PHYSICAL REVIEW B VOLUME 34, NUMBER 4 15 AUGUST 1986

Microscopic wave functions for the fractional quantized Hall states at $\nu=\frac{2}{5}$ and $\frac{2}{7}$

R. Morf
Labortories RCA, Limited, CH-8048 Zürich, Switzerland

N. d'Ambrumenil
Department of Physics, University of Warwick, Coventry, England

B. I. Halperin
Lyman Laboratory of Physics, Harvard University, Cambridge, Massachusetts 02138

(Received 24 March 1986)

New microscopic trial wave functions are proposed for fractional quantized Hall states at $\nu=2/(2p+1)$. Results for $\nu=\frac{2}{5}$ and $\frac{2}{7}$ based on Monte Carlo and exact numerical computations are presented. For $N\leq 10$ electrons on a sphere, energies differ from the exact ground-state energy by less than 0.3%. For even p, such as $\nu=\frac{2}{5}$, the trial wave function may be regarded as a microscopic realization of the condensed quasiparticle state postulated in hierarchical schemes.

In a seminal paper, Laughlin[1] introduced the idea that the fractional quantized Hall effect is a consequence of the condensation of the two-dimensional electron system into a novel ground state: an incompressible fluid with fractionally charged excitations. He constructed an explicit trial wave function for states where the filling factor ν of the lowest Landau level has the form $\nu=1/m$ (m =an odd integer). Studies by exact numerical diagonalization of the Hamiltonian for small systems (up to $N=9$ electrons) both in the plane[2,3] and on the surface of a sphere[4] showed that this trial wave function captures the essential properties of the ground state at $\nu=\frac{1}{3}$ and $\nu=\frac{1}{5}$ (Ref. 5) and gives an excellent upper bound for the ground-state energy. The structure of the ground state (GS) at other filling fractions, e.g., $\nu=\frac{2}{5}$, $\nu=\frac{2}{7}$, etc., is less well understood because Laughlin's wave function cannot be used in these cases. Two alternative attempts have been made for the description of the quantized Hall states at such filling factors: One is based on a hierarchical scheme[6,7] in which, e.g., the $\nu=\frac{2}{5}$ state of an N-electron system is pictured as an N-electron $\nu=\frac{1}{3}$ Laughlin state in which $N/2$ quasiparticles with charge $e/3$ are condensed again into a Laughlin-type fluid state. This approach makes use of *pseudo-wave-functions* for the quasiparticles, which are treated as point particles. The approximations which are thereby made are not well controlled and lead only to crude estimates for the GS energy, although they provide the correct quantum numbers.

The second approach is based upon *microscopic* trial wave functions (MTWF's). Several types of MTWF's for states at $\nu=\frac{2}{5}$, $\frac{2}{7}$, etc., have been proposed: In many cases, such as the wave functions which involve multiple derivatives and/or integrations,[6,8,9] evaluation is very difficult even for systems with very few electons. Consequently, no exact numerical results for its energy are available.[10] Another MTWF, based on the principle of forming pairs of electrons, was introduced by Halperin.[9] However, Monte Carlo calculations[11] have shown that it produces poor results for $\nu=\frac{2}{5}$. There are several reasons why it is useful to have MTWF's, if they are simple enough to allow physical interpretation as well as accurate computations: (i) they provide the basis for tests of approximate theories, e.g., the aforementioned hierarchical scheme;[6,7] (ii) they serve as starting states ψ_1 for exact computations in finite systems, based on the principle of vector iteration, where one diagonalizes the Hamiltonian H in the basis generated by $\psi_n=H\psi_{n-1}=H^{n-1}\psi_1$. Convergence can be very rapid if ψ_1 has a large overlap with the exact GS.

