mixing effects. Fig. 6.11 shows the order parameter for the ground state at $N_\Phi = 13, 15, 17, 19$, and $21$ for various $w/\ell_0$ as a function of $\kappa$. Here the order parameter vanishes for $\kappa = 0$ and increasing $\kappa$ drives the system into the MR universality class and $\langle \phi \rangle$ becomes more negative for increasing $\kappa$.

Finally we investigate the lowest few energy eigenstates of Eq. (5.1) in the torus geometry using the hexagonal unit cell for $N_e$ odd in Fig. 6.12. States with negative (positive) order parameter are indicated by a filled (open) symbol. The first excited state has $\langle \phi \rangle > 0$ but the rest have $\langle \phi \rangle < 0$. Thus, although the second, third, fourth, and fifth excited states look like an exciton on the MR ground state, in that they have a negative expectation value of the order parameter and therefore belong in the MR universality class, the first excited state does not. It, instead, looks like the $a\text{Pf}$ state. This is consistent with conclusions from the overlaps, but can only occur in small systems.

### 6.7 Entanglement Properties and Phase Diagram

From the preceding calculations, we have seen the following concomitant behaviors: a sharp drop in the energy gap, a corresponding drop in the overlap between the ground state and the MR wave function, a negative expectation value of a particle-hole symmetry-breaking order parameter. The first of these vanishes at the phase transition to a competing phase.

This phase transition point can also be identified by computing the bipartite entanglement entropy, which is the von Neumann entropy of the reduced density matrix \cite{117, 118, 119, 120, 121}, discussed in Sec. 6.4. Fig. 6.13 shows that the resulting entanglement entropy displays two nearby peaks as a function of $\kappa$ (only a single peak for $w/\ell_0 > 1.5$). The position of the two peaks coincides with the vanishing of the overlap which, in turn, coincides with the vanishing of the energy gap, as per Fig. 6.4. These peaks in the entanglement entropy indicate phase transitions \cite{128}.

In the bottom panel of Fig. 6.13, we see that there are two distinct peaks in the entanglement entropy at $\kappa = 0$ at $w/\ell_0 = 0$, while in the top panel, we see that the two peaks are barely distinguishable at $w/\ell_0 = 1$. Intriguingly, the ground state
Figure 6.13: Top Panel: Entanglement entropy and wavefunction overlap with the MR state for width $w/\ell_0 = 1$. Bottom panel: Entanglement entropy and the absolute difference of the MR Pfaffian and aPf overlaps for width $w/\ell_0 = 0$. In both cases the spherical geometry was used with $N_0 = 29$ and $S = 3$. The red vertical lines in the bottom panel are just a guide to the eye to indicate the peaks in the entanglement entropy.
has higher overlap with the aPf wavefunction in the intermediate phase between the two entanglement entropy peaks although both overlaps are quite small. We speculate about this in Sec. 6.8.

It is instructive to discuss the nature of all the phases mentioned in relation with the corresponding entanglement spectra for $w/\ell_0 = 0$ shown in Fig. 6.7. Comparing the spectra at $\kappa = 0.2$ and $\kappa = 0.53$ in Fig. 6.7 (upper and lower left panels) we observe that, with increasing Landau level mixing strength, the universal part of the entanglement spectrum gets absorbed by the "generic" spectrum above it. This leads to a decrease of the "topological gap" [122] as shown in Fig. 6.8.

Between the two peaks of entanglement entropy, at approximately $\kappa = 0.66$, the low-lying levels of the spectrum have positive slope (upper right panel of Fig. 6.7). This indicates that in this phase there exists an edge mode propagating in the direction opposite to the MR Pfaffian edge. However, both the energy gap and entanglement gap are quite small, so to say anything definitive about this state would require much larger system sizes (compared to what is currently available using exact diagonalization). In the phase diagram shown in Fig. 6.14, this state is located between the two black lines indicating the entropy peaks.

The entanglement spectrum for stronger Landau level mixing has a completely different nature as shown in the bottom right panel of Fig. 6.7. We defer the discussion of this regime to later work.

Finally, we discuss an approximate quantum phase diagram (QPD) for the FQHE at $\nu = 5/2$ in Fig. 6.14. The QPD is determined with two distinct measures: energy gap and entanglement entropy. The energy gap depicted is for the largest system with $N_\Phi = 33$ while the entanglement entropy is for $N_\Phi = 29$. Fig. 6.14 shows a contour plot of the energy gap for $S = 3$, as functions of $\kappa$ and $w/\ell_0$. We also indicate the position of the first peak in the entanglement entropy (black circles), clearly showing that it occurs where the energy gap becomes very small for $N_e = 18$ (presumably indicating that it vanishes in the thermodynamic limit). The results presented in Fig. 6.14 are in agreement with overlaps with the MR state as well. This QPD can serve as a guide for experimental searches for robust FQHE at $\nu = 5/2$ and is the first approximate QPD calculated at $\nu = 5/2$ including both Landau level mixing and finite width.

### 6.8 Conclusions

Our results demonstrate that the $\nu = 5/2$ state for small non-zero $\kappa$ and $0 \leq w/\ell_0 \leq 4$ is in the universality class of the Moore-Read Pfaffian state. In the small $\kappa$ limit, our approximations are controlled: we use the correct Hamiltonian to $O(\kappa)$, and all corrections to our Hamiltonian are of higher-order in $\kappa$ and,
Figure 6.14: Quantum phase diagram obtained from a color map of the energy gap (difference between the two lowest eigenstates for the system with $N_\phi = 33$) plotted versus well width and $\kappa$. Contours plot specific values of the extrapolated gap. Lines with black circles and black diamonds show the positions of the entanglement entropy peaks for $N_\phi = 29$ and represent the approximate phase boundaries. All the states to the left from the line connecting the black circles belong to the MR Pfaffian universality class. The top $x$-axis is the magnetic field for GaAs samples. All results are obtained on the sphere.
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therefore, can be neglected for sufficiently small $\kappa$. Our results are in qualitative agreement with the results of Ref. [105]. We reached our conclusion by computing several properties of the ground state. They all validate the use of overlaps in this case. Our results are in disagreement with the results of Ref. [23], which found a ground state in the aPf universality class.

Finite-size effects might be a potential source of error in our study. This is especially true since we are using, in a finite-system, pseudopotentials that were originally derived for the infinite system. This should make no difference for sufficiently large systems and, therefore, in the thermodynamic limit. However, it can affect our ability to make an extrapolation from small systems to the thermodynamic limit. Hence, we have checked the perturbative contribution to the energy difference using size-dependent spherical pseudopotentials in Section 6.12; our results are qualitatively unchanged.

Finally, the phase that emerges at $\kappa$ just larger than the gap closing is an interesting open problem. The energy gap and the entanglement gap are too small for us to say anything reliable at present. However, the overlap with the aPf is larger than the overlap with the MR state and the entanglement spectrum is consistent with a counter-propagating edge mode, so it is possible that the aPf state occurs in this narrow window, albeit with much smaller energy gap (possibly more in line with experimental gap values). In this context, we note that the experiment of Bid et al. [129] found evidence for a counter-propagating neutral mode in a $\nu = 5/2$ state at $B \approx 5T$ ($\kappa \approx 1.12$), consistent with the anti-Pfaffian state, which supports the scenario that a different $5/2$ state occurs at larger $\kappa$ and that this state is the anti-Pfaffian. Another possibility is a strong pairing phase [115].

Note that small $\kappa$ corresponds to relatively high magnetic fields, e.g., $\kappa = 0.5$ is a magnetic field of 25 T for GaAs samples. The range of magnetic fields and quantum well widths over which there is a $\nu = 5/2$ state in both experiments and our numerics is the range $6T \leq B \leq 12T$ and $w/\ell_0 \sim 2 - 4$. For $B \lesssim 6$ T, we do not find a quantum Hall state at $5/2$ even though experiments see a $5/2$ plateau all the way down to $B \sim 1 - 2$ T [72, 81]. There are two distinct possible explanations for this discrepancy between our results and experiments.

One is that our effective Hamiltonian is simply not quantitatively correct for $\kappa \gtrsim 1$ and including higher order corrections in $\kappa$ would shift the phase transition to lower magnetic fields. While we do not know the precise LL mixing strength $\kappa$ beyond which our effective Hamiltonian is no longer valid, the large-$\kappa$ discrepancy between our results and experiments indicates that higher-order corrections become important in the vicinity of $\kappa = 0.6$. Nevertheless, we choose to also present the results of our model at higher $\kappa$ since they may still correctly capture the trends in the $\kappa$ dependence and since they will be useful guidance and motivation for the future studies attempting to incorporate higher order corrections and thus
understand the nature of the incompressible state at low fields. Additionally, we note that for widths beyond $\frac{w}{\ell_0} \gtrsim 5$, real experimental systems are often better described as two-component systems.

The other possibility is that some of the experimental observations at low fields are spin-unpolarized states – a possibility that we have ignored in this work since we have assumed that the system is fully spin-polarized. Although there exist experimental studies [27] that demonstrate the spin-polarized nature of the $5/2$ state for certain magnetic field and finite width this doesn’t exclude the possibility that there exists a spin-unpolarized incompressible region of the phase diagram that has not been probed by NMR. It is an open question as to the effect of Landau level mixing and finite width have on the spin polarization and whether the ground state, if unpolarized, is or is not in the universality class of the MR Pfaffian or aPf phase. These questions will have to await future studies.

Our results demonstrating the strong suppression of the gap by Landau level mixing are in good qualitative agreement with the experimental observations [126] and should in turn motivate the experimental community searching for a non-Abelian phase to explore higher magnetic fields where a more stable $5/2$ state in MR Pfaffian universality class is predicted by our model.

6.9 Appendix A: Models for Non-Zero Width

We include non-zero width of the two-dimensional electron system using two approaches. In the first approach, we, for $\kappa \neq 0$, assume that the electrons are confined to an infinitely deep square quantum well in the $z$-direction so that the $z$-dependence of the wave function for the $n^{th}$ subband is $\phi_n(z) = \sqrt{\frac{2}{w}} \sin((n + 1)\pi z/w)$ with $w \in [0, d]$ and subband energy $\epsilon_n = (n + 1)^2 \pi^2 \hbar^2 / (2m_z w^2)$. Here $m_z$ is the effective electron mass in the quantum well (see Ref. [29] for details).

In the second approach we choose an alternative Gaussian model to demonstrate that the above choice of finite thickness model does not change our results qualitatively or quantitatively. We fix $\kappa = 0$ and take the $z$-dependence to have a Gaussian form $\phi(z) = (\sigma^2 2\pi)^{-1/4} e^{-z^2/4\sigma^2}$ (this wave function is the solution of a parabolic potential but since we use it only for $\kappa = 0$ we do not consider any subband mixing effects).

