Final Report on:
Numerical Studies of Collective Phenomena in Two-Dimensional Electron and Cold Atom Systems

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CONTENTS

A. INTRODUCTION

Electrons confined to two-dimensional Landau levels (LL) exhibit a host of intriguing phenomena. The most notable among these is the fractional quantum Hall effect. The recent discoveries of quantum Hall plateaus in the first excited LL have focused attention on a new breed of quantum Hall states. Among these are paired "superconducting" states (at 5/2 and 3/8 LL fillings) and their generalization to higher groupings of particles (at 12/5 LL filling) and other possible novel states at 7/3 and 8/3 fillings. In addition, ultra-cold atoms in rapidly-rotating traps share similar characteristics with the electron systems and provide yet another probe of collective phenomena in condensed matter. Atoms, unlike electrons, come in both fermion and boson flavors. Remarkably, they also allow tuning of the inter-atom interaction potential by means of Feshbach resonance. Many of the states described above for electrons can in principle be seen in the boson atom systems with dipolar interactions. Numerical calculations were carried out to investigate a number of outstanding questions in both systems.

These projects aimed to increase our understanding of the properties of and prospects for non-Abelian states[1] in quantum Hall matter[2, 3]. Experimentally, these states may be realized in both the first excited Landau level (LL) of a two-dimensional electron system in high magnetic fields and in rapidly rotating trapped atomic Bose gases[4, 5]. In the first case, a prime candidate for a non-Abelian state is the 5/2 effect[6–8]. Following the finding[9–11] that the Moore-Read (MR) non-Abelian state[1] is relevant to the 5/2 effect, there has been considerable progress in elucidating various properties of this state. As with all paired states, the quasi-particles of the MR phase carry a charge of $\nu^* e/2$[1], where $\nu^* = \nu - 2 = 1/2$ is the partial filling of the $n = 1$ Landau level. Recent experiments[12–14] report detection of charge $e/4$ quasi-holes, which is a direct confirmation of the pairing nature of the state. However there are many other candidates, such as the $\Psi_{3,3,1}$[15] state or even a strong pairing phase (condensation of charge $2e$ bosons into a $\nu = 1/8$ boson Laughlin[16] state), which have this property.

Another example of a non-Abelian state[17] may be the plateau at 12/5 LL filling[8], which by all indications is extremely weak. The mobility gap for the quasi-particle excitation obtained by transport measurements is 70 mK. Although many experiments see a clear minima in ρ_{xx} at 12/5, only in the very high mobility sample[8] has a plateau been resolved. Other prominent plateaus in the $n = 1$ Landau level are at 8/3 and 7/3 fillings[7, 8]. A recent measurement of the gap for 7/3 is 600 mK[8]. It is interesting that the gap ratio of 12/5 to 7/3, in the same sample, is approximately 0.12. This relative weakness of 12/5 to 7/3 is in disagreement with the predictions of composite fermion theory[18] and experiments[19] in the lowest LL for 2/5 and 1/3. Such a discrepancy, together with the existence of a strong plateau at half filling, and the reentrant[20] (widely believed to be crystalline[21–25]) phases strongly suggests that the electronic environment in the $n = 1$ LL is fundamentally different from the lowest LL. This in turn may indicate that either the 7/3 or 12/5 (or both) are unrelated to their counterparts in the lowest LL, which has piqued interest in studies of new candidates for the 12/5 filling. One such possibility is a state which is the generalization of pairing to clusters of k particles by Read and the PI[26]—the so called z_k parafermion sequence, the first two members of which ($k = 1$ and 2) are the Laughlin and MR states. Again, as in the case of 5/2, numerical evidence[17] supports a non-Abelian phase in a region of parameter space which is near the physical Coulomb value for the $n = 1$ LL. Contiguous to this phase is the Jain 12/5 composite fermion state[27] which is stabilized as the short range part of the Coulomb potential (the V_1 pseudo-potential) is stiffened. Unlike the MR state, which can be constructed as a $p_x - ip_y$ BCS-type pairing of fully polarized composite fermions[1, 28], the z_3 parafermion state for 12/5 is unrelated to composite fermions and will be breaking new ground if it is confirmed experimentally.

Apart from the fundamental physics perspective, non-Abelian states offer the potential for quantum computation[29–33]. For $k \neq 1$, 2, and 4, the parafermion sequence supports universal quantum computation, which is, in part, responsible for the surge of interest in non-Abelian Hall states. For the MR wavefunction the non-Abelian statistics has been directly verified[34–36].

In parallel with studies of electron systems, boson quantum Hall states have been studied in relation to rapidly rotating trapped atomic Bose gases at ultracold temperatures[37, 38]. Cooper et. al.[4] were the first to numerically study such systems using the contact potential. This potential produces the Laughlin state at $\nu = 1/2$ and obtains a large overlap with the MR state at $\nu = 1$. It also shows strong gaps and very good overlaps with the parafermion sequence. Unfortunately, the system sizes were far too small for concrete conclusions. For just the short-range contact potential, the case for MR remains strong but is, at best, inconclusive for the z_3 state and beyond. The parafermion states, z_3 and z_4, however, become robust in the presence of dipolar interactions[5, 39]. For example, a Chromium condensate[40] under rapid rotation may be a prime candidate for such phases since Chromium atoms possess permanent dipole moments. Despite considerable progress in rapid rotations, experiments have not yet reached the correlated regime. Nonetheless, the realization of non-Abelian phases in systems with generic interactions is highly significant.