In this note, we introduce new MTWF's for states at $\nu=2/(2p+1)$ which are related to the pair wave functions of Ref. 9 and which also allow studies both by Monte Carlo (MC) as well as by exact numerical calculations. For p even, such as $\nu=\frac{2}{5}$, the MTWF may be regarded as microscopic realization of the condensed quasiparticle state postulated in hierarchical schemes.[6,7] We report results of MC calculations with up to $N=60$ electrons as well as exact numerical results for systems with up to $N=12$ electrons on the surface of a sphere. At $\nu=\frac{2}{5}$, for $N=10$ electrons, the overlap between this new MTWF and the exact ground state is 97.2% and the difference in the Coulomb energy is about 0.3%. For the $\nu=\frac{2}{7}$ state and $N=8$ electrons we obtain 99.6% for the overlap and 0.04% for the energy difference. At our suggestion, computations based on our new MTWF have been carried out also by Fano, Ortolani, and Colombo.[5] Their results for $\nu=\frac{2}{5}$ with up to $N=6$ electrons agree with ours and they have also obtained promising results for $\nu=\frac{2}{9}$.

Our new MTWF, like the one introduced by Halperin,[9] is based on the principle of grouping electrons into pairs. The motivation for this has been discussed in detail in Ref. 11. In the spherical geometry, our MTWF has the form

$$\psi_T=\mathbf{A}\phi_T=\mathbf{A}\left\{\psi_m^{\mathrm{LJ}}\prod_{n}^{N/2}(u_{2n}v_{2n-1}-v_{2n}u_{2n-1})^{-t}\prod_{\substack{n,n'\\(n<n')}}^{N/2}[u_{2n}u_{2n-1}v_{2n'}v_{2n'-1}+v_{2n}v_{2n-1}u_{2n'}u_{2n'-1}-\tfrac{1}{2}(u_{2n}v_{2n-1}+v_{2n}u_{2n-1})(u_{2n'}v_{2n'-1}+v_{2n'}u_{2n'-1})]^{s}\right\}, \quad (1)$$

where ψ_m^{LJ} is the Laughlin-Jastrow wave function[1,6]

$$\psi_m^{LJ} = \prod_{\substack{i,k \\ (i<k)}}^{N} (u_i v_k - v_i u_k)^m , \tag{2}$$

and u_k and v_k are the spinor variables, $u_k = \cos(\theta_k/2)e^{i\phi_k/2}$, and $v_k = \sin(\theta_k/2)e^{-i\phi_k/2}$. The symbol **A** denotes the antisymmetrizer and m,t,s are integers satisfying $s \geq 0$, $m - t \geq 1$, and odd, so that ϕ_T is antisymmetric under exchange of electrons belonging to the same pair. The wave function ψ_T is associated with a number of flux quanta $N_\Phi = m(N-1) + s(N/2-1) - t$ and thus corresponds to a filling factor $\nu \equiv N/N_\Phi$ which tends to $\nu = 2/(2m+s)$ as $N \to \infty$. Our MTWF is an eigenstate of the operator $\mathbf{L}^2$ with eigenvalue $L = 0$,[12] so that ψ_T is rotationally invariant and the state therefore has a uniform charge distribution on the sphere. In the disk geometry, our new MTWF takes the form

$$\begin{aligned} \psi_D &= \mathbf{A}\phi_D \\ &= \mathbf{A}\left[\psi_m \prod_{n}^{N/2} (z_{2n} - z_{2n-1})^{-t} \right. \\ &\quad \left. \times \prod_{\substack{n,n' \\ n<n'}}^{N/2} (z_{2n}z_{2n-1} + z_{2n'}z_{2n'-1} - 2Z_nZ_{n'})^s \right], \end{aligned} \tag{3}$$

where

$$\psi_m = \prod_{\substack{i,k \\ (i<k)}}^{N} (z_i - z_k)^m \exp\left(-\sum_k^N \frac{|z_k|^2}{4l_0^2} \right) \tag{4}$$

is the Laughlin-Jastrow trial wave function[1] in the disk geometry. Here, l_0 denotes the magnetic length $l_0 = (\hbar c/eB_0)^{1/2}$ in a magnetic field of strength B_0. The position of electron k is denoted by the complex coordinate $z_k = x_k - iy_k$, and Z_n stands for the center of mass $Z_n = (z_{2n} + z_{2n-1})/2$ of the pair of electrons $(2n, 2n-1)$. Wave function ψ_D differs from the original pair wave function[9] only in the pair-pair "interaction" term [last product in Eq. (3)]. The previous form is obtained if the factor $(z_{2n}z_{2n-1} + z_{2n'}z_{2n'-1} - 2Z_nZ_{n'})$ is replaced by $(Z_n - Z_{n'})^2$. The new forms (1) and (3) were actually found when we attempted to generalize $(Z_n - Z_{n'})^2$ to a form valid for electrons on the surface of a sphere.