Fig. 6.15 shows that the energy gaps (extrapolated to the thermodynamic limit) are very similar for both models of non-zero width. To compare each model at a similar width we considered each energy gap as a function of the variance of the wave functions, $\text{var} = \sqrt{\langle z^2 \rangle - \langle z \rangle^2}$, that is, $\text{var} = \sigma/\ell_0$ for the Gaussian wave function and $\text{var} = 0.180756(w/\ell_0)$ for the infinite square well wave function.
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Figure 6.15: Extrapolated quasiparticle-quasihole (left panel, filled symbols) and exciton (right panel, open symbols) energy gaps as a function of well width. Each gap is calculated with spherical and planar pseudopotentials (p.p.) for two different models of the finite thickness, Gaussian and infinite square well (ISQ), cf. Section 6.9. The solid black circles (marked in the legend with an asterisk *) are the same as the solid red squares but are obtained from an extrapolation of only $N_e = 10$ and 14 electrons. The solid black circles reproduce the width dependence obtained in Ref. [43] (Fig. 14b) to show that using more particles in the extrapolation (the other data points use $N_e = 10, 14$ and 18 electrons) leads to larger gaps.
6.10 Appendix B: Exciton and Quasiparticle-Quasihole Gaps

To estimate the gap on the sphere in the thermodynamic limit, we generally follow Ref. [43]. We take energy differences and perform a linear (in $1/N_e$) extrapolation to infinite system sizes after we multiply the energy difference by the factor $\sqrt{N_\Phi/2N_e}$, [43]. We calculate energy difference (and therefore the gap) in two distinct ways:

(i) The exciton gap is the energy difference between the ground and the lowest excited state with total angular momentum $L = N_e/2$ or $L = N_e/2 - 1$ for $N_e/2$ even or odd, respectively. This excited state contains a quasi-particle and quasi-hole, maximally separated on the sphere [43]. The quasi-particle and quasi-hole are assumed to have charges $\pm e/4$ and to be separated by the diameter of the sphere $2\sqrt{N_e}\ell_0$ so we subtract the energy of the quasi-particle-quasi-hole ideal Coulomb attraction $-\frac{1}{32}\frac{1}{\sqrt{N_e}}$ (this is $A_{q=1/4}(\nu = 1/2)$ in Ref. [43]). This exciton gap is calculated for $N_e = 8, 10, 14, 16, 18$ ($N_e = 12$ is aliased with a composite fermion state at $\nu = 3/5$ and is ambiguous [11]). Note that the background energy does not enter into this definition of the gap since its contribution explicitly cancels.

(ii) Alternatively, one can compare the ground state energy at $N_\Phi$ to the ground state energies with one additional/fewer flux quantum. These are states with two quasiholes or two quasiparticles, respectively. While more subtle than in the case of the exciton gap, the background energies cancel again. The resulting gap, sometimes called the quasiparticle-quasihole (qp-qh) gap [43], is calculated for $N_e = 10, 14, 18$. Other system sizes are aliased (see Table III in Ref. [43]).

Although we present both gap calculations, we consider the exciton gap a more reliable gap estimate in the thermodynamic limit due to the less severe aliasing problem. Only estimates using exciton gap are used in the main text.

In Fig. 6.15 we illustrate the differences between the various ways of calculating the thermodynamic limit of the energy gap. The gap is roughly the same for an infinite square well potential as it is for a Gaussian $z$-dependence (once they are taken such that the wavefunction variance is the same) and for spherical and planar pseudopotentials. However, there are some quantitative differences: (i) if one extrapolates based on larger system sizes, the width dependence of the qp-qh gap is less pronounced and can only account for a 13% decrease of the gap compared to 28%; (ii) although in agreement qualitatively, using planar pseudopotentials instead of spherical ones tends to give higher gap estimates; and (iii) the exciton gap is larger than the qp-qh gap.
6.11 Appendix C: Particle-Hole Symmetry Breaking Order Parameter for an Illustrative Model Hamiltonian

In Section 6.6, we introduced an order parameter (Eq. (6.4)) for particle-hole symmetry breaking. We now show that this order parameter has negative expectation value in the MR trial wave function and positive expectation value in the aPf trial wave function. Fig. 6.16 shows \( \langle \phi \rangle \) for the ground state of \((1 - \alpha)H(0, 0, 1) + \alpha H_3\) and the ground state of \((1 - \alpha)H(0, 0, 1) + \alpha H_3^*\). Here \( H_3 \equiv \sum_{i<j<k} \hat{P}_{ijk}(m = 3) \) and \( H_3^* \) is the particle-hole conjugate of \( H_3 \). As may be seen from the \( \alpha \to 1 \) behaviour in Fig. 6.16, when the ground state is in the MR universality class, \( \langle \phi \rangle < 0 \) and when it is the aPf wave function, \( \langle \phi \rangle > 0 \). Moreover, the order parameter interpolates smoothly between zero and these values, as \( \alpha \) is increased from zero.

These calculations were performed on the sphere and on the torus for comparison. For the spherical geometry, \( \langle \phi \rangle \) is calculated at \( N_{\Phi} = 2N_e - 1 \), which is the particle-hole symmetric value of the shift on the sphere. Thus, at \( \alpha = 0 \), there is no particle-hole symmetry-breaking due to finite-size effects. At \( N_{\Phi} = 2N_e - 1 \) the ground state of \( H_3 \) is not the MR wave function, but the MR wave function with 4 MR quasiholes, and the ground state of \( H_3^* \) is the aPf wave function with 4 aPf quasiparticles. On the torus, we use the rectangular unit cell and show the results for the corner of the Brillouin zone for \( N_e = 8 \) electrons, i.e., \( K = (N_0/2, N_0/2) \). The other \( K \) points corresponding to the MR state display similar behaviour. Note in this choice of unit cell we find \( \langle \phi \rangle = 0 \) for \( \alpha = 0 \), while in the hexagonal unit cell for an even number of electrons this is not the case.

6.12 Appendix D: Finite-Size Effects, Planar and Spherical Pseudopotentials, \( m > 8 \) Pseudopotentials

In our model Hamiltonian, we used planar pseudopotentials. Although spherical pseudopotentials approach planar ones in sufficiently large systems, our use of planar pseudopotentials can be a source of systematic error in small spherical systems. In this section, we analyze the differences between spherical pseudopotentials and the planar ones used in the results reported in section 6.2. We also perform an extrapolation in system size to ensure our conclusions hold in the thermodynamic limit. We restrict our discussion here to small \( \kappa \), which is the limit in which our Hamiltonian is exact on the plane.
To consider the difference between planar and spherical pseudopotentials in Eq. (5.1), we compute the spherical pseudopotentials using a program kindly provided by Steve Simon, which was also used in Ref. [31]. We obtain the spherical three-body pseudopotentials for each of our relevant system sizes along with the three-body pseudopotentials carefully extrapolated to infinite system size. Compared to Ref. [31] we were able to include a few larger system sizes which lead to better agreement between the pseudopotentials corrections obtained in this way numerically and the corrections obtained analytically [29]. We compare the ex-
Figure 6.17: Extrapolation of the differences between the corrections to the three-body pseudopotentials to the sphere of infinite radius. Compare to Fig. 2 in Ref. [31]. The difference to Ref. [31] is that few larger system sizes were used for extrapolation in both LLs and $N\phi$.

For our biggest systems the pseudopotentials could not be calculated directly and we used the values obtained from extrapolation in $1/N\Phi$. The extrapolations used are shown in Fig. 6.17. The pseudopotentials dependence on $1/N\Phi$ we find is somewhat softer than presented in [31] but has a clear linear dependence hence using the extrapolated values is justified. The code used [31] only gives us the differences of the pseudopotentials (e.g., $V_5 - V_3$). A constant shift of the three-body pseudopotentials does not influence the many-body state as can be checked numerically. We choose this shift so that the finite-size spherical $V_3^{(3)}$ is equal to the extrapolated planar $V_3^{(3)}$. 

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6.12 Appendix D: Finite-Size Effects, Planar and Spherical Pseudopotentials, $m > 8$ Pseudopotentials

Table 6.1: The extrapolated three-body pseudopotentials obtained numerically in spherical geometry compared to those obtained analytically in Ref. [29] (see Table 2). Compare to Table 2 in Ref. [31].

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<th>Table 2 in Ref. [29]</th>
<th>our extrapolation</th>
</tr>
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</tr>
<tr>
<td>$\delta V_6 - \delta V_3$</td>
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<td>0.0046</td>
</tr>
<tr>
<td>$\delta V_7 - \delta V_3$</td>
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<td>0.0144</td>
</tr>
<tr>
<td>$\delta V_8 - \delta V_3$</td>
<td>0.0138</td>
<td>0.0137</td>
</tr>
</tbody>
</table>

In Fig. 6.18, we display the lowest-order perturbative (per particle) energy contributions of the three-body terms of $H(w/\ell_0 = 0, \kappa = 0.1, 1)$ given in Eq. (5.1) using spherical pseudopotentials, rather than the planar pseudopotentials used in Fig. 6.2. The top panel of the Fig. 6.18 uses the pseudopotentials obtained by extrapolating the spherical pseudopotentials to the thermodynamic limit and listed in Table 6.1. In principle, this should be precisely the same as in Fig. 6.2, but there are small differences since the extrapolation from these system sizes does not give precisely the planar values. The lower panel, in turn, shows the same expectation values with spherical pseudopotentials used at each system size. Three-body contributions were again evaluated in the Coulomb ground state in both cases. The results are qualitatively consistent with those obtained using planar pseudopotentials: the energy is lowered more at $S = 3$ than at $S = -1$ for each individual system size as well as in the thermodynamic limit.

Finally, we estimate the importance of higher three-body pseudopotentials, not included in our effective Hamiltonian. While $V_m^{(3)}$ with $m \leq 8$ are scalar, most of the higher pseudopotentials are matrices. This complicates their inclusion in exact diagonalization calculations, and we have not yet incorporated this. Ref. [30] gives the value of $V_9^{(3)}$. To obtain a rough qualitative estimate of the expectation value for $m = 9$ three-body pseudopotential we used a scalar value $-0.001025 e^2/\epsilon \ell_0$ obtained by averaging the entries of the 2-by-2 matrix given in [30]. The next higher three-body pseudopotential is scalar, $V_{10}^{(3)} = 0.000145 e^2/\epsilon \ell_0$, and was treated exactly.

In Fig. 6.19 we extend Fig. 6.3 with results for the $m = 9$ and $m = 10$ three-body pseudopotentials, calculated as described above. We observe that both pseudopotentials do not noticeably contribute to the difference between the Pfaffian and anti-Pfaffian states, and thus should not affect the central conclusion of the present work. Both expectation values are however non-zero, indicating that higher three-body pseudopotentials might have to be considered for quantitative comparisons.
Figure 6.18: Three-body energy contributions are calculated with system size-dependent (bottom panel) and extrapolated (top panel) spherical pseudopotentials. The energy difference between the extrapolated values are $0.000066 \frac{e^2}{\epsilon \ell_0} = 0.045 \kappa |V_{3}^{(3)}|$ (bottom panel) and $0.00019 \frac{e^2}{\epsilon \ell_0} = 0.13 \kappa |V_{3}^{(3)}|$ (top panel). Although relatively small, these values are per particle and should thus provide extensive energy separation between the two states in the thermodynamic limit.
Figure 6.19: Top Panel: Expectation value of the three-body terms in the MR and aPf trial wavefunctions as a function of angular momentum $m$, i.e., $\langle \Psi_{\text{trial}} | H_{\text{3body}}(m) | \Psi_{\text{trial}} \rangle$ where $H_{\text{3body}}(m) = V^{(3)}_m(w/\ell_0, \kappa) \sum_{i<j<k} \hat{P}_{ijk}(m)$, and $\Psi_{\text{trial}} = \Psi_{\text{MR}}$ or $\Psi_{\text{aPf}}$. Bottom Panel: Expectation value of the three-body terms for the $S = 3$ and $S = -1$ ideal Coulomb ground states as a function of angular momentum $m$. 

$N_\Phi = 33$, $w/\ell_0 = 0$, $\kappa = 0.2$
to experiments.

