PHYSICAL REVIEW B VOLUME 39, NUMBER 16 1 JUNE 1989

Equivalence of fractional quantum Hall and resonating-valence-bond states on a square lattice

Z. Zou,* B. Doucot,† and B. S. Shastry‡
Joseph Henry Laboratories, Princeton University, Princeton, New Jersey 08544
(Received 21 October 1988)

We show that a fractional quantum Hall state is equivalent to one particular resonating-valence-bond (RVB) state, the "flux phase" on a square lattice. The fictitious magnetic flux is dynamically generated in the RVB state. The fractional quantum Hall wave function for the flux phase is explicitly shown to be a singlet.

It was proposed by Kalmeyer and Laughlin[1] that the frustrated Heisenberg antiferromagnet in two dimensions, such as a triangular lattice, possessed a liquidlike ground state well characterized by the fractional quantum Hall (FQH) state for bosons at half filling. This establishes the connection between the FQH and resonating-valence-band (RVB) states.[2,3] There is a growing amount of theoretical and experimental evidence that the notion of a ground state similar to the FQH state existing in high-T_c superconductors must be taken seriously.

Kalmeyer and Laughlin considered the quantum antiferromagnetic Heisenberg model (QAFM) on a triangular lattice. The model was first mapped into a hard-core boson lattice gas by the Holstein-Primakoff transfromation. However, the kinetic energy term for the bosons has a wrong sign which makes the boson energy bands disperse down as one moves away from the center of the Brillouin zone. This problem was remedied by introducing a fictitious magnetic field. The magnitude of the fictitious magnetic field corresponds to one flux quantum per spin of the original QAFM or one flux quantum for 1/2 boson. In terms of the Heisenberg model, one is merely performing a unitary transformation in the spin space by an operator $U=2\prod_{n\in L}\sigma_n^z$, where the Laughlin sublattice L may be viewed as a square lattice with twice the lattice constant in each direction. The system is a bosonic analog of the two-dimensional electron gas with short-range interactions in a strong magnetic field. If the ground state is liquidlike, the approximate wave function is well described by the $m=2$ FQH wave function for $N=N_0/2$ bosons (N_0 is the number of the lattice sites):[1]

$$\Psi_{g,s}^B(z_1,\ldots,z_N)=\prod_{\substack{j,k\\ j<k}}(z_j-z_k)^2\exp\left[-\frac{1}{4l_0^2}\sum_{i=1}^{N}|z_i|^2\right] , \quad (1)$$

where $z_i=x_i+iy_i$ is the complex lattice coordinate of the ith particle and l_0 is the magnetic length given by $4\pi l_0^2=\sqrt{3}a^2$, a being the lattice constant. In this paper, we shall show that the FQH wave function may also be a useful variational wave function for the QAFM on a square lattice. In fact, a similar wave function has been proposed by Mele[4] in a continuum representation.

A fiercely debated question is whether or not each individual Cu-O layer in high T_c materials is antiferromagnetically ordered at $T=0$. Some numerical simulations[5] appear to indicate ordering at $T=0$, but disordered RVB-type states seem energetically competitive. We take it as self-evident that an RVB-like state with no Néel order is an interesting and crucial starting point in the consideration of the Hubbard model with holes and relatively large U. Nevertheless, one expects that the intrinsic connection between the FQH fluid and the RVB spin liquid may exist on a square lattice. In the present instance the fictitious magnetic flux is spontaneously generated due to dynamical effect of the RVB. This is best seen in the so-called "flux phase" of Affleck and Marston[6] or the "$s+id$" phase of Kotliar.[7] The flux phase is obtained by performing a mean-field theory of the QAFM,[6]

$$H=-J\sum_{\langle i,j\rangle}\chi_{ij}^{\dagger}\chi_{ij}+\text{const} , \quad (2)$$

with $\chi_{ij}^{\dagger}=\sum_\sigma c_{i\sigma}^{\dagger}c_{j\sigma}$. This Hamiltonian, written in terms of electron operators, is subject to the constraint of one particle per site, $\sum_\sigma c_{i\sigma}^{\dagger}c_{i\sigma}=1$. There is a hidden local SU(2) symmetry[8] in this Hamiltonian which plays an important role in the RVB. Here we are merely interested in the U(1) part of the SU(2) group,[9] namely the invariance of the Hamiltonian under the local gauge transformation $c_{i\sigma}\rightarrow e^{i\theta_i}c_{i\sigma}$. The simplest mean-field theory corresponds to taking the mean value of the "order parameter" $\chi_x=\langle\chi_{i,i+\tau_x}\rangle$ and $\chi_y=\langle\chi_{i,i+\tau_y}\rangle$. The relative phase between χ_x and χ_y is of most importance. The choice of $\chi_x=\chi_y$ leads to the extended s-wave state as done in Ref. 9.[10] Another choice, $\chi_x=i\chi_y$, gives rise to the flux phase as done in Refs. 5 and 6. The flux phase is energetically favorable from both mean-field and numerical calculations.[11] The excitation spectrum of the flux phase has a gap everywhere except at four isolated Fermi points:

$$E_k=\pm J\chi_0(\cos^2k_x+\cos^2/k_y)^{1/2} . \quad (3)$$

This single-particle excitation spectrum is not gauge invariant and because of that constraint only particle-hole excitations, which are gauge invariant, are permitted.