For $\nu = 2/(2p+1)$, with even p, we expect the lowest energy is obtained by choosing $m = p$, $s = t = 1$.[3,9,11] (For $\nu = \frac{2}{5}$, we have checked that the alternative choice $m = 1$, $s = 3$, and $t = 0$ leads to higher values for the energy.[13]) Our first studies were carried out in the disk geometry based on the methods outlined in Ref. 11. This involved MC importance sampling with weight $|\phi_D|^2$ (i.e., the not-fully-antisymmetrized part of wave function ψ_D) and led to an unexpected difficulty: It turned out that for $N \gtrsim 12$ electrons, distribution $|\phi_D|^2$ corresponds to a state of broken symmetry in which members of a pair get separated by distances of order of the disk radius and the separation vectors $\mathbf{r}_{2n} - \mathbf{r}_{2n-1}$ are aligned in parallel. Also, this state is characterized by a *non*uniform density $\rho(r)$ with a minimum at the disk center and a monotonic increase toward the edge. Clearly, such a state $|\phi_D|^2$ cannot be used as a basis for systematic calculation of antisymmetrization corrections (cf. Ref. 11). In the spherical geometry, the same state of broken symmetry occurs for $N \gtrsim 46$ electrons. This phase transition can be avoided by use of a different MC sampling weight,[13,14] and we believe the problem is absent in the antisymmetrized wave function. The result for the Coulomb energy $\tilde{E}$ of the nonantisymmetrized state at $\nu = \frac{2}{5}$ is $\tilde{E}/N \approx (-0.4190 \pm 0.0005)e^2/\epsilon l_0$ and antisymmetrization corrections due to two-electron interchanges[11,13] decrease the energy by 2.1% while three- and four-electron exchanges lead to a further reduction by about 0.7%, leading to a value $E/N \approx (-0.4307 \pm 0.0010)e^2/\epsilon l_0$.

Let us now turn to exact numerical computations based on our MTWF ψ_T. For this purpose, we expand ψ_T in terms of Slater determinants $D(l_1, l_2, \ldots, l_N)$ of the basis functions[6] $u_i^{l_i} v_i^{2S-l_i}$, where $0 \leq l_i \leq 2S = N_\Phi$ and, for definiteness, $l_1 > l_2 > \ldots > l_N$. Let us order these determinants according to decreasing values of the "variance" $\Delta = \sum_{i=1}^{N} (S - l_i)^2$. It is easy to verify that the determinant with maximum variance Δ_1 included in ψ_T (for $\nu = \frac{2}{5}$, i.e., $m = 2$, $s = t = 1$) is $D(2S, 2S-1, 2S-5, 2S-6, \ldots, 1, 0)$ where $2S = N_\Phi = 5N/2 - 4$. All remaining determinants included in ψ_T can be generated by iteratively applying operators $L_j^+ L_i^-$ $(i,j = 1,2,\ldots,N$ and $j > i)$ thereby simultaneously raising l_j and lowering l_i by one unit and thus reducing the variance Δ. Because ψ_T is rotationally invariant, the coefficients c_Δ of the expansion $\psi_T = \sum_\Delta c_\Delta D(\Delta)$ satisfy a set of linear equations which is obtained from the condition $L^+ \psi_T \equiv 0$ and which can be solved recursively. It turns out that for systems with up to $N = 12$ electrons these linear equations in fact have a unique solution in terms of c_{Δ_1} (which is defined by normalization of ψ_T) and the coefficients c_Δ can be written as integer multiples of c_{Δ_1}. The uniqueness of the decomposition results from the special property of ψ_T that many determinants such as $D(11,10,9,2,1,0)$, and $D(11,10,8,3,1,0)$, for the case $N = 6$, do not occur in ψ_T. (A similar property is observed in Laughlin's wave function ψ_m^{LJ} at $\nu = 1/m$.) Based on the decomposition of ψ_T we now solve the Schrödinger equation in the $L = 0$ subspace of dimension D using as basis vectors the iterates $H^{p-1}\psi_T = V^{p-1}\psi_T$ $(p = 1,2,\ldots,D)$. (The interaction potential projected onto the lowest Landau level is denoted by V.)