In Fig. 6.20 we show the effect of the higher three-body pseudopotentials on the energy gap and on the trial wavefunction overlap. We emphasise that the matrix pseudopotential $V^{(3)}_9$ can not be treated exactly in our code. Therefore the data presented in Fig. 6.20 is an attempt to test the robustness of the ground state and to qualitatively estimate the significance of higher three-body pseudopotentials but is not a precise representation of their effects. From these available calculations we observe that the corrections from the higher pseudopotentials are relatively small and thus should not change the qualitative picture established using the cut off $m \leq 8$. Precise treatment of the higher pseudopotentials may be needed if one is to exactly determine the value of $\kappa_c$, corresponding to the phase transition.

Recent work [130] that considered the model Hamiltonian similar to the one used in this work but also included the single major contribution (out of 4) of $V^{(3)}_9$ suggested that the competition between Pfaffian and anti-Pfaffian can be sensitive to this particular pseudopotential which was absent in our model. Future careful study including higher three-body pseudopotentials will be needed in order to examine this possibility.
Figure 6.20: Top Panel: Energy gap (difference between the two lowest eigenvalues) calculated at "Pfaffian" shift $S = 3$ in a system with 16 electrons. Bottom Panel: MR Pfaffian overlap. Black data points correspond to the Hamiltonian used in the main text where only the three-body pseudopotentials $V_m^{(3)}$ with $m \leq 8$ are used. Red data points correspond to the case when also $V_9^{(3)}$ and $V_{10}^{(3)}$ are included.
7 Enigmatic 12/5 fractional quantum Hall effect

We numerically study the fractional quantum Hall effect at filling factors \( \nu = 12/5 \) and 13/5 (the particle-hole conjugate of 12/5) in high-quality two-dimensional GaAs heterostructures via exact diagonalization including finite well width and Landau level mixing. We find that Landau level mixing suppresses \( \nu = 13/5 \) fractional quantum Hall effect relative to \( \nu = 12/5 \). By contrast, we find both \( \nu = 2/5 \) and (its particle-hole conjugate) \( \nu = 3/5 \) fractional quantum Hall effects in the lowest Landau level to be robust under Landau level mixing and finite well-width corrections. Our results provide a possible explanation for the experimental absence of the 13/5 fractional quantum Hall state as caused by Landau level mixing effects.

The work presented here was published in Ref. [2]. Michael Peterson double-checked the numerical results and coordinated the project. Yang-Le Wu provided the numerically calculated \( Z_3 \) Parafermion wavefunctions used to calculate overlaps and reference entanglement spectra. All other calculations were performed by the author of the thesis.

7.1 Introduction

There is interest across physics, mathematics, engineering, materials research, and computer science in finding robust experimental manifestations of topologically ordered phases with non-Abelian anyonic low-energy excitations. Not only are non-Abelian anyons (i.e., neither fermions nor bosons) suitable for topological quantum computation, but they are described by topological quantum field theories (TQFT) of intrinsic fundamental interest [9]. The fractional quantum Hall effect [13, 131, 11] (FQHE) is the canonical example of a system supporting topologically ordered phases and is widely thought to support non-Abelian anyons in the second orbital electronic Landau level (LL), most probably at filling factor \( \nu = 5/2 \) [61]. There is a possibility that the experimentally observed FQHE at \( \nu = 12/5 \) supports
7.1 Introduction

particularly exotic topologically ordered phases described by the $Z_3$ parafermionic Read-Rezayi states [16, 132, 133, 134, 25, 135, 136, 137], exemplifying an exotic SU(2)$_3$ TQFT (in contrast to the 5/2 FQH state belonging to the SU(2)$_2$ TQFT). Since SU(2)$_3$ TQFT supports a richer version of non-Abelian anyons that can realize universal fault-tolerant quantum computation [9], there is a great deal of interest in the 12/5 FQHE. In this work, we focus on the enigmatic FQHE at $\nu = 12/5$.

Compared to the rather ubiquitous $\nu = 5/2$ FQHE, the experimental literature for $\nu = 12/5$ (= 2 + 2/5 filling) is sparse with only a few experimental reports of its observation. The 12/5 FQHE was observed in a 30 nm wide GaAs quantum well with electron densities of $n \sim 3 \times 10^{11}$ cm$^{-2}$ at magnetic field strengths of $B \sim 5$ Tesla at temperatures $T \sim 6$-36 mK [68, 74, 69, 70, 138, 139]. In addition to its fragility (the 12/5 FQHE is observed only in the highest quality samples with little disorder), the real enigma is that the corresponding particle-hole conjugate FQHE at 13/5 (= 5 − 12/5) has never been observed in spite of other FQHE in the second LL (e.g., 7/3 and 8/3, 11/5 and 14/5) showing both particle-hole conjugate states with roughly equal strength. This discrepancy is puzzling because in the lowest LL the FQHE at $\nu = 2/5$ and 3/5 are both routinely observed, are to good approximation particle-hole conjugates of one another [140, 141, 142], and are well-described by the composite fermion (CF) theory [143, 11]. Exotic, rather than CF-like nature of the 12/5 state has been discussed based on the analysis of the experimentally measured energy gap [74]. Interestingly, the 12/5 and 13/5 FQHE (with roughly equal strength) are observed in systems where two subbands are occupied (e.g., bilayers, thick quantum wells) such that the chemical potential is in the lowest LL (but in the higher subband so two LLs are completely full) [77, 144, 145]. In this work we provide a possible explanation for the absence (presence) of 13/5 (12/5) FQHE in the second LL as arising from the LL mixing effect that explicitly breaks the particle-hole symmetry.

Several candidate wave functions for $\nu = 12/5$ have been proposed and studied [133, 134, 25] under idealized conditions, using the Coulomb interaction without particle-hole symmetry breaking. Two recent numerical studies [134, 25] reinforced initial results [16, 132] that the ground state at $\nu = 12/5$ is in the non-Abelian $Z_3$ Read-Rezayi (RR) phase. Both studies perturbed the interaction finding a finite region of stability around the Coulomb point. All works considered particle-hole symmetric two-body Hamiltonians so all conclusions made therein regarding the $\nu = 12/5$ state are equally valid for the particle-hole conjugate state at $\nu = 13/5$. Thus, existing theories provide evidence that the experimentally observed 12/5 and (unobserved) 13/5 FQHE are both in the RR $Z_3$ phase but cannot explain why one (i.e., 12/5) exists experimentally and the other (i.e., 13/5) does not. We provide a plausible explanation for this puzzle.

LL mixing breaks particle-hole symmetry through emergent three-body (and
higher) terms in an effective realistic Hamiltonian [112, 29, 30, 31]. The importance of LL mixing can be parameterized by the ratio \( \kappa \) of the Coulomb energy \( e^2/\epsilon l_0 \) to the bare cyclotron energy \( \hbar \omega \) (i.e., the LL gap): 

\[ \kappa = \frac{e^2}{\epsilon l_0} / \hbar \omega \]

where \( \epsilon \) is the background lattice dielectric constant, \( l_0 = \sqrt{\hbar c/eB} \) is the magnetic length, \( e \) is the electron charge, and \( \omega = eB/mc \) is the cyclotron frequency. For GaAs, \( \kappa \approx 2.5/\sqrt{B} \) [T]. For most experiments in the second LL, \( \kappa \) is of order unity, making LL mixing an important correction. One attempt at incorporating LL mixing at \( \nu = 12/5 \) used the approximation of including additional basis states within exact diagonalization [146], but did not investigate 13/5.

In the present work, we numerically study a realistic model of the FQHE (described in Chapter 5) in the second LL using exact diagonalization, systematically including LL mixing effects due to (the infinite number of) all other LLs. We find that the LL mixing-induced particle-hole symmetry breaking strongly favors the \( \nu = 12/5 \) FQHE over the 13/5 in the second LL, qualitatively in agreement with experimental observations. By contrast, in the lowest LL we do not find significant particle-hole symmetry breaking between \( \nu = 2/5 \) and 3/5 FQHE. Our work gives a probable explanation for the presence (absence) of 12/5 (13/5) in the second LL and the existence and equal strength of 2/5 and 3/5 FQHE in the lowest LL. Our work also strengthens the claim that at finite LL mixing 12/5 FQHE arises from a RR parafermionic non-Abelian state (rather than from Abelian composite fermion states as for the 2/5 and 3/5 FQHE).

Model

The effective Hamiltonian is given by Eq. 5.1. Note, that the notation for the pseudopotentials in this Chapter includes the Landau level index \( N \): \( V_{2\text{body},m}^{(N)}(w/\ell_0, \kappa) \) for the two-body and \( V_{3\text{body},m}^{(N)}(w/\ell_0, \kappa) \) for the three-body pseudopotentials.

We use the spherical geometry [60, 11] where the total magnetic flux \( N_\phi = N_e/f - S \) where \( N_e \to \infty \), of the \( N^{th} \) LL and \( S \) is the shift [113]. The experimental filling factor is \( \nu = f + 2N \) where \( 2N \) arises from completely filling the lower \( N \) spin-up and down LLs. FQHE states are gapped uniform density ground states with total angular momentum \( L = 0 \). The RR \( Z_3 \) state describes \( f = 3/5 \) with \( S = 3 \) while the particle-hole conjugate RR state, \( \text{conj}(Z_3) \), describes \( f = 2/5 \) with \( S = -2 \). The CF states for \( \nu = 2/5 \) and 3/5 have shifts of \( S = 4 \) and \(-1 \), respectively. Although the pairs of particle-hole conjugate states appear at different shifts, in the absence of LL mixing (\( \kappa = 0 \)) they have identical spectra and all eigenstates are particle-hole conjugates of each other. Hence, by considering properties like energy gaps, overlaps, and entanglement spectra we can isolate the effects of LL mixing.

Eq. (5.1) has a well-defined exact limit as \( \kappa \to 0 \), hence, we can determine the leading order effects of LL mixing on the FQHE. Most experimental observations
of the 12/5 FQHE occur at fields of $B \sim 5.15$ T (see Ref. [74]) giving a quantum well width (30 nm) of $w/l_0 \approx 2.65$ and $\kappa \approx 1.1$. We estimate (an exact self-consistent calculation is possible for a particular device [59]) that an infinitely deep quantum well of $w/l_0 \approx 3$ provides approximately the same confinement as the real quantum well, and we consider $w/l_0 \leq 4$ and $\kappa \neq 0$ to model realistic samples under realistic conditions. We assume fully spin-polarized [25] single-component states throughout this work.

### 7.2 Overlap, perturbation theory, and entanglement spectra

We first investigate whether the system remains in the $Z_3$ RR phase under realistic conditions. The ground state of Eq. (5.1) is uniform with $L = 0$ for the RR shifts for all system sizes up to $N_\phi = 37$ for $\kappa \neq 0$ and $N_\phi = 42$ for $\kappa = 0$ (we have not studied $\kappa \neq 0$ for $N_\phi = 42$). The ground states have $L \neq 0$ for the CF shifts for zero and non-zero $\kappa$, for most system sizes. The Bonderson-Slingerland (BS) non-Abelian state for $\nu = 12/5$ [147] has $L = 0$ at $\kappa = 0$ but a smaller gap than the RR state [133]—this behavior remains with $\kappa \neq 0$, see Section 7.6. Similar qualitative results were recently found in the $\kappa = 0$ limit [134, 25].