Although the order parameter χ_{ij} per se is not gauge invariant, the phase of the elementary plaquette variable

$$P(i,j,k,l)=\langle \chi_{ij}\chi_{jk}\chi_{kl}\chi_{li}\rangle \quad (4)$$

is gauge invariant and observable. The local U(1) gauge invariance can be represented manifestly by a vector potential living on the link joining two neighboring sites,

$$\chi_{ij}=|\chi_{ij}|\exp\left[\frac{2\pi i}{\phi_0}\int_i^j d\mathbf{s}\cdot\mathbf{A}(s)\right], \quad (5)$$

where $\phi_0=hc/e^*$ is the quantum of flux and e^* is the fictitious charge. The elementary plaquette variable $P(i,j,k,l)$ has a negative sign in the flux phase corresponding to flux π through the plaquette due to the vector potential $\mathbf{A}$, and $P(i,j,k,l)$ has a positive sign in the extended s-wave phase. Since both the mean-field theory and numerical calculations indicate that the flux phase is energetically stable, we conclude that half a flux quantum per plaquette is spontaneously generated in the flux phase. Thus, our effective Hamiltonian can be written as

$$H_{\text{eff}}=-J\sum_{\langle ij\rangle}\chi_{ij}(c_{i\uparrow}^\dagger c_{j\uparrow}+c_{i\downarrow}^\dagger c_{j\downarrow})+H_{\text{int}}, \quad (6)$$

where χ_{ij} is given by (5) and H_{int} is the residual interaction term. The constraint is, of course, to be implemented. This effective Hamiltonian without H_{int} describes a tight-binding model for two species of particles (up and down spin) with a strong uniform "magnetic" field corresponding to one-half flux quantum per square. The complete spectrum of this model with "rational field" was obtained by Hofstadter.[12] In particular, for our case, the ratio of flux through a lattice cell to one flux quantum, $\alpha=\frac{1}{2}$, there are two subbands whose dispersions are given precisely by those of our flux phase [Eq. (3)]. If one uses the periodic boundary conditions, a complete set of single-particle wave functions can be obtained, from which one may construct a many-body trial wave function. However, the eigenstates of the model with the periodic boundary condition involve the ϑ functions and it is rather difficult to construct a relatively simple Jastrow wave function.[13] While work on this problem is in progress, we shall, for the time being, appeal to the FQH wave function approach. The reason for adopting the FQH wave function approach is the physical precedent of its success in describing the FQH effect, as emphasized by Kalmeyer and Laughlin.[1] We believe that this approximation is valid and it gives qualitatively correct physical results. The philosophy of what we are doing here is the same as that of Laughlin.[14]

Thus, if the two species of particles were independent of each other (without the constraint), the ground-state (GS) wave function of such a system would be approximated by a product of two $m=1$ FQH wave functions for N fermions,[15]

$$\Psi(z_{1\uparrow},\ldots,z_{N\uparrow};z_{1\downarrow},\ldots,z_{N\downarrow})=\Psi_\uparrow\Psi_\downarrow=\prod_{\substack{i,j\\ i<j}}(z_i-z_j)_\uparrow\exp\left[\frac{-1}{4l_0^2}\sum_{i=1}^N|z_{i\uparrow}|^2\right]\prod_{\substack{k,l\\ k<1}}(z_k-z_l)_\downarrow\exp\left[\frac{-1}{4l_0^2}\sum_{i=1}^N|z_{i\downarrow}|^2\right], \quad (7)$$

where l_0 is the magnetic length on the square lattice given by $\pi l_0^2=a^2$. The constraint, however, introduces strong correlations between up-spin and down-spin particles. A straightforward way to impose the local constraint is by the Gutzwiller projection P_G which prohibits two particles with opposite spin from occupying the same site:

$$\Psi_{\text{GS}}=P_G\Psi=\prod_i(1-n_{i\uparrow}n_{i\downarrow})\Psi .$$

In order to carry out the Gutzwiller projection explicitly, we adopt the procedure of Shastry,[16] which corresponds to a transformation of the repulsive Gutzwiller projector between up-spin electrons and down-spins electrons into an attractive projector between up-spin electrons and down-spin holes. Specifically, we make a unitary transformation U, followed by another transformation P,

$$U=\prod_{n=1}^{N_0}(c_{n\downarrow}^\dagger+c_{n\downarrow}) . \quad (8)$$

The effect of U on down-spin electrons is

$$Uc_{n\downarrow}U^\dagger=c_{n\downarrow}^\dagger ,$$
$$Uc_{n\downarrow}^\dagger U^\dagger=c_{n\downarrow} . \quad (9)$$