In Table I we list our results for the energy E/N at $\nu = \frac{2}{5}$ for our MTWF ψ_T, the exact GS ψ_C and for the "hard-core" wave function ψ_{HC}, which is the GS when the electron-electron interaction is infinitely short range compared to l_0.[6] For the computation of the Coulomb energy we use the "chord" distance between two electrons. As unit of energy, instead of the conventional $e^2/\epsilon l_0$, we use $e^2/\epsilon l_0'$ where the length unit $l_0' = (N_\Phi \nu/N)^{1/2} l_0$ is chosen such that the areal electron density is $\rho = \nu/2\pi(l_0'^2)$ independent of N.[15] Also listed in Table I are the results for the overlaps $\langle \psi_T | \psi_C \rangle$ and $\langle \psi_{HC} | \psi_C \rangle$ between the exact GS ψ_C and wave functions ψ_T and ψ_{HC}, respectively. In the second column the dimension D of the $L = 0$ subspace is tabulated. Since for $N = 4$ electrons, only one $L = 0$ state exists, our MTWF becomes the exact GS. As can be seen, both the results for the energy and for the overlap show that our MTWF is a close approximation to the ex-

TABLE I. Coulomb energy and overlap of trial wave function ψ_T with exact ground state ψ_C at $\nu=\frac{2}{5}$. Results for the "hard-core" ground state are denoted by ψ_{HC}.

N	D	E/N (ψ_T)	E/N (ψ_C)	E/N (ψ_{HC})	$\langle\psi_T\mid\psi_C\rangle$	$\langle\psi_{HC}\mid\psi_C\rangle$
4	1	−0.426 104	−0.426 104	−0.426 104	1	1
6	3	−0.427 641	−0.428 517	−0.428 502	0.988 40	0.999 84
8	8	−0.428 283	−0.429 543	−0.429 368	0.977 12	0.995 91
10	52	−0.428 939	−0.430 258	−0.429 987	0.971 54	0.990 83
12	418	−0.429 327				
∞		−0.4310	−0.4330	−0.4326		

act GS, with values for the energy E/N which are too high by less than $\frac{1}{2}$%.

On the other hand, the hard-core wave function ψ_{HC} has a remarkably low Coulomb energy, just about 0.1% too high. Indeed, one might call ψ_{HC} the proper generalization to arbitrary filling factors ν of the original Laughlin state ψ_m, with which it coincides at $\nu=1/m$.[16] However, the usefulness of ψ_{HC} at arbitrary ν is more limited since it is no easier to compute than the exact GS ψ_C and, unlike our MTWF ψ_T, ψ_{HC} cannot be used in MC calculations which are of particular interest for the study of larger systems ($N\gtrsim 10$) as well as of excited states which tend to exhibit large finite-size corrections. We also note that the convergence to the exact GS is very rapid as the number of iterates $V^{p-1}\psi_T$ ($p=1,2,\ldots,M$) is increased: Deviations from the exact GS energy are 0.31% ($M=1$, ψ_T, cf. Table I), 155 ppm ($M=2$, ψ_T, and $V\psi_T$), 16 ppm ($M=3$), and 4 ppm ($M=4$).

Our values for the bulk limit of the energy E/N ($N\to\infty$) are obtained by extrapolation in $1/N$. The value $E/N\approx -0.4330$ for the exact GS ψ_C (cf. Table I) is somewhat higher than Su's value[17] $E/N\approx -0.434$ obtained at $\nu=\frac{2}{5}$ for $N=8$ electrons in the plane and subject to periodic boundary conditions. The bulk limit $E/N\approx -0.4310$ obtained for the MTWF ψ_T is consistent with our MC results $E/N\approx -0.4307\pm 0.0010$ discussed above which demonstrates the convergence of the antisymmetrization corrections to the energy. This, in turn, may be interpreted as evidence that the pair structure of the *non*antisymmetrized state ϕ_T has a physical relevance.