Fig. 7.1(a) presents the overlap between the exact ground state $|\psi\rangle$ of Eq. (5.1) with the model wave functions $|Z_3\rangle$ and $\text{conj}(Z_3)$. For small $\kappa$ the overlap remains relatively unchanged but the 12/5 overlap with $\text{conj}(Z_3)$ is larger than the overlap with $Z_3$ at 13/5 for $\kappa \lesssim 0.5$ for all system sizes—the overlap at 13/5 decreases monotonically with $\kappa$ and both overlaps are found to collapse to zero near $\kappa \approx 1$ though some finite size effects are observed for larger $\kappa$.

Since the overlaps are relatively flat for small $\kappa$, we study the eigenstates obtained in the absence of LL mixing, at $\kappa = 0$ (denoted $|\psi_0\rangle$). We calculate $\langle\psi_0|H^{(3)}(\kappa = 0.1)|\psi_0\rangle$ where

$$H^{(3)}(\kappa) = \sum_m V^{(N)}_{3\text{body},m}(w/l_0, \kappa) \sum_{i<j<k} \hat{P}_{ijk}(m)$$

[shown in Fig. 7.1(b)]—this represents the lowest-order perturbative contribution to particle-hole symmetry breaking induced by LL mixing. The thermodynamic limit extrapolation of $\langle\psi_0|H^{(3)}(\kappa = 0.1)|\psi_0\rangle$ per particle for $\nu = 12/5$ is more than ten times smaller than for 13/5, indicating that LL mixing more severely affects the energetics of 13/5 compared to 12/5. While the ground state energies are lowered by the three-body terms, the excited states are lowered as well, reducing the energy gap at 13/5 and increasing the gap at 12/5. In the inset of Fig. 7.1(b) we show that $V^{(1)}_{3\text{body},3}$, $V^{(1)}_{3\text{body},5}$, and $V^{(1)}_{3\text{body},6}$ are the three-body pseudopotentials that contribute most to particle-hole symmetry breaking between $\nu = 12/5$ and 13/5.
Enigmatic 12/5 fractional quantum Hall effect

Figure 7.1: (a) Wave function overlap between $Z_3$ and $\text{conj}(Z_3)$ and the exact ground state of Eq. (5.1) at $\nu = 13/5$ and 12/5, respectively, as a function of $\kappa$ for $N_\phi = 37$ (14 holes/electrons). A finite well width increases the overlaps and $\kappa$ breaks particle-hole symmetry yielding higher overlaps with $\text{conj}(Z_3)$ for 12/5 compared to $Z_3$ for 13/5. The inset shows the overlaps in more detail. (b) Expectation values of the three-body terms per particle $N_p$ of Eq. (5.1) for $\kappa = 0.1$ and $w/l_0 = 0$, evaluated for the ideal Coulomb ground and first excited states (both denoted $|\psi_0\rangle$) at 12/5 and 13/5, respectively, as a function of inverse LL degeneracy $1/(N_\phi + 1)$ extrapolated to the thermodynamic limit. $N_\phi = 27$ is aliased with $\nu = 1/3$ and left out. (Inset) Expectation values for each three-body term $[H_L^{(3)} = V_{3\text{body},L}(w/l_0, \kappa = 0.1) \sum_{i<j<k} \hat{P}_{ijk}(L)]$ for $N_\phi = 37$. Lines are a guide to the eye except in the main plot of (b) where they represent linear extrapolations.
7.2 Overlap, perturbation theory, and entanglement spectra

![Graph](image)

Figure 7.2: (a) Entanglement spectrum for the exact ground state of Eq. (5.1) for $w/l_0 = 3$ and $\kappa = 0.1$ at $\nu = 13/5$ (shift $S = 3$) and (b) at $\nu = 12/5$ (shift $S = -2$) for $N_\phi = 37$. The counting for the low-lying levels is 1, 1, 3, 6 up to $\Delta L^z_A = 5$ agreeing with $Z_3$ and $\text{conj}(Z_3)$. The orbital cuts, using the notation of Ref. [122], are $P[0|0]$ for $S = 3$ and $P[1|1]$ for $S = -2$. $\Delta L^z_A = L^z_A - (L^z_A)_{\text{root}}$ where (a) $(L^z_A)_{\text{root}} = 120$ and (b) $(L^z_A)_{\text{root}} = 60.5$. The topological gap is indicated by the green arrow and defined as the difference between the two lowest lying levels at $\Delta L^z_A = 1$ (see Section 7.3).

The $Z_3$ state has a relative abundance of three-body clustering by construction [16] and large expectation value of $H^{(3)}(\kappa)$ (not shown), similar to $|\psi_0\rangle$ at $\nu = 13/5$. In contrast, the three-body terms have little effect on $12/5$.

Overlaps may depend on short-range physics, so we investigate orbital entanglement spectra [117, 118, 119, 120, 122, 121]. If the ground state is in the RR phase, the counting of the low-lying levels of the entanglement spectra will be related to the SU(2)$_3$ TQFT describing the edge excitations [122]. The counting of the low-lying levels for $\nu = 13/5$ and $12/5$ for $w/l_0 = 3$ and $\kappa = 0.1$ (Fig. 7.2) matches the counting for $Z_3$ and $\text{conj}(Z_3)$, respectively, (including $\kappa = 0$, see Ref. [134]).

The results above confirm that the ground state of Eq. (5.1) remains in the RR phase under LL mixing. Further, LL mixing affects $\nu = 13/5$ more than $12/5$ and introduces strong particle-hole asymmetry.
Figure 7.3: Energy gap for $N_\phi=37$ at $\nu = 12/5$ and $13/5$ for $w/l_0 = 0-4$ (a)-(e). Similar results are obtained for smaller system sizes. (f) Width dependence of the gap for $N_e=8, 12, 14, \text{ and } 16$ for $\nu = 12/5$ for $w/l_0 = 0, 2, \text{ and } 3$ and $\kappa = 0$. (Inset) The gap as a function of $w/l_0$ at $\kappa = 0$ for $N_e=16$ ($N_\phi = 42$). Finite width reduces the gap by approximately 25% at $w/l_0 = 3$ relative $w/l_0 = 0$ for the largest system size. Note the similarities in (f) to Fig. 1(b) in Ref. [134].
7.3 Energy gap and topological gap

The neutral gap is related to the experimentally measured activation gap and the physical robustness of the FQHE. It is the difference between the two lowest energies at constant $N$, if the ground state has $L = 0$, otherwise it is taken to be zero.

Fig. 7.3(a)-(e) show energy gaps for our largest system ($N = 37$) for $w/l_0 = 0$-4. LL mixing breaks particle-hole symmetry producing a larger energy gap for $\nu = 12/5$ compared to $13/5$. The gap at $w/l_0 \neq 0$ for $12/5$ increases with $\kappa$ while the $13/5$ gap is suppressed (the suppression is found for all non-aliased system sizes and values of $w/l_0$, however an increasing gap at $\nu = 12/5$ for non-zero width is only found for the two largest system sizes $N = 37$ and $32$). Hence, LL mixing strengthens the $12/5$ FQHE for finite $w/l_0$ while weakening $13/5$ (strengthening of the FQHE gap with LL mixing does not happen for $\nu = 5/2$ [59]).

The thermodynamic extrapolation suffers from finite-size effects ($N = 12$ and 17) and aliasing ($N = 27$). The energy gaps at the remaining $N$ are shown in Fig. 7.3(f). Without LL mixing, finite width decreases the gap from $0.012e^2/\epsilon l_0$ at $w/l_0 = 0$ to $0.009e^2/\epsilon l_0$ at $w/l_0 = 3$ [values given are for $N = 42$ shown in the inset of Fig. 7.3(f)]. In the limit of small LL mixing, (i.e., high magnetic fields) it should be possible to observe more robust $12/5$ states in narrow quantum wells.

We expect that the equivalence of various models of finite width demonstrated for $\nu = 5/2$ [59] also holds here. Thus, to determine the effective width $w/l_0$ corresponding to a certain experimental device one would first calculate (for instance using a Schrödinger-Poisson solver) or measure [148] the square of the absolute value of the electron wave function in the direction perpendicular to the 2DEG and determine its variance (as defined in Ref. [59]). Then $w/l_0$ should be chosen such that the variance in the ground state of an infinitely deep quantum well of width $w/l_0$ is the same as in the given experimental sample.

Fig. 7.4 shows the energy gap as a function of $\kappa$ for $N = 32$ and $37$ (12 and 14 electrons (holes) for $\nu = 12/5$ (13/5), respectively) to the experimental value of $\kappa \sim 1.1$ for $w/l_0 = 3$. All the sharp features in the $\kappa$-dependence are associated with the change of $L$ in the first excited states. The behavior of the different system sizes is consistent up to $\kappa = 0.6 - 0.7$ and demonstrates a larger energy gap at $12/5$ than at $13/5$. Finite-size effects are observed for larger $\kappa$ which could be a result of our perturbative (in $\kappa$) approach to LL mixing breaking down or the smallness of the energy gap.

Finally, we investigate the topological gap. Following Ref. [122] we define the topological gap as the difference between the two lowest-lying levels in the entanglement spectrum at $\Delta L_A^z = 1$ (see Fig. 7.2). It represents the "energy
7.4 Second versus lowest Landau level

Finally we compare the second with the lowest LL. In Fig. 7.6(a) we show the relative energy gap difference induced by LL mixing between \( \nu = 12/5 \) and 13/5 and between \( \nu = 2/5 \) and 3/5 as a function of particle number. The LL mixing induced difference is much larger in the second LL than in the lowest LL (the sign is also different between the two with 12/5 strongly favored in the second LL while 3/5 is slightly favored in the lowest LL). The LL mixing induced gap difference between 12/5 and 13/5 grows with system size and is likely a robust feature in the thermodynamic limit.

We can further quantify the particle-hole symmetry breaking by calculating the
Figure 7.5: Topological gap for \( \frac{12}{5} \) and \( \frac{13}{5} \) as a function of \( \kappa \) for \( w/l_0 = 0-4 \) and \( N_\phi = 37 \).

overlap between the exact ground state \( |\psi\rangle \) at \( \nu = \frac{12}{5} \) (2/5) and the particle-hole conjugate of the exact ground state \( \text{conj}(\psi) \rangle \) at \( \nu = \frac{13}{5} \) (3/5). At \( \kappa = 0 \), this overlap is unity since the two states are particle-hole conjugates. In Fig. 7.6(b) particle-hole symmetry is much more strongly broken for the \( \nu = \frac{12}{5} \) (13/5) FQHE than for the \( \nu = \frac{2}{5} \) (3/5) FQHE. In fact, particle-hole symmetry is hardly broken at all in the lowest LL (in the lowest LL \( \langle \psi|\text{conj}(\psi)\rangle \gtrsim 0.9 \) up to \( \kappa \sim 2.4 \)). This apparent particle-hole symmetry could be a property of the lowest LL or of the CF-like states in any LL.
Figure 7.6: (a) Relative gap difference $\delta \Delta_\nu = (\Delta_\nu - \Delta_{1-\nu})/\Delta_\nu$ (induced by $\kappa = 0.1$) between particle-hole-conjugates at $12/5$ ($13/5$) and $2/5$ ($3/5$). $N_p$ is the number of particles for $\nu = 12/5$ and $2/5$ or number of holes for $\nu = 13/5$ and $3/5$. (b) Particle-hole symmetry breaking (quantified by $\langle \psi | \text{conj}(\psi) \rangle$) in the second LL compared to the lowest LL for $w/l_0 = 0$ and $3$. The system sizes are $N_\phi = 32$ for $\nu = 12/5$ ($13/5$) and $N_\phi = 31$ for $\nu = 2/5$ ($3/5$).

