Properties of Paired Quantum Hall States at $\nu = 2$

F. G. Pikus $^a$ and A. M. Tikofsky $^b$

$^a$ Department of Physics, University of California, Santa Barbara, CA 93106
$^b$ Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106

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The energetic properties of a paired quantum Hall state at Landau level filling $\nu = 2$ are investigated using variational Monte Carlo techniques. Pairing is found to be energetically favorable in small magnetic fields because it introduces correlations between up and down spins that are absent in the conventional $\nu = 2$ state. We find that pairing survives extrapolation to the thermodynamic limit.

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The traditional view of the Integral Quantum Hall Effect (IQHE) treats the system as a gas of non-interacting electrons in a background magnetic field. The corresponding spectrum consists of Landau levels separated from each other by an energy gap $\Delta = \hbar \omega_c = \hbar c / m^* B$ where $m^*$ is the band effective mass of the electrons and $B$ is the external magnetic field. It is presumed that $B$ is so large that many-particle interactions can essentially be ignored because they encourage the occupation of higher Landau levels. Recent experiments [1,2] have led one of the authors [3] to propose that the traditional picture is incomplete. For small enough $B$, it was argued that a new even IQHE exists that is distinct from the old one and whose stability relies on the existence of the many-particle interactions as well as the occupation of higher Landau levels. In this letter, we investigate the energetic properties of such a state at Landau level filling fraction $\nu = 2$ and argue that it is more stable than the conventional $\nu = 2$ state for small magnetic fields.

The investigation of new low magnetic field IQHE states is motivated by an experimental phase diagram that is inconsistent with an IQHE insensitive to many-particle interactions [1,2]. At low magnetic fields, a direct second order phase transition from a state with $\nu = 2$ to an insulator ($\nu = 0$) has been observed with no experimental evidence for an intermediate $\nu = 1$ phase in the transition region. However, in the non-interacting picture, $\nu$ measures the number of filled Landau levels below the Fermi energy and the system must decrease the number of these levels by one at a time and therefore pass through a $\nu = 1$ phase in the transition from $\nu = 2$ to $\nu = 0$. It was therefore proposed that an unconventional $\nu = 2$ quantum Hall state, which can make a direct continuous transition to an insulator, arises in low magnetic fields. This state will be called the $2b$ state and is distinct from the conventional spin-unresolved $2a$ state. At any finite magnetic field, the $2a$ state is adiabatically connected to the $2a$ state at infinite magnetic in which the lowest Landau level for each spin is completely filled.

The essential idea behind the $2b$ quantum Hall state is that all up- and down-spin electrons pair to form spinless bosons. At electronic filling fraction $\nu = 2$, these bosons form their own Landau levels with filling fraction $\nu_b = \nu/4 = 1/2$. When $\nu_b^{-1}$ is an even integer, bosons can form a Laughlin state that is analogous to the Laughlin fractional quantum Hall states that exist when $\nu^{-1}$ is an odd integer [4].

The transition from $\nu = 2$ to an insulator is the allowed transition from the $\nu_b = 1/2$ bosonic quantum Hall state to an insulating state.

A proposed spin-singlet many-electron wavefunction [3] for the 2b state is

$$\Phi = \prod_{k<l} (u^*_k v^*_l - u^*_l v^*_k) \text{ Per } F(|u_i v_j - u_j v_i|),$$  \hspace{1cm} (1)

where $(u_i, v_i)$ is the complex coordinate of the $i$th electron on the sphere, $(u^*_k, v^*_k)$ is the complex coordinate of the $k$th spin $\sigma$ electron, and $\text{Per}$ denotes the Permanent of the symmetric matrix whose $(i,j)$th component is $F(|u_i v_j - u_j v_i|)$. Because $F$ in not analytic, the $2b$ state has a significant occupation of higher Landau levels. This is required because any candidate $2b$ state must be thermodynamically distinct from the conventional spin-unpolarized $2a$ state, the unique state at $\nu = 2$ in the lowest Landau level. In addition, $\Phi$ has total filling fraction $\nu = 2$ as the total angular momentum of this state is identical to that of the $2a$ state.