B. COMPLETED WORK

In this section the completed work is described in some detail. Also included is a list of the PI's contributions as an invited speaker in national and international conferences. This list is given first:

I. Invited Talks at National and International Conferences

1. Participated in the EPQHS International Worksop on " Emergent Phenomena in Quantum Hall Systems", held in Taos, New Mexico, July 7-9, 2005.

2. "Z_3 Parafermion Incompressible State of Rapidly-Rotating Bosons With Dipolar Interactions", talk presented at the "Low D Quantum Condensed Matter 2005" workshop, held in Amsterdam July 25-30, 2005.

3. "Universality of Edge Tunneling Exponents of Fractional Hall Liquids", presented at the 2006 APS March Meeting "Quantum Hall Edges" Symposium March 2006, Baltimore, Maryland.

4. "Finite-Size Studies of Non-Abelian Hall States", presented at the international conference on "Strongly Correlated Low Dimensional Systems", July 2006, Ascona, Switzerland.

5. "Non-Abelian Phases in Atomic Bose Gases and Quantum Hall Systems", presented at the international workshop on "Interactions, excitations and broken symmetries in quantum Hall systems", October 2006, Max Planck Institute, Dresden, Germany.

6. "Non-Abelian Hall Phases in Fermi and Bose gases", presented at the international workshop on "Emergent Phenomena in Quantum Hall Systems-2:FQHE beyond the First 25 Years", held June 13-16, 2007, the Pennsylvania State University, University Park, Pennsylvania.

7. "Non-Abelian phases in Fermi and Bose gases: a finite-size perspective", presented at the international workshop on "Quantum Phases of Matter", held June 1-August 31, 2007 (attended June 18-July 1, 2007), the Kavli Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing, China.

8. "Non-Abelian phases in High Landau levels and atomic Bose Gases", presented at the "Workshop on Topological Phases of Condensed Matter", held October 24-26, 2008, the Institute for Condensed Matter Theory, the University of Illinois, Urbana, Illinois.

II. Publications

The following manuscripts have appeared in print:

1. "Exact diagonalization study of domain structure in integer filling factor quantum Hall ferromagnets", E. H. Rezayi, T. Jungwirth, A. H. MacDonald, and F. D. M. Haldane *Phys. Rev. B* **67**, 201305R (2003).

2. "Disorder-Driven Collapse of the Mobility Gap and Transition to an Insulator in the Fractional Quantum Hall Effect", D. N. Sheng, X. Wan, E. H. Rezayi, K. Yang, R. N. Bhatt, and F. D. M. Haldane, *Phys. Rev. Lett.* **90**, 256802 (2003).

3. "Coexistence of Composite Bosons and Composite Fermions in $\nu = 1/2+1/2$ Quantum Hall Bilayers", S. H. Simon, E. H. Rezayi, and M. V. Milovanovic, *Phys. Rev. Lett.* **91**, 046803 (2003).

4. "Universality of the Edge-Tunneling Exponent of Fractional Quantum Hall Liquids", X. Wan, F. Evers, and E. H. Rezayi, *Phys. Rev. Lett.* **94**, 166804 (2005).

5. "Mobility gap in fractional quantum Hall liquids:Effects of disorder and layer thickness", Xin Wan, D. N. Sheng, E. H. Rezayi, Kun Yang, R. N. Bhatt, F. D. M. Haldane, *Phys. Rev. B* **72**, 075325 (2005).

6. "Incompressible Liquid State of Rapidly Rotating Bosons at Filling Factor 3/2", E. H. Rezayi, N. Read, and N. R. Cooper, Phys. Rev. Lett. 95, 160404 (2005).

7. "Vortex Lattices in Rotating Atomic Bose Gases with Dipolar Interactions", N. R. Cooper, E. H. Rezayi, and S. H. Simon, Phys. Rev. Lett. 95, 200402 (2005).

8. "Vortex lattices in rotating atomic Bose gases with non-local interactions", N. R. Cooper, E. H. Rezayi, and S. H. Simon, Solid State Comm. 140 (2), 61 (2006).

9. "Competing compressible and incompressible phases in rotating atomic Bose gases at filling factor $\nu = 2$, N. R. Cooper and E. H. Rezayi, Phys. Rev. A 75, 013627 (2007).

10. "Construction of a paired wave function for spinless electrons at filling fraction $\nu = 2/5$", Steven H. Simon, E. H. Rezayi, N. R. Cooper, and I. Berdnikov, Phys. Rev. B 75, 075317 (2007).

11. "Generalized quantum Hall projection Hamiltonians", Steven H. Simon, E. H. Rezayi, and Nigel R. Cooper, Phys. Rev. B 75, 075318 (2007).

