Monte Carlo study of Bose Laughlin wave function for filling factors $1/2$, $1/4$ and $1/6$

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Abstract. – Strongly correlated two-dimensional electronic systems subject to a perpendicular magnetic field at lowest Landau level (LLL) filling factors: $1/2$, $1/4$ and $1/6$, are believed to be composite-fermion (CF) Fermi liquid phases. Even though a Bose Laughlin wave function cannot describe these filling factors, we investigate whether such a wave function provides a *lower energy bound* to the true CF Fermi liquid energies. By using Monte Carlo simulations in disk geometry we compute the Bose Laughlin energies and compare them to corresponding results for the spin-polarized LLL CF Fermi liquid state and avalable data from the literature. We find the unexpected result that, for filling factors $\nu = 1/4$ and $1/6$, the Bose Laughlin ground-state energy is practically identical to the true CF liquid energy while this is not the case at $\nu = 1/2$ where the Bose Laughlin ground-state energy is sizeably lower than the energy of the CF Fermi liquid state.

Modulation doped $GaAs/Al_xGa_{1-x}As$ heterojunctions provide an almost ideal experimental realization of a two-dimensional electron gas (2DEG). In these devices, the application of a strong perpendicular magnetic field quenches the kinetic energy and eventually brings the electrons in a regime where correlations are of utmost importance. In cases where the perpendicular magnetic field is very strong, all electrons partially occupy the lowest Landau level (LLL) and have their spins fully polarized in the direction of the magnetic field. The phase diagram of a 2DEG in a strong perpendicular magnetic field at filling factors $0 < \nu \leq 1$ is intricate with competing liquid and Wigner solid phases. At filling factors, $\nu = 1/3$, $2/5$, $3/7$, ... and $\nu = 1/5$, $2/9$, ... electrons condense into an incompressible liquid state and the fractional quantum Hall effect (FQHE) occurs. [1] It is believed that at even-denominator filling factors, $\nu = 1/2, 1/4$ and $1/6$ the electrons form a compressible liquid state [2–4] while for filling factors, $0 < \nu \leq 1/7$, Wigner crystallization occurs [5–8].

On the theoretical side, the accurate prediction of the critical filling factor, ν_c, where the liquid-solid transition occurs is very difficult. For an ideal 2DEG system free of any disorder the best available theoretical estimates [5] suggest $\nu_c \cong 1/6.5$. In experimental realm, the situation is more complex. Various measurements [9] on high-quality samples, yet with a finite amount of disorder, show the existence of a re-entrant solid-like phase around the FQHE state, $\nu = 1/5$ which likely represents an electronic solid phase pinned to fluctuations of the potential.

The majority of theoretical studies which are based on models free of any disorder agree that the critical filling factor, ν_c below which the Wigner crystal forms is close to and probably slightly larger than filling factor $\nu = 1/7$ in excellent agreement with the estimate of Lam and Girvin [5]. A recent study [10] based on the exact diagonalization method found strong evidence that the Wigner crystal forms at filling factors, $\nu \leq 1/7$. Such study considered the filling factors, $\nu = 1/6, 1/7$, and $1/8$. It was found that for $\nu = 1/8$, as well as $\nu = 1/7$ the translational symmetry (signature of liquid phase) is broken and the system has 2D crystalline order. However, the system continued to have its translational symmetry for the case of filling factor $\nu = 1/6$, suggesting that the value of the critical filling factor, ν_c is between slightly above $1/7$, but below $1/6$.

The principal FQHE states at $\nu = 1/3$ and $1/5$ are thoroughly explained and very well described by the Laughin wave function [11] while the other FQHE states at filling factors, $\nu = p/(2mp + 1)$ (p, m integer) are readily understood in terms of the composite fermion (CF) theory. [12] The limit ($p \to \infty$) of such FQHE states [13, 14] corresponds to even-denominator filled states, $\nu = 1/(2m)$ which are believed to be compressible Fermi liquid states qualitatively different from the FQHE states of the originating sequence [15]. The basic understanding now is that the low-temperature phase of fully spin-polarized electrons at filling fraction $\nu = 1/(2m)$ is a CF Fermi liquid phase. A trial wave function for the CF Fermi liquid ground state at $\nu = 1/(2m)$ has been written down by Rezayi and Read [16] and reads:

$$\Psi_{Fermi} = \hat{P}_{LLL} \left[\det|e^{i\vec{k}_\alpha \vec{r}_i}| \; \Psi_{Bose} \right] \;, \tag{1}$$

where Ψ_{Bose} is the Bose Laughlin wave function for filling factor $\nu = 1/(2m)$:

$$\Psi_{Bose} = \prod_{i<j}^{N} (z_i - z_j)^{2m} \; \exp \left[-\sum_{j=1}^{N} \frac{|z_j|^2}{4l_0^2} \right] \;. \tag{2}$$