7.5 Conclusion

LL mixing strongly breaks the particle-hole symmetry between $\nu = 12/5$ and $13/5$ FQHE in the second LL, but has little effect on $\nu = 2/5$ and $3/5$ FQHE in the lowest LL. Our work implies that the absence of $13/5$ FQHE in the second LL is likely a direct consequence of LL mixing effects. This is mainly due to the suppression of the energy gap at $\nu = 13/5$ – the FQHE might simply be too fragile (in terms of energy gap) since LL mixing affects $13/5$ more severely than $12/5$, and because in experimental measurements, at constant density, $\kappa$ is larger at $13/5$ compared to $12/5$ (since the magnetic field at $13/5$ is smaller than at $12/5$). The $12/5$ ground state at shift $S = -2$ remains in the non-Abelian parafermionic (conjugate) RR $Z_3$ phase when finite-width and non-zero LL mixing are taken into account extending the validity of previous conclusions [134, 25, 16, 132, 146] obtained for idealized conditions. We do not rule out the $\nu = 13/5$ FQHE in the $Z_3$ RR phase, but establish that the $13/5$ FQHE is always much weaker than $12/5$. Future experiments with smaller $\kappa$ could show a very weak FQHE at $\nu = 13/5$ in extremely high mobility samples at ultra-low temperatures with a very small activation energy.
7.6 Appendix A: Energetics at the Bonderson-Slingerland shift

In this appendix we explore the perturbative change in the FQHE gap Landau
level mixing induces at the shifts corresponding to the Bonderson-Slingerland (BS) state and its corresponding particle-hole conjugate. Shown in Fig. 7.7 are the expectation values of the three-body terms of our effective Hamiltonian [Eq. (5.1)] for the ground and first excited states (the results are presented in the same way as in Fig. 1b). Both the ground and excited states reduce their energy by approximately the same amount at 12/5. For 13/5 the energy of the excited state is reduced significantly more than that of the ground state meaning that the gap of 13/5 is reduced whereas the gap of 12/5 remains relatively constant.

7.7 Appendix B: Robustness of the composite fermion states for the 2/5 and 3/5 FQHE under Landau level mixing

To further characterize the evolution of the states in the lowest Landau level we approximate the CF-like states at 2/5 and 3/5 with the exact ground state of a "hardcore" model Hamiltonian with $V_1 \neq 0$ and all other $V_m = 0$ at $N_\phi = 5N_e/2 - 4$ and $N_\phi = 5N_e/3 + 1$, respectively. This Hamiltonian produces the $1/m$ Laughlin state exactly as the zero-energy ground state for $N_\phi = m(N_e - 1)$ and produces ground states with large overlaps ($> 0.99$) with CF wave functions for filling factor $\nu = n/(2pm + 1)$ at the appropriate flux as checked via Monte Carlo. As shown in Fig. 7.8 the overlap remains stable under Landau level mixing and only starts to significantly decrease around $\kappa = 3 - 4$, well beyond the typical experimental values.

It is an open question whether the observed robustness of the FQH states at 2/5 and 3/5 is due to their CF-like nature or to the specific form of the effective interaction in the lowest Landau level.
7.7 Appendix B: Robustness of the composite fermion states for the 2/5 and 3/5 FQHE under Landau level mixing

Figure 7.8: Overlap between the realistic ground state and the ground state of the hardcore ($V_1 \neq 0$ and $V_m = 0$ for all other $m$) Hamiltonian for $N_\phi = 31$. $w=0$ (left panel) and $w=3$ (right panel).
We investigate InAs/GaSb double quantum wells in the non-inverted semiconducting regime and in the inverted regime where electrons and holes coexist. We explain an unconventional Landau level spectrum with energy gaps modulated by the magnetic field applied perpendicular to the quantum wells observed in experiment in terms of an effective low-energy theory that possesses the symmetries of the quantum well and reproduces the first-principles band-structure of the experimental device.

The results of this chapter were published in Ref. [4]. The experimental work was performed in the group of Prof. Klaus Ensslin by Matija Karalic, Susanne Mueller and Christopher Mittag. The samples were grown by Thomas Tschirky in the group of Prof. Werner Wegscheider. The first-principles calculation of the band structure to which our effective model was fitted were performed by Quan-Sheng Wu who also calculated the $Z_2$ invariant for the inverted (non-inverted) band structures [149, 150] to confirm their topological (trivial) nature. Alexey A. Soluyanov provided general theoretical guidance and his notes for the action of symmetry operations on the elements of the basis (Equations 8.2-8.6) we used for the Hamiltonian. Thomas Ihn coordinated the project, double-checked some of the derivations, helped to include Zeeman term and analyse the results of the simulations. The derivation of the effective Hamiltonian, identification of the parameters corresponding to the experimental samples, derivation and numerical calculation of the Landau levels was performed by the author of the thesis.
8.1 Introduction

8.1.1 Quantum spin Hall effect, topological insulators and topological quantum computations

Quantum spin Hall effect (QSHE) is a time-reversal-invariant, two-dimensional, topological state of matter where the bulk is insulating and the helical edge states are protected from dissipation by the time-reversal symmetry (see Ref. [151] for a review). The QSHE and the IQHE discussed here are two examples of the topological band structure (allow non-interacting, single-particle description) phases that can in general be ordered into a "periodic table" according to their dimensionality and presence of certain symmetries [151, 152, 153].

QSHE is related to the integer quantum Hall effect and its discovery [154] was in part motivated by the realization of the topological nature of IQHE. Thouless, Kohmoto, Nightingale, and Nijs (TKNN) [17] considered a 2D system of electrons on a lattice subject to a magnetic field and showed that the calculation of the Hall conductivity $\sigma_{xy}$ using the Kubo formalism is similar to the calculation of the Chern number, an integer topological invariant that can be calculated for any given band structure. This explained the precise quantisation of $\sigma_{xy}$ observed in IQHE.

Haldane [19] considered a model (now known as "Haldane model") of graphene where he added a magnetic field so that it satisfies the spacial symmetry of the honeycomb lattice of graphene and cancels out over a unit cell, yet breaks the time-reversal symmetry. Haldane showed that this state is a quantum Hall state with $\sigma_{xy} = e^2/h$ which can be understood in terms of the Chern invariant that is found to add from the two Dirac points in the graphene dispersion. Breaking the time-reversal symmetry is essential in this construction since otherwise the contributions from the two Dirac points would cancel out leading to zero Chern number.

Quantum spin Hall effect can be roughly thought of as a combination of two copies of the (time-reversal breaking) Haldane model for each of the two spin species into a single time-reversal symmetric state. Its first realisation was constructed [154] in a similar setting of the 2D graphene where the time-reversal symmetry was preserved (no magnetic field) but a spin-orbit interaction was added. Chern number is 0 in this time-reversal symmetric system. It was however realised [155] that the topological nature of this phase can be characterised by a different topological $Z_2$ invariant, which has a relatively simple interpretation in terms of the bulk-boundary correspondence [151]. Namely, one can tell apart the two topologically distinct classes by counting the number of Kramers pairs of edge modes crossing the Fermi energy $E_F$.

The edge modes of the QSH state are non-chiral - they carry the two spin species
in opposite directions at every point on the edge. As long as the disorder respects
time-reversal symmetry the backscattering for the edge modes is forbidden. It can
also be shown [154] that the scattering due to electron-electron interaction can be
suppressed at low enough temperature.

Besides the fundamental physics interest the QSH state can be used to imple-
ment topological quantum computing [156, 157]. When combined with a super-
conductor and a magnet the QSH phase can be used to create Majorana fermions
and thus be a building block of the topological quantum computer.

The existence of the QSH state has been proposed in the quantum well struc-
tures made of the heavier elements and thus featuring stronger spin-orbit in-
teraction [158], which brings us to the discussion of the QSH phase in the semiconductor
heterostructures continued in the next section.

8.1.2 QSH phase in the coupled InAs/GaSb quantum wells

The peculiar band lineup of coupled InAs/GaSb quantum wells (QW) can lead
to the coexistence of electrons and holes at the charge neutrality point [159, 160].
According to a recent prediction [161], this material system displays a topological
insulator phase, whose existence and strength can be tuned by gate voltages and
which hosts the quantum spin Hall (QSH) state [155, 154, 162]. The topological
insulator phase arises if the band ordering is inverted and coupling between electron
and hole states opens a hybridisation gap at the charge neutrality point. So far,
several groups have performed experiments on InAs/GaSb QWs demonstrating
edge transport [163, 164] and conductance quantisation consistent with the QSH
state [165, 166, 167, 168]. However, the aforementioned works have not shown spin
polarization of edge currents, as has been done in HgTe QWs [169]. Indeed, recent
experiments [170, 171] have detected edge transport in the topologically trivial
phase of InAs/GaSb QWs, providing room for an alternative explanation for edge
transport in general in this system. Therefore, it is of utter importance to clearly
and consistently distinguish the two phases and to understand their properties
under applied electric and magnetic fields.

Our theoretical work and numerical simulations were motivated by the experi-
mental results obtained at the Solid State Physics Laboratory of the Department
of Physics at ETH Zurich for the two samples of different InAs well widths, one of
them in the topological regime (inverted band alignment and hybridisation gap,
topologically non-trivial phase, TI sample) and the other in the semiconducting
regime (non-inverted band alignment and normal gap, topologically trivial phase,
NI sample). Both samples have comparable mobilities. The experiments unravel
the energy dispersion qualitatively and the charge carrier occupations of electrons
and holes quantitatively. The experimental data shows unique fingerprints of the
inverted band structure and band hybridisation, such as a suppression of the resis-
8.2 Experimental observations

An important property of the experiment is the presence of the top gate that allows one to adjust the electron and hole densities in the sample by changing the voltage on it: $V_{tg}$. The charge neutrality point (CNP) where the carrier density of electrons is equal to that of holes is found to be at $V_{tg} = -6.08\,\text{V}$ for the TI sample.
Quantum spin Hall effect in the coupled InAs/GaSb quantum wells

and $V_{tg} = -2$V for the NI sample. For $V_{tg}$ higher than the CNP the conductance is dominated by electrons and for lower by holes.

The total density in our TI device follows the experimentally determined relation $n_{tot}(V_{tg}) = n - p = c(V_{tg} - V_{tg}^{\text{CNP}})$ for the whole gate voltage range, with $c = 1.41 \times 10^{11} \text{cm}^{-2}\text{V}^{-1}$. Assuming parabolic dispersions for electrons and holes, we find an approximately linear decrease (increase) of the hole (electron) density with gate voltage. Under the same assumption the band overlap between the electron dispersion in InAs and the hole dispersion in GaSb also depends linearly on gate voltage. In Ref.172 the validity of such a model incorporating screening effects via quantum capacitances was shown.

In Fig. 8.1, we present the experimentally measured conductivity $\rho_{xx}$ as a function of $V_{tg}$ and $B_\perp$ for the TI sample. This map shows the Landau fan of electrons for $V_{tg}$ above the CNP, and that of holes below. Filling factors $\nu$ are indicated in the figure (negative for hole, positive for electron Landau levels). A remarkable, regular pattern appears in the electron region above $B_\perp \approx 2$T. The minima in $\rho_{xx}$ corresponding to integer filling factors $\nu$ are modulated in strength with magnetic field. A similar effect, although less pronounced, is visible on the hole side (at $\nu = -1$, see arrows). Other inverted samples (not shown) demonstrate a stronger pattern on the hole side.