12. "Pseudopotentials for multiparticle interactions in the quantum Hall regime", Steven H. Simon, E. H. Rezayi, and Nigel R. Cooper, Phys. Rev. B 75, 195306 (2007).

13. "Bipartite entanglement entropy in fractional quantum Hall states", O. S. Zozulya, M. Haque, K. Schoutens, and E. H. Rezayi, Phys. Rev. B 76, 125310 (2007).

14. "Density Matrix Renormalization Group Study of Incompressible Fractional Quantum Hall States", A. E. Feiguin, E. Rezayi, C. Nayak, and S. Das Sarma, Phys. Rev. Lett. 100, 166803 (2008).

15. "Paired composite fermion phase of quantum Hall bilayers at $\nu = \frac{1}{2} + \frac{1}{2}$", Gunnar Möller, Steven H. Simon, and Edward H. Rezayi, Phys. Rev. Lett. 101, 176803 (2008).

16. "Trial Wavefunctions for $\nu = \frac{1}{2}+\frac{1}{2}$ for Quantum Hall Bilayers", Gunnar Möller, Steven H. Simon, and Edward H. Rezayi, Phys. Rev. B 79, 125106 (2009).

17. "Non-Abelian quantized Hall states of electrons at filling factor 12/5 and 13/5 in the first excited Landau level", E. H. Rezayi, N. Read, Phys. Rev. B 79, 075306 (2009).

18. "Spin polarization of the $\nu = 5/2$ quantum Hall state", A. E. Feiguin, E. Rezayi, Kun Yang, C. Nayak,S. Das Sarma, Phys. Rev. B 79, 115322 (2009).

III. Description of the published work

1. Tilted Fields and Domain Walls in Quantum Hall Ising Ferromagnets

Tilting the magnetic field away from the direction perpendicular to the plane of a two-dimensional electron gas can trigger transitions between highly correlated ground states of the system. Such a transition seems to have appeared[41] in high ($\nu = 6$, for example) completely filled Landau levels at an extreme tilt angle of 82 degrees. The transport becomes highly anisotropic and, taken at face value, seems to indicate a quantum phase transition to a broken symmetry state previously observed at half-filled Landau levels (at 9/2 and 11/2 fillings). These arise purely from electron-electron interactions. However, there is an additional single-body component here that needs to be taken into account. The experimental anomaly occurs at a tilt angle that lines up the lowest Landau level of the second subband ($N = 0, i = 2$) with the first excited Landau level of the first subband ($N = 1, i = 1$). These have opposite spins and we found no trace whatsoever of a broken symmetry ground state (GS); instead the GS at this point is always uniform and can be described as an Ising ferromagnet (with complete Z_2 symmetry). The self-consistent local-spin-density-functional approach (LSDA) was used (with the appropriate sample parameters) to calculate the single particle wavefunctions and their energies as well as the interaction potential $v(q_x, q_y)$ in the presence of the tilted field. The latter was then used in many-particle calculation of a finite-size system to investigate the nature of the GS. A clear domain wall excitation was found above the Ising ferromagnetic GS, which was dominant in the system size we studied. The proliferation of such domain walls at the critical tilt angle could account for the magnetotransport anomalies. This is because charge transport occurs along the walls, which will be oriented either parallel or perpendicular to the in-plane field. The determination of the precise domain wall orientation relative to the tilted field requires much larger sizes as the differences in the energies are very small. It can best be determined by a self-consistent Hartree Fock rather than a full many-particle calculation. Experimentally, the domain walls are parallel to the in-plane field as this is the "easy" direction for conduction.

The results were published in Physical Review B as a Rapid Communications(publication 1).

2. Calculation of Quantum Hall Conductance for $\nu = 1/3$

In this work we have carried out a quantitative study of the effects of random disorder in the fractional Hall regime. This is the first such calculation of its kind. It was first recognized by Thouless and co-workers, in the case of the integer filling, that the Hall conductance is related to a topological invariant called the first Chern integer on the torus. This number is obtained by calculating the Berry phase in the parameter space of twisted boundary conditions (as formulated in references 20 and 21). Because of the topological order of fractional quantum Hall states, the GS at 1/3 is 3-fold degenerate in the absence of disorder on the torus. In addition, by inserting flux quanta through the "donut" hole of the torus, one can cycle through the GS manifold[44]. Thus, there is no physically meaningful distinction between the members of the GS manifold and one needs to assign the average Chern number to each of the ground states. For the quantum Hall state at 1/3 filling this number would be 1/3, with very little fluctuation. On the other hand, deviation from 1/3 and/or large fluctuations in this number will signal the collapse of the quantum Hall state.

In a finite size system, disorder will lift these degeneracies into quasi-degeneracies; however below the mobility gap, the group of 3 near-degenerate levels will have a robust (total) Chern number (of 1) and thus a quantum Hall conductance (average Chern number) of 1/3. At or above the mobility gap this trend breaks down and these states can no longer support dissipationless current flow. This provides a reliable numerical method for finding the mobility gap. We obtained the mobility gap as a function of random disorder (provided disorder is not too weak) and found the critical disorder for destruction of quantum Hall states. Using standard models for electron scattering from the disorder potential, we obtained (for an infinitely thin layer) the dependence of the experimental gaps[45, 46] on the sample mobility. The overall trend agreed with the experiments but the theoretical gaps were shifted up in energy. Including a more realistic 2-D layer with a finite thickness obtained much better agreement with experiment.