The Rezayi-Read (RR) CF Fermi wave function is obtained after the product of the Bose Laughlin wave function with a Slater determinant of plane waves is fully projected into the LLL by means of the projection operator, $\hat{P}_{LLL}$. In the above expressions, N is the number of electrons that occupy the N lowest-lying single-particle plane-wave states labeled by the momenta $\{\vec{k}_\alpha\}$ consistent with an ideal 2D spin-polarized Fermi gas, $z_j = x_j + iy_j$ is the position coordinate for the j-th electron in complex notation, $l_0 = \sqrt{\hbar/(eB)}$ is the magnetic length, B is the perpendicular magnetic field and $-e(e > 0)$ is the electron's charge.

A straightforward motivation to study the Bose Laughlin wave function in relation to the true CF liquid state is justified on the naive expectation that, because of the Bose statistics, the Bose Laughlin energy may constitute a reasonable *lower energy bound* to the CF Fermi liquid energies for the given even-denominator filling factors. While this is an expectation that we cannot prove exactly, an *a posteriori* justification may be provided if the numerical results are consistent with it (although we caution that this is not a definitive proof in any way). The assumption that corresponding Bose Laughlin and CF liquid ground-state energies should be reasonably different from each other (given the very different nature of the wave functions) is more relevant to us in contrast to the question of whether the Bose Laughlin wave function is an exact lower energy bound of the true CF liquid energy.

The main result of this work is not to assert the relevance of the Bose Laughlin wave function at filling factors $1/2$, $1/4$, and $1/6$, but to report a surprising and unexpected finding, namely that the energy of the Bose Laughlin wave function at $\nu = 1/4$ and $1/6$ (but not $1/2$) is practically identical to the energy of the corresponding true CF Fermi liquid state.

The model that we adopt consists of N fully spin-polarized electrons moving in a two-dimensional (2D) space subject to a strong perpendicular magnetic field. The electrons are embedded in a uniform neutralizing background of positive charge which is spread uniformly within a finite disk of area $\Omega_N = \pi R_N^2$ and radius R_N. The electrons can move freely all over the 2D space and are not constrained to stay inside the disk. The uniform density of the system is $\rho_0 = \nu/(2\pi l_0^2)$. The radius of the disk is determined from the condition: $\rho_0 = N/\Omega_N$ which gives a finite disk radius $R_N = l_0\sqrt{2N/\nu}$. The kinetic energy per electron corresponding to the Bose Laughlin wave function is $\langle \hat{K} \rangle/N = \hbar\omega_c/2$, where ω_c is the cyclotron frequency. Since the kinetic energy per electron is a mere constant, the problem reduces to calculate the expectation value of the potential energy operator which consists of three terms:

$$\hat{V} = \hat{V}_{ee} + \hat{V}_{eb} + \hat{V}_{bb} \; , \tag{3}$$

where $\hat{V}_{ee}, \hat{V}_{eb}$ and $\hat{V}_{bb}$ are, respectively, the electron-electron, electron-background and background-background potential energy operators. For a pure Coulomb interaction they are given by

$$\hat{V}_{ee} = \sum_{i<j}^{N} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \;\; , \;\; \hat{V}_{eb} = -\rho_0 \sum_{i=1}^{N} \int_{\Omega_N} \mathrm{d}^2 r \, \frac{e^2}{|\vec{r}_i - \vec{r}|} \;\; , \;\; \hat{V}_{bb} = \frac{\rho_0^2}{2} \int_{\Omega_N} \mathrm{d}^2 r \int_{\Omega_N} \mathrm{d}^2 r' \, \frac{e^2}{|\vec{r} - \vec{r}\,'|} \; . \tag{4}$$

Monte Carlo (MC) simulations in disk geometry [17, 18] are used to calculate the expectation value of the electron-electron and electron-background interaction potentials, $\langle \hat{V}_{ee} \rangle/N$ and $\langle \hat{V}_{eb} \rangle/N$, respectively. The background-background interaction energy can be calculated exactly and is

$$\frac{\langle \hat{V}_{bb} \rangle}{N} = \frac{8}{3\pi}\sqrt{\frac{\nu N}{2}} \frac{e^2}{l_0} \; . \tag{5}$$