Finally, let us discuss the radial distribution function $g(R)$ in the limit of small separation R. Following Yoshioka,[2] let us write $g(R)=\sum_k c_k R^{2k}$. Our values for c_1 in the bulk limit are 0.116, 0.105, and 0.103 for wave functions ψ_T, ψ_C, and ψ_{HC}, respectively.[18] Numbers given are in units of l_0^{-2}. Clearly, c_1 is minimum for the hard-core wave function ψ_{HC}. This actually constitutes a possible definition of ψ_{HC} (for $\nu>\frac{1}{3}$, for $\frac{1}{3}>\nu>\frac{1}{5}$ the conditions are $c_1=c_2\equiv 0$, c_3 minimum).[6] On the other hand, the exact GS ψ_C leads to a remarkably low value for c_1, just 2% larger than the minimum (cf. Ref. 4).

An important property of our MTWF, is that it led us to the natural sequence of $\nu=\frac{2}{5}$ states for which the number of flux quanta $N_\Phi=5N/2-4$. This coincides with the sequence suggested by hierarchical schemes.[6] It turns out that other sequences, where $N_\Phi'=N_\Phi+\text{const}$ all correspond to GS's which, in the language of the hierarchical schemes, have additional defects (quasiparticles or quasiholes).[19] As a consequence, for those "unnatural" sequences, the energy E/N shows marked finite-size effects. By contrast, for our sequences of states the size dependence of E/N is very smooth and basically linear in N^{-1} (cf. Table I and Ref. 15).

Let us now turn to the $\nu=\frac{2}{7}$ state which is obtained by setting $m=3$ and $s=1$. The most obvious choice for t might seem $t=0$.[11] However, for $N=4$ electrons ($N_\Phi=10$) no $L=0$ state exists, which contains ψ_3^{LJ} as a factor and ψ_T vanishes after antisymmetrization.[19] The "natural" sequence of states has in fact a number of flux quanta $N_\Phi=7N/2-2$,[4,6] which is obtained for $t=-2$. This meets all requirements ($m-t\geq 1$ and odd). More generally, states at $\nu=2/(2p+1)$ with p odd are represented by our MTWF setting $m=p$, $s=1$, and $t=-2$. In Table II we list the results obtianed from this MTWF ψ_T for $\nu=\frac{2}{7}$.[20] The total number D of $L=0$ states is listed together with the number D' of those containing ψ_3^{LJ} as a factor. The results for both the energy E/N and the overlap $\langle\psi_T\mid\psi_C\rangle$ demonstrate that our MTWF is a very close approximation to the exact GS. For $N=4$ electrons our MTWF actually coincides with the hard-core GS ψ_{HC} since only one $L=0$ state exists which contains ψ_3^{LJ} as a factor.

TABLE II. Coulomb energy and overlap of trial wave function with exact ground state at $\nu=\frac{2}{7}$.

N	D	D'	E/N (ψ_T)	E/N (ψ_C)	$\langle\psi_T\mid\psi_C\rangle$
4	2	1	−0.386 004	−0.386 012	0.999 939
6	10	2	−0.384 527	−0.384 626	0.997 163
8	80	2	−0.383 671	−0.383 811	0.996 293

The physical interpretation of our MTWF for $\nu=\frac{2}{5}$ is quite natural: Members of a pair of electrons come somewhat closer, thus representing the charge accumulated at the position of a quasiparticle. The interpretation of the $\nu=\frac{2}{7}$ state MTWF is not so clear: We have not yet investigated the properties of the nonantisymmetrized state ϕ_T. In particular, we do not know if the pairs in the presence of the additonal repulsive term $(z_{2n}-z_{2n-1})^2$ maintain their character. If they do and if the antisymmetrization corrections are small, we might conclude that the pairs would be associated with the quasiholes of the hierarchical picture. Otherwise, the precise physical significance of our MTWF at $\nu=\frac{2}{7}$ remains unclear, but in any case it is an excellent MTWF with a very large overlap with the exact GS.

We wish to acknowledge helpful discussions with G. Fano, D. Yoshioka, P. Béran, E. Tosatti, and P. W. Anderson. Two of us (R. M. and N. d'A.) also thank the International Center for Theoretical Physics, Trieste, for its hospitality. Work at Harvard University was supported by National Science Foundation Grant No. DMR85-14638.

---

[1]R. B. Laughlin, Phys. Rev. Lett. **50**, 1395 (1983).