The first paper was published in Physical Review Letters and a longer paper incorporating layer thickness and variants of the disorder potential was published in Physical Review B (publications 2 and 5).

3. *A Double Layer Quantum Hall State at $\nu_T = 1/2 + 1/2$ Filling*

The quantum Hall effect in bi-layer systems at a total filling factor of one continues to attract considerable interest. One important aspect of this problem that remains controversial is the nature of the correlated to uncorrelated transition. Experimentally such a transition is seen in the transport[47, 48] (as well as the tunneling[49]) as the inter-layer distance is varied. In the strongly correlated phase (small layer separation), the system develops inter-layer coherence and shows a plateau in the magneto- transport. For large separation (experimentally, $d_c \geq 1.7$ magnetic lengths ℓ) the ground state consists of two uncorrelated composite fermion (CF) Fermi liquid states without a Hall plateau. The correlated phase is described by the so called one-one-one state (Ψ_{111}), which can be interpreted in a number of equivalent ways: as a BEC of interlayer excitons, a pseudo-spin planar ferromagnet, or a quantum Hall condensate of interlayer composite bosons (CB) (an electron in one layer binding a zero of the wavefunction in the other layer). Unfortunately, in the absence of a microscopic picture for the transition, it is notoriously difficult to extract its nature from brute-force numerics. Accordingly, we constructed a series of wavefunctions (on the order of the number of particles) that smoothly interpolate between the two phases, from Ψ_{111} in the correlated regime to two uncorrelated CF Fermi liquid states in each layer. The underlying physical picture is that of two inter-penetrating CF and CB liquids in the transition region. While a phase-separated two-fluid model will predict a first order transition[50], our wavefunctions give a continuous transition. We have tested these wavefunctions against the exact ground state as a function of the distance and indeed find that they describe the transition region rather well; our wavefunctions (in a 5-electron per layer system), with 0, 1, 2, 3, 4, and 5 CF states, progressively describe the actual ground state as the distance was increased through its critical value.

The results of this study have been published in Physical Review Letters (publication 3).

4. *Universality of Edge Tunneling Exponent at 1/3 Landau Level Filling*

It has been argued by Wen[51] that quantum Hall states describe a novel phase of condensed matter that possesses topological order. This is more subtle than the order associated with broken symmetry, which is commonly described by a measurable order parameter. A possible method of "measuring" the topological order is by tunneling into the edge of a quantum Hall fluid. In this case, as a consequence of the topological order, the physics of the edge is described by a chiral Luttinger liquid[52] (instead of a normal Fermi liquid) and the tunneling $I - V$ characteristics will be non-Ohmic: $I \propto V^\alpha$. The exponent is determined by the bulk and, for states at fillings 1/3, 2/5 or $n/(2n+1)$, $\alpha = 3$. For 1/3 filling this exponent has been verified for the Laughlin state; however a smaller non-universal value was reported for the GS of the more generic Coulomb potential. This deviation was largely attributed to the long-range nature of the Coulomb potential. (The Laughlin state is the (zero energy) GS of an ultra-short-range interaction potential.) If true, this directly contradicts the concept of topological order and undermines many of the phenomena associated with it (such as the edge physics of quantum Hall states or the possibility of using quantum Hall fluid excitations for topological quantum computing[32]).

Motivated in part by this and in part by the actual measurements[53–55] that reported differing non-universal values, we investigated the conditions under which such deviations could occur. In particular we studied the effects of the edge confining potentials on α.

For a strong confining potential (such as a hard edge) the exponent always deviated from the universal value while for weak confining potential the exponent was 3. On the other hand we did not find any evidence for dependence of the exponent on the range of the interaction potential. Our findings are completely consistent with topological order and provide a plausible explanation of variations in the experimental exponents; they appear to be the result of different edge confining potentials.

This paper was published in Physical Review Letters (publication 4).

5. *Rapidly-Rotating Ultra-Cold Atoms: Broken Symmetry and Highly Correlated states*

Rotating Bose-Einstein condensates (BECs) have shown fascinating ground states with crystalline arrangements of vortices. These occur in weakly interacting Bose gases where the dominant scattering is short-ranged and in the s-wave channel. This is modeled by a repulsive contact pseudo-potential. Such a model exhibits the vortex lattice phases observed in experiments. The recent discovery of BEC in chromium has opened the door to the experimental study of boson systems with dipolar interactions. Accordingly we have undertaken a study of possible phases of rotating atoms where both contact as well as dipolar interactions are present. Our study is restricted to states within the lowest Landau level. Such a condition can now be experimentally achieved[56], which makes the new phases we find accessible to direct experimental probing. These, plus studies of incompressible fluids of vortices, are described below.