A Fourier analysis of the Landau fan in Fig. 8.1 (not shown) combined with the low-field Hall effect measurements lead to an estimate of a depletion voltage of holes (electrons) $V_{tg}^{(p)} = 2$V ($V_{tg}^{(n)} = -9$V). Using these values we find the electron density at charge neutrality to be about $3 \times 10^{11} \text{cm}^{-2}$. The band overlap increases linearly with gate voltage from approximately 3meV at $V_{tg} = -9$V to 76meV at $V_{tg} = 2$V. These numbers imply that the band alignment becomes non-inverted for $V_{tg} < -10$V. The band overlap will determine the constant in our theoretical low-energy model that fixes the relative position of the electron and hole dispersions (see Fig. 8.7 and Section 8.3.3).

A zoom into a region of the electron Landau fan is shown in Fig. 8.2. The modulation of the $\rho_{xx}$ minima was studied by measuring the associated activation energies for $\nu = 3, 4, 5$ at the points marked in Fig. 8.2. It was confirmed that the modulation of $\rho_{xx}$ is caused by a modulation of energy gaps in the Landau level spectrum. The values of the activation energies are unexpectedly small: with an electron mass of $m_{\text{InAs}}^* = (0.03-0.04)m_0$ [173], the bare Landau level splitting is $\hbar c/m_{\text{InAs}}^* = 2.9\text{--}3.9$meV/T. The Zeeman splitting increases with magnetic field at a rate of $g^*\mu_B = 0.6\text{--}0.9$meV/T if we use $g^* = 10\text{--}15$ [174, 175]. The values for the activation energies in Fig. 8.2 are two orders of magnitude smaller than these expectations. The possible explanation of this fact within our theoretical model is presented in the Section 8.4.2.
8.2 Experimental observations

Figure 8.2: Zoom-in of Fig. 8.1, where each row is normalized according to \( \rho_{xx}/\rho_{xx}(B_{\perp} = 0) \) (a.u.). The numbers on the outside indicate filling factors \( \nu \). The dashed lines are guides to the eye, marking the evolution of selected filling factors as a function of \( V_{tg} \) and \( B_{\perp} \). Along the dotted (dash-dotted) line, even (odd) filling factors are enhanced and odd (even) filling factors are suppressed. The activation energy \( \Delta \) at the positions of the symbols is found by fitting the temperature dependence of the minima of the longitudinal conductivity \( \sigma_{xx} = \rho_{xx}/(\rho_{xx}^2 + \rho_{xy}^2) \) with an exponential function of the form \( \sigma_0 e^{-\Delta/(2k_B T)} \) (\( \sigma_{xx} \) in the smallest gaps, \( \nu = 4 \) at \( B_{\perp} = 5.7 \) T and \( \nu = 5 \) at \( B_{\perp} = 8 \) T, can be fit equally well with \( \sigma_0 e^{-(\Delta/(2k_B T))^{1/2}} \), but the resulting \( \Delta \) is within 10% of those values given in Fig. 8.2). The unit of \( \Delta \) is \( \mu eV \).
Figure 8.3: $\rho_{xx}$ as a function of $V_{tg}$ and perpendicular magnetic field $B_\perp$ at $T = 130\text{mK}$. The numbers indicate filling factors $\nu$, where we assign positive $\nu$ to electron and negative $\nu$ to hole Landau levels. The horizontal stripe visible around $B_\perp = 7\text{T}$ is due to the sample being unstable.

In order to compare the TI and NI samples we show in Fig. 8.3 $\rho_{xx}$ as a function of $V_{tg}$ and $B_\perp$ for the NI sample, in analogy to Fig. 8.1. The Landau fan branching out into the electron region resembles that of a conventional two dimensional electron system, where the energy spectrum in $B_\perp$ is determined by cyclotron and Zeeman energies. The fan lacks the strongly modulated energy gaps observed for the TI sample. Interestingly, even in the NI sample the minima of the odd filling factors oscillate weakly (as indicated exemplarily by the arrows).
8.3 Theoretical analysis

8.3.1 Hamiltonian

We would like to derive the most general $4 \times 4$ Hamiltonian that respects the symmetry group of the host structure. The four basis states are the conduction band states of electrons in InAs (spin up and down) and heavy hole valence band states in GaSb (spin up and down). The interesting physics in our system happens at the interface between the two quantum wells made of InAs and GaSb. We thus can restrict ourselves to a two-dimensional plane defined by the interface.

Both InAs and GaSb have the cubic crystal structure and zincblende unit cell shown in Fig. 8.4. The interface defining our 2D space is perpendicular to the structure growth direction $[001]$ which is the vertical $z$ axis in Fig. 8.4. We identify the symmetry group in question as $C_{2v}$ that contains a 180 degrees rotation axis ($C_2$, $z$ axis) and two mirror symmetries (reflection planes are defined by a diagonal in the horizontal plane and $z$ axis). Note that this structure does not have a 4-fold rotation symmetry that would mean the equivalence of $x$ and $y$ axis and that is present for the Hamiltonian used in Ref. [161].

As any hermitian $4 \times 4$ matrix the Hamiltonian can be expanded in the basis constructed of a Kronecker product of two Pauli matrices:

\[
H = \sum_{ij} a^{ij} b_{ij} = \sum_{ij} a^{ij} \tau_i \otimes \sigma_j,
\]

(8.1)

where $i, j = 0, 1, 2, 3, 4$, $b_{ij}$ is a basis vector, $a^{ij}$ real valued expansion coefficients and $\tau_i$ acts on the electron-hole and $\sigma_j$ on the spin subspace.

We consider two spatial dimensions and require that the Hamiltonian is invariant under the $C_{2v}$ point symmetry group of our structure. Besides, we also impose the time-reversal symmetry which our system should possess in the absence of the magnetic field. The symmetry matrices in our basis read:

\[
C_2 = i \tau_z \otimes \sigma_z
\]

(8.2)

\[
\sigma_x = i I \otimes \sigma_x
\]

(8.3)

\[
\sigma_y = i \tau_z \otimes \sigma_y
\]

(8.4)

\[
\Theta = i I \otimes \sigma_y K
\]

(8.5)

In Section 8.4.1 we will study the importance of the inversion symmetry-breaking terms. The inversion symmetry reads

\[
P = \tau_z \otimes I
\]

(8.6)
Quantum spin Hall effect in the coupled InAs/GaSb quantum wells

Example

As an example let us consider the 03 element in the sum 8.1: $a^{03}(k_x, k_y)b_{03} = a^{03}(k_x, k_y)\tau_0 \otimes \sigma_3$.

The invariance of the Hamiltonian under a symmetry operation $\hat{S}$ means that it commutes with the Hamiltonian $H(\hat{S}k)\hat{S} = \hat{S}H(k)$. Multiplying by $\hat{S}^{-1}$ on both sides we obtain

$$H(k) = \hat{S}H(\hat{S}^{-1}k)\hat{S}^{-1}. \quad (8.7)$$

We consider all symmetry operations $\hat{S}$ from the $C_{2v}$ point group plus time-inversion. Calculating the right-hand side of Eq. 8.7 we find that it evaluates to $a^{03}b_{03}$ for $\hat{S} = C_2$ and to $-a^{03}b_{03}$ for both mirror symmetries and time-inversion.

Figure 8.4: Zincblende unit cell [176].
8.3 Theoretical analysis

Considering the action of the $C_2, \sigma_v^x, \sigma_v^y, \Theta$ symmetries on the wave vector $k$ we obtain for the coefficients correspondingly

$$a^{03}(k_x, k_y) = a^{03}(-k_x, -k_y)$$  (8.8)
$$a^{03}(k_x, k_y) = -a^{03}(-k_x, k_y)$$  (8.9)
$$a^{03}(k_x, k_y) = -a^{03}(k_x, -k_y)$$  (8.10)
$$a^{03}(k_x, k_y) = -a^{03}(-k_x, -k_y).$$  (8.11)

We observe that the only expression that satisfies all four constraints is $a^{03}(k_x, k_y) = 0$. For other cases we might however find that the coefficient $a^{ij}(k)$ must be odd or even in $k_x$ or $k_y$.

**General second order Hamiltonian**

The symmetries give the following conditions on the coefficients $a^{ij}$ as functions of the momentum $k$: $a^{03} = a^{10} = a^{23} = a^{11} = a^{12} = 0$ and $a^{00}, a^{30}, a^{21}$ are even in both $k_x$ and $k_y$; $a^{13}, a^{02}, a^{32}$ are odd in $k_x$ and even in $k_y$; $a^{20}, a^{01}, a^{31}$ are even in $k_x$ and odd in $k_y$ and finally $a^{22}$ is odd in both $k_x$ and $k_y$.

The above conditions fully specify the Hamiltonian. To make it useful for practical numerical study we expand each of the coefficients as a power series in $k_x$ and $k_y$. The Hamiltonian up to the 2nd order in $k$ has 16 parameters and reads

$$\begin{pmatrix}
(C^{00}_{00} + C^{00}_{10} + C^{00}_{20} + C^{00}_{30})k_x^2 + (C^{02}_{00} + C^{02}_{10} + C^{02}_{20} + C^{02}_{30})k_y^2
 & (C^{00}_{11} + C^{00}_{12} + C^{00}_{13})k_x k_y
 & (C^{00}_{10} + C^{00}_{11} + C^{00}_{12} + C^{00}_{13})k_x
 & (C^{00}_{22} + C^{00}_{23})k_y
 & (C^{00}_{30} + C^{00}_{31} + C^{00}_{32} + C^{00}_{33})k_x
 & (C^{02}_{10} + C^{02}_{11} + C^{02}_{12} + C^{02}_{13})k_y
 & (C^{02}_{20} + C^{02}_{21} + C^{02}_{22} + C^{02}_{23})k_x
 & (C^{02}_{30} + C^{02}_{31} + C^{02}_{32} + C^{02}_{33})k_y
\end{pmatrix}
\begin{pmatrix}
(C^{m}_{00} + C^{m}_{10} + C^{m}_{20} + C^{m}_{30})k_x^2 + (C^{m}_{02} + C^{m}_{12} + C^{m}_{22} + C^{m}_{32})k_y^2
 & (C^{m}_{11} + C^{m}_{12} + C^{m}_{13})k_x k_y
 & (C^{m}_{10} + C^{m}_{11} + C^{m}_{12} + C^{m}_{13})k_x
 & (C^{m}_{22} + C^{m}_{23})k_y
 & (C^{m}_{30} + C^{m}_{31} + C^{m}_{32} + C^{m}_{33})k_x
 & (C^{m}_{20} + C^{m}_{21} + C^{m}_{22} + C^{m}_{23})k_y
 & (C^{m}_{32} + C^{m}_{33})k_x
 & (C^{m}_{33})k_y
\end{pmatrix}
\begin{pmatrix}
m_{00} & m_{01} & m_{02} & m_{03}
& m_{10} & m_{11} & m_{12} & m_{13}
& m_{20} & m_{21} & m_{22} & m_{23}
& m_{30} & m_{31} & m_{32} & m_{33}
\end{pmatrix}
$$

where $m_{ij}$ is the matrix element in $k^{th}$ row and $l^{th}$ column and $C^{lm}_{ij}$ are the real constants with indices $ij$ relating them to the indices of the expansion coefficients $a^{ij}$ they originated from; $l$ is the power of $k_x$ and $m$ is the power of $k_y$. The corresponding basis is $|H+\rangle$, $|H-\rangle$, $|E-\rangle$, $|E+\rangle$, where $H$ stands for hole, $E$ for electron and the sign indicates the spin.