In our MC simulations we adopt the well-known Metropolis algorithm [19]. In this algorithm, the expectation value of any operator is estimated by averaging its value over numerous electronic configurations of $\{\vec{r}_1, \ldots, \vec{r}_N\}$ coordinates. Our runs consist of 100000 "equilibration" MC steps (a step consists of attempts to move all the electrons one by one) and up to 2×10^6 "averaging" MC steps used to calculate the expectation value of chosen operators. The simulations are done for systems of $N = 4, 16, 36, 64, 100, 144, 196, 256, 324$ and 400 electrons. The correlation energy per particle in the thermodynamic limit ($N \to \infty$) is obtained by fitting the finite-N energies, $\langle \hat{V} \rangle/N$ to a second-order polynomial function as described in ref. [17]. The resulting polynomial fits are

$$\begin{cases} \frac{\langle \hat{V} \rangle_{1/2}}{N} = \left(-0.4841(5) + \frac{0.1017(68)}{\sqrt{N}} - \frac{0.0280(07)}{N} \right) \frac{e^2}{l_0} \; , \\ \frac{\langle \hat{V} \rangle_{1/4}}{N} = \left(-0.3614(03) + \frac{0.0306(964)}{\sqrt{N}} - \frac{0.0184(964)}{N} \right) \frac{e^2}{l_0} \; , \\ \frac{\langle \hat{V} \rangle_{1/6}}{N} = \left(-0.3013(31) + \frac{0.0133(206)}{\sqrt{N}} - \frac{0.0151(46)}{N} \right) \frac{e^2}{l_0} \; . \end{cases} \tag{6}$$

The finite-N correlation energies per particle for the Bose Laughlin state at $\nu = 1/2, 1/4$ and $1/6$ and their thermodynamic limit values are displayed in table I. We estimated that the statistical uncertainty (which scales as $1/\sqrt{\text{MC steps}}$) of the energy data reported in table I is in the fifth digit after the decimal point which is rounded. Similarly, the statistical uncertainty of the extrapolated values is in the fifth digit after the decimal point. We also computed the single-particle density function, $\rho(\vec{r}) = \left\langle \sum_{i=1}^{N} \delta(\vec{r} - \vec{r}_i) \right\rangle$ and the pair distribution function

Table I – *Correlation energy per particle for the Bose Laughlin state at filling factors $\nu = 1/2$, $1/4$ and $1/6$. Results obtained from a standard Monte Carlo simulation in disk geometry. Energies are in units of e^2/l_0. The statistical uncertainty in the last digit of energy is shown in paranthesis.*

N	1/2	1/4	1/6
4	−0.4402(8)	−0.3506(9)	−0.2984(7)
16	−0.4603(8)	−0.3548(1)	−0.2988(6)
36	−0.4679(7)	−0.3568(2)	−0.2995(6)
64	−0.4719(2)	−0.3579(0)	−0.2999(6)
100	−0.4743(2)	−0.3585(7)	−0.3002(1)
144	−0.4759(2)	−0.3590(2)	−0.3003(6)
196	−0.4770(5)	−0.3593(2)	−0.3004(7)
256	−0.4779(0)	−0.3595(5)	−0.3005(5)
324	−0.4785(3)	−0.3597(2)	−0.3006(0)
400	−0.4790(4)	−0.3598(4)	−0.3006(3)
∞	−0.4841(5)	−0.3614(03)	−0.3013(31)

which for a liquid with uniform density ρ_0 is $\rho_0\, g(r) = \frac{1}{N} \left\langle \sum_{i=1}^{N} \sum_{j\neq i}^{N} \delta(r - |\vec{r}_i - \vec{r}_j|) \right\rangle$. The single-particle density of the Bose Laughlin state shows the expected non-uniformity near the disk boundary (see fig. 1). Note that the non-uniformity near the disk edge always persists and increases as the filling factor decreases. The pair distribution function for $\nu = 1/2, 1/4$ and $1/6$ obtained after a MC simulation in disk geometry for $N = 400$ electrons is shown in fig. 2.