Background: A stationary quasi-two-dimensional trap with parabolic confinement, in the absence of interactions, is described by a 3-dimensional asymmetric harmonic oscillator with $\omega_{\|} >> \omega_{\perp} = \omega_0$. Here the parallel direction is along the rotation axis and is taken to be the z-axis. At low temperatures, $K_bT << \hbar\omega_{\|}$, the motion along the z-axis is quenched (and will be neglected) and becomes quasi-two-dimensional in the $x-y$ plane. There is now a series of wavefunctions of the form $\Psi_m(z) \propto z^m \exp(-z\bar{z}/4)$, where m is the angular momentum, $z = x+iy$ is the complex coordinate, and the overbar indicates complex conjugation. Except for $m = 0$, which is the non-degenerate ground state, $m > 0$ describes excited states of the trap with energy $E_m = (m+1)\hbar\omega_0$. When rotated at angular velocity Ω_0 along the z-axis and in the rotating frame, the Hamiltonian is Legendre transformed to $H_{\text{rot}} = H - \Omega_0 L_z$, where L_z is the total angular momentum. In the rotating frame, the single particle energy of the above series becomes: $\epsilon_m = \hbar(m+1)(\omega_0 - \Omega_0) + \hbar\Omega_0$. As Ω_0 approaches the trap frequency ω_0, one recovers the lowest Landau level physics[37, 38], except that the underlying particles are Bose atoms. It is in fact remarkable that the conditions of the lowest Landau level have already been achieved experimentally[56]. For low temperatures, the low energy interactions among atoms can be modeled by an s-wave contact pseudo-potential $g\sum_{i<j}\delta(\vec{r}_i - \vec{r}_j)$, where $g = 4\pi\hbar^2 a_s/m$, a_s is the s-wave scattering length and m is the atom mass. The conditions of lowest LL occupation will be maintained as long as the interactions are sufficiently weak or the system is sufficiently dilute. It is assumed throughout that these conditions are satisfied.

Another remarkable property of this system is that the strength of the potential can be altered by means of the Feshbach resonance[57]. It is assumed that the strength of the s-wave scattering potential is tunable, particularly when dipolar interactions are considered. In this lowest LL regime, the physics of the problem is controlled by the interaction potential and the filling factor ν, which in this context is defined as $\nu = N/N_v$, where N_v is the number of vortices and N is the number of atoms. For a low density of vortices[58] a vortex lattice phase is readily observed[59]. It is instructive to draw a parallel to the fractional quantum Hall effect (FQHE) where, at low electron densities, a Wigner crystal is formed. Thus the filling factors in the two problems, loosely speaking, seem dual to one another: $\nu_{atom} \sim 1/\nu_{FQHE}$. At a sufficiently high density of vortices, on the order of the density of the particles, the vortex lattice is unstable and the system enters the highly correlated regime of FQHE. The best estimate of the critical filling for an s-wave contact potential model is $\nu_{crit} \approx 6$. For $\nu > \nu_{\text{crit}}$ and an s-wave pure contact potential, a hexagonal vortex lattice was observed by Cooper et. al.[4] For longer range potentials, however, the phase diagram of the system is considerably enriched. This new physics is the subject of 4 publications (6-9).

Broken Symmetry Crystalline States: We studied the broken symmetry states by minimizing the Gross-Pitaevskii energy functional under the constraint of no admixing of the excited Landau level states. We also imposed periodic boundary (or toroidal) conditions (PBC). This geometry is particularly well suited to detection of crystalline phases in numerical calculations. Our goal was to investigate the effect of dipolar interactions. As a result of varying the parameter that quantifies the relative strength of the s-wave component (V_0 pseudo-potential) to the dipole potential (defined by $\alpha = V_2/V_0$, where V's are Haldane pseudo-potentials), we indeed found several different crystalline phases. In addition to the previously discovered hexagonal lattice, we found square lattices as well as phases with stripe order. When we added a d-wave component to the tunable s-wave potential, we found qualitatively the same physics as in the full dipolar potential. Only quantitative differences were observed. This indicates the new phases are quite robust and quantum phase transitions, driven by α, occur when dipolar-type longer-range potentials are added to the s-wave potential.

Correlated States of Vortices: Attempts by the PI to extend the calculations of Cooper et. al.[4] to larger systems at $\nu = 3/2$ filling failed to produce concrete evidence of an incompressible Hall state. For example, the pair correlation function for 24 bosons on the sphere shows a rather widely oscillating tail[5], which is more consistent with a broken symmetry crystalline order than the exponential decay (to the background value at large distances) expected of a gapped phase. Strictly speaking, this does not rule out a gapped phase; it may merely indicate a rather weak (very small gap) incompressible phase when the system size is smaller than the correlation length of the system. The latter length scale determines the smallest system size beyond which the large N physics is seen. On the other hand, the inclusion of the dipolar interaction, when $0.2 \leq \alpha \leq 0.4$, has a dramatic effect[5]. It produces the doublet of ground states (excluding the center of mass degeneracy of 2) on the torus expected of the z_3 non-Abelian state. The ground states also obtain a huge overlap with the doublet of the z_3 parafermion states (publication 6). A similar, but weaker, signature is seen for the z_4 state (publication 9).