The behavior of the $2b$ state described by Eq. (1) is governed by the function $F$. For $F = 1$, $\Phi$ is the conventional $2a$ state consisting of two filled Landau levels. If $F$ is short-ranged then it can be thought of as a pair wavefunction and its effective size is the coherence length. For distances much longer than this coherence length, $F$ acts like a $\delta$-function and

$$\Phi \sim \prod_{k<l} (u^*_k v^*_l - u^*_l v^*_k)^2 \text{Det } \left[ \delta^2 (|u^*_i v^*_j - u^*_j v^*_i|) \right].$$  \hspace{1cm} (2)

When $F$ is approximated as a $\delta$-function, there is a well-defined pair coordinate and $\Phi$ vanishes as the second power of the complex pair coordinate as two pairs approach each other. $\Phi$ therefore acts like a $\nu_b = 1/2$ Laughlin state of charge $e^* = 2e$ bosonic pairs.

At first, the existence of a pairing state stabilized by repulsive Coulomb interactions seems counterintuitive. Moreover, because a pairing wavefunction is constructed...
by occupying higher Landau levels, we lose kinetic energy that must be compensated by a gain in interaction energy. However, we only lose interaction energy among the two electrons in a pair; we gain repulsive energy because the Laughlin $\nu_0 = 1/2$ state keeps the pairs well separated. The maximum possible gain in energy can be estimated by approximating the pairs as tightly bound point objects thus ignoring the energy cost for forming the pairs. We can then calculate the interaction energy for all electrons not in the same pair. This is just the Coulomb energy of a $\nu_0 = 1/2$ state of spinless charge $e^* = 2e$ bosons. Laughlin’s interpolation formula for $E_m$ [6], the Coulomb energy of a projected $\nu = 1/m$ state, gives an energy per electron for the $2b$ state of $U_{2b} = -0.49(e^*)^2/\ell l^* = -1.39e^2/\ell l$ where $l$ is the magnetic length. In contrast, the energy of the $2a$ state is $E_{2a} = -\sqrt{\pi/8} e^2/\ell l$. Forming a paired state has yielded an energy gain per pair of $2(E_{2a} - U_{2b}) = 1.53e^2/\ell l$.

In this paper, we will argue that the gain in interaction energy between pairs, associated with a $2b$ state, outweighs the energy cost of forming pairs. In order to make the formation of pairs as inexpensive as possible, we consider pairing functions $F$ costing the least Coulomb energy. If $F(r)$ is strongly peaked at $r = 0$, electrons in a pair have large overlap and pair formation is expensive. We give $F$ the variational freedom to reduce the cost of pair formation by taking

$$F(r) = (r - \beta) \exp(-\alpha r^2), \quad (3)$$

where pairing is indicated by a nonzero inverse pair size $\alpha$ and $\beta$ is a variational parameter chosen to minimize the cost of pair formation. If we had only two electrons, one of each spin, then the many body wavefunction in Eq. (1) would simply be $F$. The cost of pair formation, which is the expectation value of the Coulomb interaction in this state, is easily shown to be minimized for $\beta \alpha = 1 - 1/\sqrt{2}$. In contrast, one might have expected that giving $F$ a node at $r = 0$ and hence taking $\beta = 0$ would yield the smallest Coulomb energy. If we rewrite $F$ as the sum of two terms as $F(r) = r \exp(-\alpha r) + (\beta) \exp(-\alpha r)$, it is easily shown that the energetic gain of having $\beta > 0$ comes from the negative overlap of these two terms. However, a large value of the second term still implies a large value of $|F(0)|$ which costs repulsive Coulomb energy. We therefore impose the additional restriction that $F(r)$ be replaced by $G(r) = \text{Max}(F(r), F(r_0))$ where $r_0$ depends on $\alpha, \beta$ and is chosen so that not more 5% of the integral $\int d^2r G(r)^2$ comes from $r < \beta$. If we fix $\beta$ then $r_0 = 0$ for small $\alpha$, becomes nonzero only for large enough $\alpha$, and then increases with $\alpha$.