The Hamiltonian is different from the one of Liu et all [161] in that it allows anisotropy between $x$ and $y$ directions and includes 2nd order terms in $k$ everywhere where they are allowed by symmetry, not only on the diagonal.

### 8.3.2 Fitting to the tight binding dispersion

We determine the parameters $C^{lm}_{ij}$ by fitting the dispersion given by our effective Hamiltonian written down above to the dispersion calculated from a tight binding model for the precise geometry corresponding to the TI and NI samples.
The procedure of obtaining the tight-binding dispersion starts with the hybrid (HSE [177, 178, 179]) functional calculation performed in VASP package [180, 181] and intended to reproduce the gap and band structure of bulk InAs and GaSb. Based on this the tight-binding parameters are extracted for each of the materials using the Wannier90 software [182, 183, 184] such that the tight-binding model reproduces the band structure of VASP. Finally, one solves the tight-binding model for a heterostructure, infinite in $x-y$ plane which consists of the two layers (InAs and GaSb) of precisely the same thicknesses as in experiment and where the hopping given by Wannier90 in the previous step are used in the corresponding material. This procedure was originally performed by QuanSheng Wu in order to determine the thicknesses of the two layers that lead to the inverted band structure, desired for the QSH state. We use the band structure supplied by QuanSheng Wu corresponding to the TI and NI devices as a reference in order to determine the parameters of our effective Hamiltonian.

The parameters of our Hamiltonian are obtained by the least-square fit of the dispersion given by the effective Hamiltonian to the tight-binding dispersion over the region $[-0.0147, 0.0147] \times [-0.0147, 0.0147]$ in $k_x k_y$ plane.

The following parameters give the best fit for the TI sample:

- $C^{00}_{00} = 0.48609248eV$;
- $C^{30}_{00} = 2.3288687e-03*0.96eV$;
- $C^{00}_{02} = 23.262313eV$;
- $C^{30}_{02} = -61.106681eV$;
- $C^{02}_{00} = 22.670352eV A^2$;
- $C^{30}_{02} = -54.735715eV A^2$;
- $C^{01}_{01} = -0.11552277eV A^2$;
- $C^{31}_{01} = -0.20876968eV A^2$;
- $C^{02}_{10} = -0.22089286eV A^2$;
- $C^{32}_{10} = -0.017056818eV A^2$;
- $C^{13}_{10} = 0.24038851eV A^2$;
- $C^{20}_{01} = -0.18792671eV A^2$;
- $C^{22}_{11} = 5.2094870e V A^2$;
- $C^{21}_{00} = -5.1760050e-04eV$;
- $C^{21}_{02} = 33.894074eV A^2$;
- $C^{21}_{20} = 35.878439eV A^2$.

These parameters assume that the unit for the energy is electronvolt and that the unit for $k$ is inverse Angstrom. The band overlap is given by $2*C^{30}_{00}$.

The dispersion of our Hamiltonian with these parameters is compared to the tight-binding result in Fig. 8.5.

The parameters for the NI sample obtained from the fit are:

- $C^{00}_{00} = 0.49154446eV$;
- $C^{30}_{00} = -3.1065179e-03eV$;
- $C^{00}_{02} = 21.963230eV A^2$;
- $C^{30}_{02} = -34.153949eV A^2$;
- $C^{01}_{01} = 0.13994709eV A^2$;
- $C^{31}_{01} = -0.38763449eV A^2$;
- $C^{10}_{10} = 1.1629283e-02 eV A^2$;
- $C^{11}_{10} = 0.38885775eV A^2$;
- $C^{10}_{20} = -5.4719899eV A^2$;
- $C^{20}_{21} = -49.480814eV A^2$.

For the TI sample we obtain the effective masses of $0.0435m_0$ for electrons and $-0.09088m_0$ for holes.
8.3 Theoretical analysis

Figure 8.5: The tight-binding dispersion for the TI sample (solid lines) and the dispersion of the effective Hamiltonian with the parameters obtained from the best fit (solid dots). The dispersion is shown for $k_x = 0$.

The effective masses that we determine from the tight-binding dispersion for the NI sample are $0.04338m_0$ for electrons and $-0.08517m_0$ for holes. We note that the hole masses appear to be smaller than reported in experimental literature [185]. We will use the masses quoted here throughout to keep our calculations consistent.

8.3.3 Dispersion as a function of gate voltage

We make an approximation that the applied top-gate voltage $V_{tg}$ only changes the band overlap given by $2 \times C_{30}^{00}$. If we are able to find out how the band overlap depends on the $V_{tg}$ we can track the dependence of the dispersion of the effective Hamiltonian on the gate voltage. The capacitor model of Ref. 172 gives such dependence, provided that the electron and hole densities as functions of $V_{tg}$ are known from the experiment.

In Fig. 8.7 we show the evolution of the dispersion in the TI sample with the top-gate voltage. The band overlap $2 \times C_{30}^{00}$ is calculated using the capacitor model and experimental densities and is the only parameter that changes between the plots with all other parameters of the effective Hamiltonian fixed to the TI best-fit
Our simplified model for the density of states does not account for the gap in energy that opens in the TI regime. Also the capacitor model is least reliable in this region. Together with the uncertainties in the masses and other parameters this explains only qualitative agreement between these results and the positions of the experimentally measured peaks in $\rho_{xx}$ in Fig. 1(a) of the main text of Ref. [4]. However it allows us to support qualitatively the assignments of the peaks suggested there. The hole bands at $V_{tg} = -10 \text{V}$ show relatively big spin-splitting which agrees with the existence of two hole species concluded based on the experimental measurements.

### 8.3.4 Landau levels calculation

Consider the magnetic field applied along $z$ direction and otherwise free electron moving in the two dimensions defined by the $xy$ plane. The Hamiltonian operator for an electron reads then
8.3 Theoretical analysis

Figure 8.7: Dispersion Y–Γ–X calculated numerically by diagonalizing the 2nd order Hamiltonian. The position of the Fermi energy is calculated based on the experimentally determined electron and hole densities. For $V_{tg} = -9$ V the bands are separated by the energy distance on the order of $10^{-2}$ meV but do not touch.

\[ H_{LLs} = \frac{1}{2m} \left( p + \frac{eA}{c} \right)^2, \]  

where the rotation of the vector potential should give the magnetic field: $\nabla \times A = B\hat{z}$.

Choosing Landau gauge $A = B(0, x, 0)$ the two-dimensional Hamiltonian becomes

\[ H_{LLs} = \frac{1}{2m} \left( p_x^2 + (p_y + \frac{eB}{c} x)^2 \right) = \frac{1}{2m} \left( \tilde{p}_x^2 + \tilde{p}_y^2 \right) = \frac{1}{m} \left( p_x^2 + p_y^2 + 2p_y^2 \frac{eB}{c} x + \left( \frac{eB}{c} \right)^2 x^2 \right), \]  

Let’s consider operators

\[ \tilde{p}_+ = \hbar \tilde{k}_+ = \tilde{p}_x + i\tilde{p}_y = p_x + ip_y + i\frac{eB}{c} x \]  

and

\[ \tilde{p}_- = \hbar \tilde{k}_- = \tilde{p}_x - i\tilde{p}_y = p_x - ip_y - i\frac{eB}{c} x. \]
Their product
\[
\hbar^2 \tilde{k}_+ \tilde{k}_- = \left( p_x + ip_y + \frac{eB}{c} x \right) \left( p_x - ip_y - \frac{eB}{c} x \right)
\]  
\[
= p_x^2 + p_y^2 + 2 \frac{eB}{c} x p_y + \left( \frac{eB}{c} \right)^2 x^2 + \frac{i e B}{c} (x p_x - p_x x)
\]  
\[
= 2m H_{LLs} + \frac{i eB}{c} i \hbar = 2m H_{LLs} - \frac{eB}{c} \hbar.
\]  
(8.18)
is related to the Hamiltonian 8.13. This allows us to rewrite the Hamiltonian in the form reminiscent of the harmonic oscillator
\[
H_{LLs} = \frac{eB \hbar}{mc} \left( \sqrt{\frac{\hbar}{2eB}} \tilde{k}_+ \ast \sqrt{\frac{\hbar}{2eB}} \tilde{k}_- + \frac{1}{2} \right)
\]  
(8.19)
which can be made precise under the definition \( a^\dagger = \sqrt{\frac{\hbar}{2eB}} \tilde{k}_+ \) and \( a = \sqrt{\frac{\hbar}{2eB}} \tilde{k}_- \):
\[
H_{LLs} = \hbar \omega_c (a^\dagger a + \frac{1}{2}),
\]  
(8.20)
with \( w_c = \frac{eB}{mc} \) and \([a, a^\dagger] = 1\).

Now, we can express \( \tilde{k}_x \) and \( \tilde{k}_y \) in terms of the ladder operators
\[
\tilde{k}_x = \frac{1}{2} \sqrt{\frac{2eB}{\hbar c}} (a^\dagger + a)
\]  
(8.21)
\[
\tilde{k}_y = \frac{i}{2} \sqrt{\frac{2eB}{\hbar c}} (a - a^\dagger).
\]  
(8.22)

Finally, replacing \( k_x \rightarrow \tilde{k}_x \) and \( k_y \rightarrow \tilde{k}_y \) in the effective \( 4 \times 4 \) Hamiltonian we obtain its expression in the Hilbert space where each of the 4 basis states is expanded with a ladder of Landau levels. Practically, one introduces a cut-off in the ladder and only considers \( N \) lowest Landau levels which results in a \( 4N \times 4N \) Hamiltonian matrix.

In the Landau level basis the representation of \( a^\dagger \) corresponds to a matrix where only the elements \((in + 1, in)\) are non-zero and equal to \( \sqrt{in} \), with \( in \) in range between 1 and \( N - 1 \). For the operator \( a \) the non-zero elements \((in - 1, in)\) of the matrix are given by \( \sqrt{in - 1} \) and \( in \) is between 2 and \( N \).

**Zeeman energy**

Zeeman energy shift is given by
\[ \Delta_{\text{Zeeman}} = \mu_{\text{Bohr}} * g * J * B, \] (8.23)

where \( \mu_{\text{Bohr}} \) is the Bohr magneton, \( g \) - Lande factor, \( J = 0.5 \) is the spin momentum magnitude and \( B \) is the magnetic field. The Lande factors we use for the numerical simulations are \( g = -10 \) for electrons and \( g = -3 \) for holes. This choice is reasonable [174, 175] but also somewhat arbitrary since no sharp values seem to be firmly established in literature.

In the \( 4 \times 4 \) Hamiltonian \( \Delta_{\text{Zeeman}} \) will appear on the diagonal having the opposite signs for the two spin components and the Lande factor corresponding to holes for \( |H⟩ \) states and to electrons for \( |E⟩ \).

### Numerical calculation of Landau levels

To obtain the Landau level spectrum the \( 4N \times 4N \) matrix is diagonalized numerically for each value of the magnetic field. The cut off was chosen to be \( N = 50 \) and was checked to not noticeably effect the results.

Note, that in case the SI units are used the expressions for the Hamiltonian do not contain the speed of light constant \( c \).

Once the eigenvalues and eigenvectors of the matrix are calculated for each eigenvalue the highest weight in the corresponding eigenvector is found. If the square of the weight is higher than \( 0.5 \) then the eigenvalue is plotted with one of the four colours corresponding to one of the \( N \)-dimensional sectors in which the highest weight was found and corresponding to one of the four basis states (spin up and down for electrons and holes). If the squared maximum weight is less than \( 0.5 \) the eigenvalue is coloured as "mixed".