6. *A Paired State at $\nu = 2/5$ and a New Sequence of Wavefunctions*

The theoretical investigation of the FQHE usually employs a "grounds up" approach[16, 27] that starts with a microscopic wavefunction, as in the BCS theory of superconductivity, from which the physical properties of the state are deduced. However, there are several components that are essential to this type of investigation. These include having a special positive semi-definite Hamiltonian[60] for which the proposed model state is the unique zero-energy ground state. Numerical studies of such Hamiltonians are (and have been) critical to understanding many of the properties of the state, including the topological order[51], the nature of quasi-particle statistics, etc. There is, in addition, the most important question of whether the system is gapped in the bulk. This is rather difficult to address by any method other than numerical calculation; although it has been argued that the system will be gapless if the corresponding conformal field theory (CFT) (for which the wavefunction in question is a correlator) is non-unitary[28, 61]. Even numerical calculation may not reach large enough system sizes to provide a definitive answer, but the trend from the 4 or 5 smallest system sizes becomes fairly apparent. Often the model Hamiltonians include p-body interactions, with p reaching as large as 5 or 6, which are non-trivial to study systematically. In publications 10-12 we developed some very useful tools for this purpose. We have classified and catalogued p-body Hamiltonians in terms of the appropriate projection operators. This method is vastly superior to the common practice of using the derivatives of many-body delta-function potentials. It becomes physically transparent which kind of many-particle correlations are favored and which are projected out. It is also much more efficient numerically. In addition, in publication 6 we have extended the idea of pseudo-potentials to p-body Hamiltonians that go hand-in-hand with these projection operators. Haldane's original formulation of pseudo-potentials was for 2-body Hamiltonians. Our formulation will be useful in calculating LL mixing effects for states in high Landau levels.

Finally, using these tools we attempted to determine whether there are any *new* sequences of correlated states of quantum Hall fluids that involve pairing, or more generally, k-particle grouping correlations that are distinct from the parafermion sequence. In publication 5 we proposed such a new series which has LL fillings of $\nu = k/(2k+1)$, $k > 1$ (and their particle-hole conjugates) for fermions and $\nu = k/(k+1)$ for bosons. Surprisingly, these fillings are identical to the Jain sequence[27]. Even the charge-flux shift S (defined as $N_\phi = \nu^{-1}N - S$) is the same for both. In fact, for $k = 2$, one obtains a very large overlap with Jain's 2/5 state. Bernevig and Haldane[62] have argued that the two differ only by the presence of a quasi-hole and quasi-particle pair and are therefore closely related. However, it appears that our sequence of wavefunctions may be correlators of non-unitary conformal field theories (for example, at 2/5 the corresponding CFT is the minimal model M(5,3)[63, 64]) and can not describe bulk phases of matter[61]. They may be critical states appropriate to quantum critical points. These issues were first raised by Read[28] in connection to the Hollow-Core model[65]. Numerical studies are consistent with a gapless phase and show a rather fast drop of the gap with system size. This raises an interesting question as to where exactly such a critical state fits in the quantum Hall phase diagram. Even more mysterious is the connection to Jain's state since the latter is known to describe a gapped phase of quantum Hall matter. Understanding these and related issues will possibly shed light on the conditions that stabilize Hall states in general and non-Abelian Hall states in particular.

7. *Topological Order and Entanglement Entropy*

Entanglement (von Neumann) entropy, a concept developed in information theory, provides a measure of the degree of quantum entanglement between two parts of a system. It can yield useful information about the nature of the underlying state, as well as the degree of correlations. It is becoming a standard tool for studying highly correlated systems and their phase transitions[66, 67]. The entanglement entropy of a subsystem A with the rest of the system B is defined as $S_A = -Tr\rho_A \ln\{\rho_A\}$, where the density matrix of subsystem A, $\rho_A = Tr_B\rho$, is obtained from the density matrix of the total system, ρ, by tracing over the degrees of freedom of the rest of the system B. The PI's interest here was in studying topological phases of quantum Hall matter. Such phases are characterized by their topological order. In a pair of remarkable papers[68, 69], it has been shown that entanglement entropy, or more precisely topological entanglement entropy, carries the signature of the topological order. By an appropriate partitioning of the system and tracing over the "exterior" variables, it can be shown that the topological entanglement entropy scales with the boundary length L of the two subsystems: $S = \eta L - \gamma$, with the remaining terms vanishing in the limit $L \to \infty$. Furthermore, γ is universal and independent of system size or other geometrical parameters and is related to the total quantum dimension of the system D by $\gamma = \ln\{D\}$, where $D = \sqrt{\sum_a d_a^2} \geq 1$ and the d_a's are the quantum dimensions of sectors of the topological field theory. They can be determined by the fusion rules of the fundamental anyons, labeled by a's, of the theory. For Abelian states, γ is less than one but it exceeds one for non-Abelian Hall states. The topological entanglement entropy can, therefore, detect whether the state is Abelian or non-Abelian. In addition, the spectrum of ρ_A conveys more detailed information, such as the number of quasi-holes or edge states[70]. Using a somewhat different partitioning method, Haque[71] et. al. obtained the entanglement entropy for the Laughlin state at 1/3 filling. Following this method, with the PI's collaboration, the calculations were extended to the Moore-Read state. We studied up to an 18-electron size system; extrapolation to infinite size yields $\gamma \approx 1.1 \pm 0.3$, in agreement with the exact value of $\ln(\sqrt{8}) = 1.0397$. The calculation was done on the sphere and extrapolation to infinite size was performed in two steps. First we chose a block of orbitals starting from the north pole and extrapolated the entropy to infinite size while keeping the number of orbitals in the north pole fixed. Then these extrapolated entropies were plotted against the square root of the number of orbitals at the north pole. The intercept yields $-\gamma$. However the error in the extrapolated S_A increases with the number of orbitals kept, introducing large uncertainties in the value of γ. The error can be somewhat controlled by using the algorithm of Bulirsh and Stoer (publication 13).