We employ a spherical geometry to calculate the energy of $\Phi$ in Eq. (4) for a finite number of electrons. Because this choice enforces a uniform density, we avoid the influence of a physical edge in our calculations [9]. As is the convention, we induce a uniform magnetic field by placing a monopole at the center of the sphere such that the total magnetic flux through the sphere is $2S$ flux quanta $\hbar c/e$ and $2S$ is required to be an integer by the Dirac quantization condition. The single particle kinetic energy operator on the sphere is the conventional $K = (\partial^2/\partial^2 + (z^2)A)^2/2m^*$, defined in spherical coordinates. A spherical system with $2N$ electrons occupying $\Phi$, a state with angular momentum corresponding to filling the lowest Landau level of each spin, has $2S = N - 1$. The corresponding magnetic length is $l_N = \sqrt{\hbar/m^*\omega} = D/\sqrt{2(N-1)}$ where $D$ is the diameter of the sphere. In addition, we define the Coulomb interaction between two electrons $i$ and $j$ to be $V_{ij} = e^2/\ell |r_{ij}|$ where $r_{ij} = u_iu_j - u_ju_i$ is the complex chord distance.

Calculating the expectation value of the energy using $\Phi$ requires evaluating multi-dimensional integrals. Integrals of such large dimension were computed using a straightforward Monte-Carlo integration on a parallel Cray T3D supercomputer. Because the values of the integrand at different random points are completely independent, the algorithm trivially parallelized and showed perfect linear speed-up. The most time-consuming step was the computation of the permanents in Eq. (1), for which an effective algorithm can be found in Ref. [8].

The calculated expectation value of the total Coulomb energy shows that that the energy gain due to the pairing correlations outweighs the energy cost of forming the pairs. The $2b$ state’s Coulomb energy is compared to the energy of two filled Landau levels, $2E_{2a} = -\sqrt{\pi/2} e^2/\ell l$, where $l$ is the $N \rightarrow \infty$ magnetic length. In Fig. 1, the potential energy gain per pair is shown for various system sizes as a function of $\alpha N = \alpha l_N$. For each value of $N, \beta$ is fixed to be that value which gives lowest expectation value for the total interaction energy at the optimal value of $\alpha N$. We see that the value of $\alpha N$ at which the energy is minimal does not change as the size of the system increases. Therefore, the gain in energy associated with pairing seems to survive the thermodynamic limit as the preferred value of the pair size $1/\alpha$ scales with the magnetic length $l_N$ and not the system size $D$. Because the filling fraction is fixed at $\nu = 2$, the pair size also scales as the interparticle spacing. In contrast, the preferred value of $\beta$ seems to be independent of $N$ and ranges from $0.12D$ to $0.22D$.

In addition to the tendency towards pairing, Fig. 1 provides further information about the behavior of the interaction energy. Because $F$ is not constant, there is an energy gain near $\alpha = 0$ due to mixing in of higher Landau levels. When $\alpha D << 1$, the pair size is much greater than the system size and the energy can not differentiate between different values of $N$. In this region, the interaction energy per particle, as a function of $\alpha$, should be independent of $N$. While this behavior is consistent with our results, it is not apparent in Fig. 1 as the energy is plotted as a function of $\alpha N$ instead of $\alpha$ in addition to being defined in units of $e^2/\ell l_N$ instead of $e^2/\ell l D$. The energy is linear in the inverse pair size $\alpha N$ in the $\alpha \rightarrow \infty$ limit as it is dominated by the Coulombic energy cost of forming pairs.