We compare the Bose Laughlin energies in the thermodynamic limit as displayed in the last row of table I to respective values of the LLL-projected spin-polarized CF Fermi liquid state energies (eq. (1)) at same filling factors. A search in the literature provides us with the following values for the CF Fermi liquid energy at $\nu = 1/2$: $-0.466\, e^2/l_0$ from ref. [20] and $-0.46557(6)\, e^2/l_0$ from ref. [21]. Both of these values are higher than the value $-0.4841(50)\, e^2/l_0$ which corresponds to Ψ_{Bose}. Reference [20] gives the energy $-0.3608\, e^2/l_0$ for the $\nu = 1/4$ state, a value that is higher than but very close to the energy, $-0.3614(03)\, e^2/l_0$, corresponding to the Ψ_{Bose} state. We were unable to find data for the energy of the Ψ_{Fermi} state at $\nu = 1/6$. While there are more data for the *unprojected* version
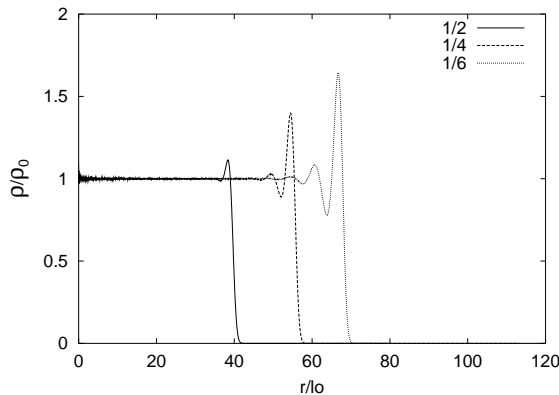

Fig. 1 – One-body density function, $\rho(r)/\rho_0$, for the Bose Laughlin states $\nu = 1/2$, $1/4$ and $1/6$ as a function of the distance r/l_0 from the center of the disk for systems with $N = 400$ electrons.

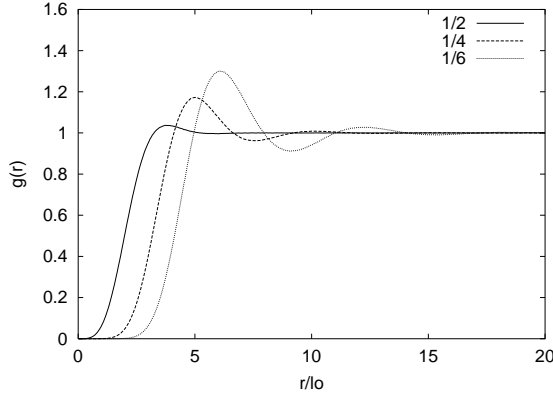Fig. 2 – Pair distribution function of the Bose Laughlin state at filling factor $\nu = 1/2$, 1/4 and 1/6 obtained after a MC simulation in disk geometry for $N = 400$ electrons.

of the CF Fermi liquid wave function obtained with different methods [22–25], we found only few results for the *fully LLL projected* CF Fermi liquid states at the filling factors considered in this work. In order to have a larger pool of results to whom to compare the $\nu = 1/2, 1/4$ and 1/6 energies, we pursue a different path and resort to interpolation formulas that give the energy per particle, $E(\nu)$ of the electronic liquid state as a function of the LLL filling factor: $0 < \nu \leq 1$. A crude empirical formula of this form has been suggested by Laughlin (L) [11] and reads:

$$E_L(\nu) = 0.814 \sqrt{\nu} \left(0.230 \, \nu^{0.64} - 1\right) \frac{e^2}{l_0} . \tag{7}$$

Another formula proposed by Levesque, Weis, and MacDonald (LWM) [26] has the form:

$$E_{LWM}(\nu) = -0.782133 \sqrt{\nu} \left(1 - 0.211 \, \nu^{0.74} + 0.012 \, \nu^{1.7}\right) \frac{e^2}{l_0} . \tag{8}$$

Both expressions, $E_L(\nu)$ and $E_{LWM}(\nu)$ are derived by fitting the energy of Laughlin wave functions and violate the particle-hole symmetry condition in the LLL.

A third interpolation formula which satisfies the particle-hole symmetry condition in the LLL and therefore provides a more accurate interpolation for the dependence of energy on the LLL filling factor is given by Fano and Ortolani (FO) [27] and has the form

$$E_{FO}(\nu) = \left[-\sqrt{\frac{\pi}{8}} \, \nu - 0.782133 \sqrt{\nu} \, (1-\nu)^{3/2} + 0.55 \, \nu \, (1-\nu)^2 - 0.463 \, \nu^{3/2} \, (1-\nu)^{5/2}\right] \frac{e^2}{l_0} . \tag{9}$$

We use the $E_L(\nu), E_{LWM}(\nu)$ and $E_{FO}(\nu)$ interpolation formulas to generate more data for the energies at $\nu = 1/2, 1/4$ and 1/6 and compare the interpolated values to Bose Laughlin energies at same filling factors. Such energies (in units of e^2/l_0) are given in table II.