8. *Density Matrix Renormalization Group Studies of Incompressible Hall States*

An extremely successful method for solving one-dimensional problems with short-range interactions is the Density Matrix Renormalization Group[72, 73] (DMRG). It is essentially a decimation scheme that successively thins out the high energy degrees of freedom, obtaining an effective Hamiltonian for the low energy degrees of freedom. The key step is to split the problem into a system and an environment. One then obtains the density matrix of the system after integrating out (or tracing over) the environment. Then a new enlarged system is constructed from the largest p eigenvalues of the density matrix plus newly added states. The steps are repeated until a convergence criterion is satisfied and the number of states kept controls the accuracy. We used the finite-size DMRG in momentum space[74]. While this technique has been applied to studies of both broken symmetry and incompressible states on the torus[25, 76], no calculations of the gap have been reported. We applied the method to the $\nu = 5/2$, quantum Hall state using the spherical geometry where larger size systems, compared to the torus, can be achieved. The work was done in collaboration with Adrian Feiguin. Our goal was to push the previous results for the gap of the 5/2[10, 75], as well as calculations of ground state properties, to as large a system size as possible. The calculation is made difficult by the proximity of the system to a critical point of phase transition. For example, experiments have shown that tilting the field away from the direction perpendicular to the 2-D electron layer causes a transition to an insulating state, which exhibits strong

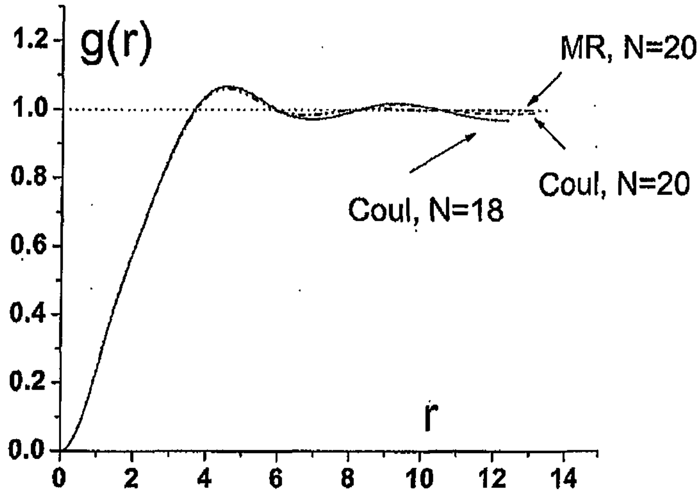

FIG. 1. Pair correlations for the Coulomb potential + $\delta V_1 (= 0.035)$ compared to MR $g(r)$. The oscillations in the tail are more strongly suppressed for $N = 20$, indicating the system is converging to the large N limit at or past 20-electron sizes. The addition of δV_1 is to avoid the phase boundary region near the pure Coulomb value, which introduces crystalline-like features (see pub. 14) in finite size systems.

anisotropies in the longitudinal transport coefficients R_{xx} and R_{yy}. This transition has also been seen numerically. The largest system size that was achieved is 26 electrons. Our calculated gap for charged excitations, which is measured in the transport experiments, was slightly higher than the previous estimate of Morf. Both calculations were carried out using spherical geometry with Coulomb interactions appropriate for the first excited Landau level. We did not account for the finite layer thickness of the experimental samples nor any LL mixing effects. All of these corrections are expected to reduce the gap. Another effect that has been neglected in all previous calculations, including ours, is the finite extent of the quasi-holes. As alluded to earlier, if the state at 5/2 is paired, then every added flux creates a pair of charge $e/4$ quasi-holes. To properly account for the repulsion of two charge $e/4$ objects, the working assumption so far has been to subtract the repulsive energy from the gap by treating the quasi-holes as a pair of point charge-$e/4$ particles pinned at opposite poles of the sphere. This causes a serious overestimation of the gap. Even in the best of circumstances, when the potential is tuned to maximize the overlap with the model Moore-Read quasi-hole excitations, the spatial extent of the quasi-holes for the Coulomb potential is comparable to the system size and they do not interact as point objects. However the DMRG calculations appear to suggest that convergence may be reached a few sizes beyond the 20-electron system, which has been corroborated by exact calculations (Fig. 1) for $N = 20$[77]. Thus a more reliable result for the gap will need to address sizes of at least $N = 20$, 22, 24, and possibly 26. We have reported a summary of our results in publication 14.