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\[ U_{2b} = \frac{\rho}{2} \int d^2r \left( g_{\uparrow\uparrow}(r) + g_{\downarrow\downarrow}(r) - 2 \right) \frac{e^2}{\epsilon r}, \tag{4} \]

that modifications of the correlation functions are responsible for the energy gain shown in Fig. 1. There is only a minor change in the behavior of the same spin correlation function \( g_{\uparrow\uparrow} \) as we vary from \( \alpha = 0 \) to its energetically preferred value. The \( 2a \) state does so well at keeping same spin particles apart that the \( 2b \) state need not do much better. On the other hand, simply filling two Landau levels yields no correlations between up and down spins and a constant \( g_{\uparrow\downarrow} \). The \( 2a \) state, given by \( \Phi \) in Eq. (3) with \( \alpha = 0 \), has only weak correlations between opposite spin electrons. Therefore, having a finite \( \alpha \) is favored energetically because it introduces strong correlations between the locations of up and down spins. These correlations minimize the repulsive Coulomb energy between up and down spins by giving them a preferred separation and thus keeping them on average farther apart.

In spite of mixing in all higher Landau levels, the loss of kinetic energy associated with the \( 2b \) state is only of order the cyclotron energy \( \hbar \omega_c \) per pair as is seen in Fig. 2. The prefactor \( \prod_{i<j,\sigma} (u_i^\sigma v_j^\sigma - u_j^\sigma v_i^\sigma) \) forces much of the \( 2b \) wavefunction into the lowest Landau level. The ability of a Jastrow prefactor to force most of the wavefunction into the lowest Landau level is well known from Jain’s construction of hierarchical quantum Hall states \[10\]. However, that work assumed that the wavefunction was not thermodynamically distinct from a wavefunction projected onto the lowest Landau level. In contrast, a paired wavefunction must necessarily involve all Landau levels. The two-particle paired wavefunction, \( \Phi \sim F(r) \), can be expressed in terms of its projection onto the \( n^{th} \) Landau level as \( \Phi = \sum_n a_n \psi_n(r) \) where \( \psi_n(r) \) is the zero angular momentum state in the \( n^{th} \) Landau level. If we do not include all terms in this series and hence all Landau levels then we do not really have pairing as \( F(r) \) will oscillate instead of vanishing exponentially at large \( r \).

The energy gain associated with the \( 2b \) state can outweigh the energy loss only for small enough magnetic field. The energy gain is Coulombic and scales as \( e^2/\epsilon l \sim B \) while the energy loss is kinetic and scales as \( \hbar \omega_c \sim B \). Therefore, there is an energy gain associated with forming a \( 2b \) state only for large enough values of the ratio

\[ y = \frac{e^2/\epsilon l}{\hbar \omega_c} = l/a^* = \sqrt{\frac{B^*}{B}}, \tag{5} \]

FIG. 1. The potential energy per pair \( 2(U_{2b} - E_{2b}) \), defined in units of \( e^2/\epsilon l_N \), as a function of \( \alpha_N = \alpha l_N \). Zero is chosen as the energy for the state formed by filling the lowest Landau for each spin \( 2(E_{2b}) \) and the data for \( 2N \) electrons are indicated by empty circles \((2N = 10)\), solid circles \((2N = 12)\), empty squares \((2N = 14)\), and empty triangles \((2N = 16)\). The dotted line was drawn through the \( 2N = 10 \) data as a guide for the eye. The Monte Carlo error bars for the \( 2N = 16 \) data are so large that they were left out for clarity.