[2]D. Yoshioka, B. I. Halperin, and P. A. Lee, Phys. Rev. Lett. **50**, 1219 (1983); Surf. Sci. **142**, 155 (1984); D. Yoshioka, Phys. Rev. B **29**, 6833 (1984).

[3]F. D. M. Haldane, Phys. Rev. Lett. **55**, 2095 (1985).

[4]F. D. M. Haldane and E. H. Rezayi, Phys. Rev. Lett. **54**, 237 (1985).

[5]G. Fano, F. Ortolani, and E. Colombo (unpublished); and (private communications).

[6]F. D. M. Haldane, Phys. Rev. Lett. **51**, 605 (1983).

[7]B. I. Halperin, Phys. Rev. Lett. **52**, 1583 (1984); **52**, 2390(E) (1984).

[8]R. B. Laughlin, Surf. Sci. **141**, 11 (1984).

[9]B. I. Halperin, Helv. Phys. Acta **56**, 75 (1983).

[10]Results on the basis of hypernetted chain calculations have been obtained by A. H. MacDonald, G. C. Aers, and M. W. C. Dharma-wardana, Phys. Rev. B **31**, 5529 (1985).

[11]R. Morf and B. I. Halperin, Phys. Rev. B **33**, 2221 (1986).

[12]Operator $\mathbf{L}=\sum_k^N \mathbf{L}_k$ is given by $L_k^+=u_k\partial/\partial v_k$, $L_k^-=v_k\partial/\partial u_k$, and $L_k^z=\frac{1}{2}(u_k\partial/\partial u_k - v_k\partial/\partial v_k)$.

[13]R. Morf and B. I. Halperin (unpublished).

[14]The phase transition can be eliminated by performing the MC sampling with weight

$$|\tilde{\Phi}_T|^2=|\Phi_T|^2\prod_n \exp-[(\mathbf{r}_{2n}-\mathbf{r}_{2n-1})^2/R_c^2]=|\Phi_T|^2 G$$

and calculating expectation values, e.g., the energy $\langle E\rangle$ by $\langle\tilde{\Phi}_T|EG^{-1}|\tilde{\Phi}_T\rangle/\langle\tilde{\Phi}_T|G^{-1}|\tilde{\Phi}_T\rangle$. The results are insensitive to the value of the cut-off R_c and the calculation of antisymmetrization corrections becomes well behaved (Ref. 13). We also tested this weighting procedure for the Laughlin state at $\nu=\frac{1}{3}$ and obtained results for the energy independent of R_c (for $R_c\gtrsim 4l_0$).

[15]The strong size dependence of the energy observed in Refs. 4 and 5 is mostly due to the variation of the areal electrons density $\rho=[N/(N-1)]\nu/2\pi l_0^2$. Measuring energies in units $e^2/\epsilon l_0'$ rather than $e^2/\epsilon l_0$, the variation of $E/N(3\leq N\leq 10)$ at $\nu=\frac{1}{3}$ is reduced by two orders of magnitude and for $N\geq 4$ basically linear in N^{-1}. Extrapolated values $(N\rightarrow\infty)$ are $E/N\approx -0.4102$ for the $\nu=\frac{1}{3}$ GS versus, consistent with MC results (Ref. 11), $E/N\approx -0.4099$ for the Laughlin state.

[16]Cf. the discussion of short-ranged potential in Ref. 6 and that of S. A. Trugman and S. Kivelson, Phys. Rev. B **31**, 5280 (1985).

[17]W. P. Su, Phys. Rev. B **32**, 2617 (1985).

[18]The hypernetted chain result of Ref. 9 is $c_1=\frac{1}{8}$.

[19]N. d'Ambrumenil, B. I. Halperin, and R. Morf (unpublished).

[20]The case $m=1$ corresponds to $\nu=\frac{2}{3}$ which is related by particle-hole symmetry to the $\nu=\frac{1}{3}$ state. Our MTWF does not satisfy this symmetry. Its overlap $\langle\psi_T|\psi_C\rangle$ with the exact GS has the values 1, 0.971, 0.954, 0.930, and 0.911 for $N=4$, 6, 8, 10, and 12. Energies are accurate to better than 0.8%.