The results in table II and the $\nu = 1/2$ results from refs. [20, 21] suggest that the $E_L(\nu)$ and $E_{LWM}(\nu)$ formulas are too crude to describe the energy of the electronic liquid states for the whole range of LLL filling factors. Clearly the Bose Laughlin energy at $\nu = 1/2$ is distinctly smaller than the CF Fermi liquid energy of refs. [20, 21] and FO interpolation energy, as well. The FO value at $\nu = 1/2$ is close to the spin-polarized CF liquid-state value [21], although we notice that it is closer to the energy of the spin-unpolarized (singlet)

Table II – *Energy per particle for the LLL states $\nu = 1/2$, $1/4$ and $1/6$ obtained from interpolation formulas eq. (7), eq. (8) and eq. (9) as compared with Bose Laughlin state energies. Energies are in units of e^2/l_0. The statistical uncertainty in the last digits of energy is shown in paranthesis.*

$E(\nu)$	1/2	1/4	1/6
E_L	-0.490632	-0.368452	-0.308033
E_{LWM}	-0.485225	-0.361930	-0.301595
E_{FO}	-0.469049	-0.361519	-0.303660
Ref. [20]	-0.46600	-0.36080	. . .
Ref. [21]	$-0.46557(6)$	. . .	. . .
E_{Bose}	$-0.4841(50)$	$-0.3614(03)$	$-0.3013(31)$

CF state, $-0.46953(7)\,e^2/l_0$ reported in ref. [21]. This is not the case for the other two filling factors, $\nu = 1/4$ and $\nu = 1/6$, where all the interpolation energies including the FO values are slightly lower than the Bose Laughlin energies, though very close to them. The more accurate polarized CF Fermi liquid state energy [20] ($-0.3608\,e^2/l_0$ at $\nu = 1/4$) is larger than the Bose Laughlin energy, though it is important to note that the two values are so close that they can be considered practically identical.

The fact that interpolation energies are slightly lower than the Bose Laughlin energies at $\nu = 1/4$ and $1/6$ surely does not invalidate the possibility of the Bose Laughlin wave function being a lower energy bound to the true CF Fermi liquid energy since it is well known [28] that the true energy at any filling factor (excluding the Laughlin filling factors) is always higher than the approximate energy obtained from L, LWM and FO interpolation formulas that are smooth functions of ν and should be handled with care. For electronic LLL Laughlin wave functions (Fermi or Bose) and a bare Coulomb potential, the Haldane pseudopotential parameters, V_m, are known to be all positive and decrease monotonically as the relative angular momentum, m, increases. In contrast to the electronic case, the Haldane pseudopotential parameters (for both bare and screened Coulomb potentials) corresponding to the CF Fermi liquid states in eq. (1) show a distinct non-monotonic behavior with some of them even becoming negative for large values of relative angular momentum [29]. In the CF language, a state with filling factor, $\nu = p/(2mp + 1)$ represents a CF system with p-filled CF LL-s which weakly interact with each other by some residual interaction. In such a case, the CF Haldane pseudopotentials (both small p and large p) show a qualitatively different behavior from the electronic LLL Laughlin pseudopotentials. Such a qualitatively different behavior is likely associated with the weakly interacting nature of the CFs as compared to pure electrons [30]. Because of the different nature of the two liquid wave functions (eq. (1) and eq. (2)) and their respective Haldane pseudopotentials, it was unexpected to find that the Bose Laughlin and the true CF Fermi liquid energies are practically identical for filling factor $\nu = 1/4$ and $1/6$, while clearly distinct for $\nu = 1/2$.

In summary, we used MC simulations to calculate the ground-state properties of Bose Laughlin wave functions at compressible filling fractions $\nu = 1/2$, $1/4$ and $1/6$. The calculated ground-state energies are compared with results for spin-polarized CF wave functions for these filling factors. We found that the Bose Laughlin wave function ground-state energy is lower than the CF Fermi liquid energy for $\nu = 1/2$, whereas for other filling factors, $\nu = 1/4$ and $1/6$, we find the surprising result that the Bose Laughlin ground-state energy is practically identical to the energy of the true CF liquid state as calculated from different studies and from estimates obtained from various interpolation schemes. Because Bose Laughlin and true CF liquid energies are very different at $\nu = 1/2$, we naively expected to see a similar tendency apply to the other two even-denominator-filled CF liquid states, $\nu = 1/4$ and $1/6$; however,

unexpectedly we found out that the Bose Laughlin and true CF liquid energies are practically identical at filling factors 1/4 and 1/6. The physical significance and robustness of this finding is not yet clear to us and further work is needed to address this issue.

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