FIG. 2. The correlation functions are shown for \( 2N = 10 \) electrons as a function of the angle \( \theta \) where \( D \sin \theta/2 \) is the chord distance. Values of \( g_{\uparrow\downarrow} \) and \( g_{\downarrow\uparrow} \) are denoted by the solid markers and empty markers, respectively. The \( \alpha \) \( = 0 \) data are indicated by circles; the data for \( \alpha = 5 \), the optimal value of \( \alpha \), are indicated by pentagons; and the data for \( \alpha = 3 \) data are indicated by solid squares. The lines are only meant as guides to the eye. As is the convention, the correlation functions are normalized so that at large distances (in the \( D \to \infty \) limit) \( g_{\sigma \sigma}(\pi) = 1 \).
at composite filling fraction $\nu_{\text{comp}} = 1/m$, that makes a direct continuous transition to an insulator. In fact, there is recent evidence for a $\nu = 3$ to insulator transition [11]. In addition, we are presently investigating a class of paired states at $\nu = 1/2$ in double layer systems that are distinct from the states that have been proposed to explain the experimental observation of a quantum Hall effect at $\nu = 1/2$ [12]. A preliminary indication of this paired state would be a direct continuous transition from the $\nu = 1/2$ state to an insulator.

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where $a^* = e^2 \hbar / m^*$ is the effective Bohr radius. For GaAs–Al$_x$Ga$_{1-x}$As, $a^* = 100\AA$ and $B^* = 6.6T$. Our calculation first gives a gain in energy for $y \sim 1$.

The numerical evidence presented does not prove unequivocally that the $2b$ state is the preferred state. A definitive calculation would compare the lowest energy $2b$ state to the lowest energy $2a$ state. Clearly, the specific form of these states would depend on the value of the external magnetic field $B$ in a complicated way. In addition, even though the lowest energy $2a$ and $2b$ states are thermodynamically distinct, they need not differ greatly in energy. It is clearly not feasible to perform an unequivocal energetic comparison of the $2a$ and $2b$ states. Instead, we compared our $2b$ state to the $2a$ state without any occupation of higher Landau levels. In so doing, we have made the case that the energetic gain of pair correlations can outweigh the energetic cost of forming pairs. In order to do any better, we need to include the effect of disorder as this is known to stabilize the experimental signatures of the $2b$ state at larger magnetic fields [13].

The energetic arguments used to justify pairing can be extended to other quantum Hall systems. For instance, the same mechanism that we have discussed would encourage the formation of a state at $\nu = m$, consisting of charge $e^* = me$ particles forming a quantum Hall state

[1] L. W. Wong et al., Phys. Rev. B51, 18033 (1995); H.W. Jiang, unpublished.
[2] H. W. Jiang et al., Phys. Rev. Lett. 71, 1439 (1993);
[3] T. Wang et al., Phys. Rev. Lett. 72, 709 (1994); R. J. F. Hughes et al., J. Physics: Cond. Mat. 6, 4763 (1994).
[4] D. Shahar et al., Phys. Rev. B52, R14372 (1996).
[5] A. M. Tikofsky and S. A. Kivelson, Phys. Rev. B53, R13275 (1996).
[6] R. Prange and S. M. Girvin, *The Quantum Hall Effect* (Springer-Verlag, New York, 1987).
[7] I. Herbut, Phys. Rev. B46, 15582 (1992).
[8] M. Henryk, “Permanents”, Ser. “Encyclopedia of mathematics and its applications”, vol. 6, Addison-Wesley Pub. Co., Mass., 1978. Given an order N matrix $M_{ij}$, the permanent $\text{Per}(M) = \sum_{\pi} \prod_{i=1}^N M_{\pi_i \pi_i}$, the product is over the $N/2$ pairs $ab$, the sum is over the possible permutations of these pairs.
[9] F. D. M. Haldane, Phys. Rev. Lett. 51, 605 (1983).
[10] G. Dev and J. K. Jain, Phys. Rev. B45, 1223 (1992); N. Trivedi and J. K. Jain, Mod. Phys. Lett. B5, 503 (1991).
[11] S. H. Song and D. C. Tsui (private communication).
[12] Y. W. Suen et al., Phys. Rev. Lett. 68, 1379 (1992); J. P. Eisenstein et al., Phys. Rev. Lett. 68, 1383 (1992); Song He et al., Phys. Rev. B47, 4394 (1993); M. Greiter et al., Phys. Rev. B46, 9586 (1992).