### 8.4 Results and discussion

Fig. 8.8 shows a comparison of numerically calculated Landau level spectra for the inverted (a) and non-inverted regime (b) of the TI sample. These calculations are based on the effective \( 4 \times 4 \) Hamiltonian with up to quadratic terms in \( \tilde{k} \) in the subspace of conduction band states in InAs and heavy hole valence band states in GaSb [see Section 8.3 for the details]. Fig. 8.8(b), calculated for \( V_{tg} = -10 \) V (TI sample, non-inverted regime) shows the two Landau fans for electrons and holes modified by Zeeman splitting and spin-orbit interaction effects. Electron and hole states do not mix appreciably. The calculated Landau fans are qualitatively the same for the non-inverted regime of the TI sample (Fig. 8.8(b)) and for the NI sample (Fig. 8.9). Corresponding experimentally measured Landau fans for the NI
Quantum spin Hall effect in the coupled InAs/GaSb quantum wells

Figure 8.8: (a) Landau level spectrum calculated numerically for the TI sample at $V_{tg} = -4\,\text{V}$, inverted regime. States dominated by electrons or holes of certain spin and mixed states are shown in corresponding colors. The vertical dashed lines indicate the magnetic fields for $\nu = 2, 3, 4$ where the Fermi energy jumps to the next unoccupied Landau level. The inset depicts the dispersion $Y-\Gamma-X$ and the position of the Fermi energy at $B_\perp = 0$. (b) As in (a), but at $V_{tg} = -10\,\text{V}$, non-inverted regime. The spectrum calculated for the NI sample is shown in Fig. 8.9.
8.4 Results and discussion

sample are shown in Fig. 8.3 and in both theory and experiment the Landau fans of holes and electrons clearly separate.

This behaviour is in contrast to the Landau level spectrum at $V_{tg} = -4$V (TI sample, inverted regime) shown in Fig. 8.8(a). Due to the inversion, the electron Landau fan starts off at lower energy than that of holes, and the two fans inevitably intersect. The off-diagonal terms in the Hamiltonian describing ordinary inter-band and spin-orbit inter-band coupling effects lead to avoided crossings of levels. These are the same terms that govern the appearance of the topological insulator gap at zero magnetic field. Due to the presence of hole-like Landau levels in the electron regime above the gap the spectrum is significantly denser than expected for pure InAs electron systems, in agreement with the smaller gaps observed in the experiment. Furthermore, if transitions of the Fermi energy between Landau levels at integer filling factors happen close to avoided crossing points of Landau levels, the gaps can be particularly small. These insights give a complete picture that is in qualitative agreement with the measurement presented in Fig. 8.1.

Figure 8.9: Landau level spectrum calculated for the NI sample.
8.4.1 Importance of the spin-orbit coupling

In Fig. 8.10 we present the Landau level spectrum for the parameters identical to Fig. 8.8(a) except that all the terms that break the inversion symmetry (including spin-orbit coupling) are switched off. We observe that some of the levels that were coupled before now turn into crossings. Importantly, the two Landau fans intersect also in this case without the inversion breaking terms and would thus result in a pattern similar to the one presented in Fig. 8.1. As we discuss in more detail in Section 8.4.2 the full Hamiltonian including all terms and of at least 3rd order is needed to quantitatively explain the experimentally measured pattern.

![Figure 8.10: Landau levels for the TI sample at $V_{tg} = -4\,\text{V}$. All the terms in the Hamiltonian that break the inversion symmetry have been set to 0.](image)

8.4.2 Origin and position of the minima of IQHE gaps

In Fig. 8.11 we show the evolution of magnetic field value corresponding to the complete filling of 3 Landau levels with $V_{tg}$. We observe that the transition point in B linearly sweeps over the B axis. Thus the second dashed black line in Fig. 8.8(a) passes through the Landau levels spectrum from left to right with increasing $V_{tg}$. 

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Figure 8.11: Calculation for the TI sample. The dependence of the magnetic field corresponding to completely filling three Landau levels (second vertical black line in Fig. 8.12) on the gate voltage.

Apparently, for certain voltages of the top gate this line will pass through a crossing or avoided crossing of two Landau levels. This voltage corresponds to a local minimum of the integer quantum Hall gap.

In Fig. 8.12 we illustrate this by showing the Landau level spectrum and the transition lines at the two nearby values of $V_{tg}$: $-4.4V$ and $-4.1V$. We see that the $\nu = 3$ IQHE gap indicated by the red dots becomes particularly small for $V_{tg} = -4.1V$.

Not all the crossings in Fig. 8.12 are gapped. One reason is that here we only consider at most the 2nd order terms in $k$, which means level $n$ can at most couple to level $n + 2$. By increasing the order in $k$ more and more crossings will become avoided. Some of them, however, are protected by symmetry remaining after the magnetic field is turned on. In experiment such symmetry could further be locally broken by any imperfections in the lattice. Thus the minimum IQHE gap measured in experiment is determined either by the matrix element responsible for a certain level anti-crossing or by disorder.

Tracking the position of the $\nu = 3 \rightarrow \nu + 1$ transition as shown in Fig. 8.13 we
Figure 8.12: Landau level spectra calculated for the TI sample at $V_{tg} = -4.4$ V (upper panel) and $V_{tg} = -4.1$ V (lower panel). The vertical black lines indicate the magnetic fields for $\nu = 2, 3, 4$ where the Fermi energy jumps to the next unoccupied Landau level due to complete filling of the Landau level degeneracy. The energies of the $\nu = 3$ and $\nu = 4$ Landau levels are indicated with the red dots at the magnetic field corresponding to complete filling of three Landau levels.
can understand the origin and the magnitude of the minima of the IQHE gap.

![Graph showing the ν = 3 IQHE gap as a function of gate voltage Vg.](image)

Figure 8.13: Calculation for the TI sample. Size of the ν = 3 IQHE gap (energy difference between the two red dots in Fig. 8.12) as a function of gate voltage Vg.

The minima shown in Fig. 8.13 are in agreement with the position of the minima (∼ 4T and ∼ 5T) presented in the experimental Fig. 8.2. Interestingly, the model up to the 2nd order can not explain the minima observed for ν = 3 around 9.5T, and the 3rd order model is required to do that.

It is important to note that although this agreement is encouraging one should keep in mind that we do not know the precise values of various parameters that enter the calculation such as the g-factor for holes. Although the presented Landau spectra are not strongly sensitive to any single parameter to compare to the experiment quantitatively one would have to identify the precise values of the input parameters first.

8.5 Conclusion

We derived the general effective low-energy 4 × 4 model for the coupled InAs/-GaSb quantum wells that respects the symmetries of the involved materials. This
model can be tuned between inverted and non-inverted regimes by changing the parameter controlled by the applied electric field and corresponding to the band overlap. We determine the remaining free parameters of our model by requiring that it reproduces the band structure obtained from the first-principles calculation, performed for the precise geometry of the experimental samples.

The Landau levels that we numerically calculate for this model allow us to qualitatively explain the Landau levels structure observed in experiment in both inverted and non-inverted regimes. We also provide an explanation for the source of the modulation of the integer quantum Hall gaps and for the unexpectedly small values of them measured in experiment. Interestingly, at least third-order in $k$ Hamiltonian is needed for a more quantitative agreement with experiment.

We conclude that the unusual pattern experimentally observed in experimental Landau levels is a signature of the inverted regime.
Conclusion and outlook

In the context of the fractional quantum Hall effect we studied the model that includes the realistic effects of Landau level mixing of strength $\kappa$ and finite thickness parametrised by the width of an infinitely deep quantum well $w$. We also established that this parametrisation is reliable and does not lead to loss of generality.

The two effects have non-trivial interplay and the existence of the phase diagram at $\nu = 5/2$ establishes probably the most important result of this work: when asking "What is the state of the 2DEG at filling factor $\nu$?" it is crucial to specify the conditions (namely $w$ and $\kappa$) as the answer may depend on them. The same might apply to the question "Is the state with a certain filling factor is fully spin-polarized?". For the limit of small but finite Landau level mixing we establish that the state is in the Moore-Read Pfaffian universality class.

Our results obtained for $\nu = 5/2$ indicate that increased Landau level mixing (decreased magnetic field) monotonously suppresses the FQHE gap. We stress that we measure our gap in units proportional to the inverse magnetic length or in other words proportional to $\sqrt{B}$. Thus the $\sqrt{B}$ dependence of the $\nu = 5/2$ energy gap on the magnetic field comes on top of the dependence shown in our phase diagram. Thus, significantly more stable $\nu = 5/2$ FQHE state is expected in an experiment at higher magnetic fields.

The model we study includes the Landau level mixing effects perturbatively to the first order in $\kappa$ and is thus exact only in the limit $\kappa \to 0$. From the results at higher $\kappa$ we can learn the qualitative trends such as the suppression of the gap at $5/2$ but can not reliably extract the quantitative parameters such as the critical value of $\kappa$, corresponding to a phase transition. Nevertheless, we observe that the effect of Landau level mixing is important and can lead to a qualitative change of the nature of the state. A natural wish for the future studies resulting from this is to improve the model (for instance by adding higher orders in perturbative expansion) in a way that would improve the reliability of the results for higher values of $\kappa$. Another possible outcome of such a model is the precise characterisation of the phases that arise beyond the phase transition that
we observed in our work. The predictive power of the effective model can also be improved by including higher 3-body pseudopotentials (only $V_L^{(3)}$ with $L \leq 8$ where used in our work).

Comparison of the energy gaps measured in experiment to the gaps calculated numerically has been a long outstanding issue in the field and it seems reasonable that the quantitative agreement may be achieved by combining a theory reliable at experimental values of $\kappa$ with a way of accounting for the effects of disorder.

Our results indicate the sensitivity of the states in the second Landau level to the form of the effective electron interaction. Therefore it is important to study other setups where this interaction may be different. For example, exploring systems and materials other than GaAs may potentially lead to observation of more robust FQHE states.

We find that Landau level mixing weakens the $\nu = 13/5$ FQHE state to the extent where it is no longer observable in experiment. At the same time no significant change for the $\nu = 3/5$ is observed over the whole range of experimentally accessible values of $\kappa$. This leaves us with an interesting open question, whether the robustness of $\nu = 2/5$ and $\nu = 3/5$ states is due to it’s position in lowest Landau level or to the composite fermion nature of the many-body state.

Our results for the states in the second Landau level indicate that both $\nu = 5/2$ and $\nu = 12/5$ (in fact also $\nu = 13/5$ should it ever be observed) support the non-Abelian anyons at finite Landau level mixing. As a result, both states persist as good candidates (at least from the theoretical point of view) to become a building block of a topological quantum computer. Especially, this is true for the $\nu = 12/5$ state, where the expected type of non-Abelian anyons is quite rare compared to the one of $\nu = 5/2$.

In the context of quantum spin Hall effect the first-principles calculations were used to identify the geometry of the devices that leads to the topological/trivial phase. The two devices, grown according to the first-principles prescriptions do indicate the signatures of the inverted band structure expected for a topological phase that could also be reproduced by the low-energy model tailored to the specific experimental samples. The approach that combines the first-principles and analytical calculations with experiment into a feedback loop has good chances to yield useful results when applied to other materials and systems.

The results for the quantum spin Hall effect are an example of a successful application of the engineering approach when one attempts to create the conditions where topological phase is stable as opposed to searching for cases where such a phase is prepared for us by Nature. This approach may gain importance on the way of turning the physical experiment into a technology.
List of publications


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