9. *A Paired Phase in Bilayer Systems at Total Filling Factor $\nu = 1/2 + 1/2$*

The quantum Hall effect at $\nu_T = 1$ has continued to attract considerable attention over the past few years. It is one of the most enduring systems in the lowest LL, exhibiting an inter-layer coherent phase for small layer separations and a correlated-uncorrelated phase transition at a separation of $d \approx 1.7$ magnetic lengths. The coherent phase, characterized as a particle-hole superfluid or a planar x-y pseudo-spin ferromagnet, has been thoroughly investigated.

Previously we proposed[78] (publication 3) a two-fluid model: a composite boson superfluid and composite fermion normal fluid. We constructed a series of wavefunctions for fixed numbers of composite bosons and composite fermions whose sum equals $N/2$—the number of electrons in one layer of an equally balanced bilayer system. This model obtains very large overlaps for almost the entire range of interlayer distances except for a small, but finite, region at intermediate distances. Our construction has two main features; it describes a continuous, probably second order, transition to the uncorrelated regime and it does not address any possible correlated state of composite fermions. This conclusion is in agreement with experiments which strongly suggest a continuous transition. In a thermodynamic system beyond the transition, it is plausible that composite fermions will dominate the physics and the possibility of a correlated state of CF's should not be ruled out. Bonesteel et. al.[79, 80] have already addressed this question and have proposed a BCS-type inter-layer pairing of composite fermions. To investigate this possibility, we assumed a BCS state but adjusted the pairing part of the wavefunction to fit the numerical data. Excellent agreement was obtained by fiting 3 to 4 parameters in the pairing wavefunction. The only difference with the proposed wavefunctions was that the pairing here is $p_x + ip_y$ instead of $p_x - ip_y$. The BCS type wavefunctions have a trivial limit, $(v(k) = 0)$, at which point one recovers the non-interacting Fermi sea of composite fermions. Thus care needs to be exercised to avoid confusing a paired phase with a Fermi liquid phase. Our numerical calculations have unmistakably identified a $p_x + ip_y$ paired phase, which appears to be contiguous to the inter-layer coherent phase as predicted by Bonesteel at al. This phase is stabilized for intermediate distances in a finite region past the transition from the inter-layer coherent phase. Thus, there is an intervening weak pairing Abelian phase. A short summary of the results has been published in Physical Review Letters and a longer, much more comprehensive paper has been published in Physical Review B (publications 15 and 16).

10. *Finite-Size Studies of quantum Hall effect at 12/5 and 13/5*

As stated earlier, the results of finite-size calculations for up to 18 electrons at 13/5 (which by particle-hole symmetry has the same spectrum as 12/5) does support the z_3, non-Abelian, parafermion phase which, in the interaction parameter space, is contiguous to the LL Jain's phase. The non-Abelian phase is stabilized for softer short-range repulsion and makes a direct transition to the Abelian phase, changing the topological order. Such transitions are expected to be continuous, but it is difficult to determine, with any degree of certainty, the order of the transition with finite-size calculations. These results have been published in Physical Review B (publication 17).

11. *Spin Polarization of the 5/2 State*

One important issue for the 5/2 effect is its spin polarization. Initially the destruction of the 5/2 plateau upon tilting the magnetic field was interpreted to mean that the underlying state is spin-singlet or possibly partially polarized. Tilting necessitates an overall increase in the magnitude of the B-field. Since the perpendicular component of B must remain fixed to maintain the same filling factor, the accompanying increase in the Zeeman energy was thought to drive the state into a compressible phase, leading to the disappearance of the quantized plateau. Subsequent numerical studies, however, have shown that the 5/2 state may be very close to a stripe ordered state and a transition to the latter can be driven by the tilted field, as has been observed experimentally. This state of affairs does not rule out an accompanying spin transition when the field is sufficiently tilted. More current direct measurements of polarization have not been definitive in establishing the spin state of the 5/2 effect. The direct evidence for full polarization comes from numerical studies. Morf compared only the energies of fully polarized and spin-singlet states at 5/2 (for 12 electrons) and found the former to be lower even if the Zeeman energy is excluded. Strictly speaking, this comparison does not rule out a ground state at partial polarization. The problem was revisited in order to address this question as well as to go beyond the 12-electron size. In a series of exact diagonalization and DMRG calculations, which extended system sizes to N=14 for both spin-singlet and partially polarized states with polarization $P = 1/2$, we found the polarized state is lowest in energy even when the Zeeman energy is excluded. The full excitation spectrum for 10 electrons shows a spin-wave mode consistent with a fully spin-polarized incompressible state. These results are reported in publication 18.

C. STUDENT SUPPORT

Four students have received support from the grant.

1. Aldo Davalos
2. Kyle Irwin (currently in the Ph.D. program at the University of California, Riverside)
3. Laurent Boue (a French exchange student, pursued a Ph.D. degree in France).
4. Michael Gaston

These students have assisted the PI, in varying degrees, in programming, running programs, data collection and analysis, as well as with analytical methods. They received training in numerical and analytical techniques for studying highly correlated systems. Davalos and Gaston are from underrepresented groups in physics (Hispanic and African American, respectively).

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