This is just a particle-hole transformation for down-spin electrons only. The effect of P on down-spin particles is

$$Pc_{n\downarrow}P^{-1}=(-1)^P c_{n\downarrow} \text{ and } Pc_{n\downarrow}^\dagger P^{-1}=(-1)^P c_{n\downarrow}^\dagger ,$$

where $(-1)^P=1$ if n is on the even sublattice and -1 if n is on the odd sublattice. After the transformations, the local constraint becomes

$$c_{n\uparrow}^\dagger c_{n\uparrow}=c_{n\downarrow}^\dagger c_{n\downarrow} , \quad (10)$$

which is equivalent to say that wherever there is an up-spin electron, there is also a down-spin hole. We recognize that the particle-hole transformation U is reminiscent of the SU(2) gauge symmetry.[8] Because the particle-hole transformation changes the sign of $c_{i\downarrow}^\dagger c_{j\downarrow}$ term in (6), the transformation P provides a Marshall[17] factor to restore the invariance of the effective Hamiltonian (6). Thus the effect of the Gutzwiller projection is simply to set $z_{n\uparrow}^p=z_{n\downarrow}^h$ in the product wave function (7), where $z_{n\uparrow}^p$ and $z_{n\downarrow}^h$ are coordinates of up-spin particle and down-spin hole, respectively. Therefore our variational wave function can be written as

$$\Psi_{g,s}(z_{1\uparrow},\ldots,z_{N\uparrow};z_{1\downarrow},\ldots,z_{N\downarrow})$$
$$=(-1)^\delta\prod_{\substack{i,j\\ i<j}}(z_i-z_j)^2\exp\left[\frac{-1}{2l_0^2}\sum_{k=1}^N|z_k|^2\right], \quad (11)$$

where $(z_i-z_j)^2$ should be understood as

$$\prod_{\substack{i,j\\ i<j}}(z_i-z_j)^2=\prod_{\substack{i,j\\ i<j}}(z^p_{i\uparrow}-z^p_{j\uparrow})(z^h_{i\downarrow}-z^h_{j\downarrow})\delta(z^p_i,z^h_i) , \quad (12)$$

and $\delta(z^p_i,z^h_i)=1$ if $z^p_i=z^h_i$, and equal to zero otherwise. In Eq. (11) we have introduced an additional phase factor in front of the wave function, ($z_j=n_j+im_j$, measured in the magnetic length)

$$(-1)^\delta=\exp\left[i\pi\sum_j^N n_j+m_j+n_jm_j\right] , \quad (13)$$

which is required for the wave function to be a spin singlet, which we shall explicitly prove shortly. We note some important features of the wave function (11) in the following.

(1) The wave function (11) is obviously symmetric in the orbital coordinates, in fact it cannot be symmetrized further. Thus it must be a spin singlet with total spin **S**=0, for it must be maximally antisymmetric in spin variables. This can be explicitly shown as follows: In the spin representation, the wave function reads

$$\Psi\{\sigma_i\}=\sum_{z_1,z_2,\ldots,z_N}\Psi_{\rm GS}\{z_i\}S^-_{z1}S^-_{z2}\cdots S^-_{zN}|\uparrow\cdots\uparrow\rangle \quad (14)$$

where $S^-_{z_i}=c^\dagger_{n\uparrow}c^\dagger_{n\downarrow}$, etc., are the Anderson pseudospin[18] lower operations which are isomorphic to the Pauli spin operators, and $|\uparrow\cdots\uparrow\rangle$ is a ferromagnetic state. Since we have no net magnetization, i.e., $S^z_{\rm tot}\equiv\sum_n S^z_n=0$, it suffices to show that

$$S^+_{\rm tot}|\Psi\{\sigma_i\}\rangle\equiv\sum_n S^+_n|\Psi\{\sigma_i\}\rangle=0 .$$

Here $S^+_{\rm tot}$ is the total spin raising operator. Applying $S^+_{\rm tot}$ on the wave function (14) and after some straightforward manipulations using the commutation relations of the spin operators, we find it sufficient to show

$$\sum_{z_i}\Psi_{\rm GS}(z_1,\ldots,z_i,\ldots,z_N)=0 , \quad (15)$$

where the sum over z_i runs over the *entire* lattice. To establish this last identity, we appeal to an identity derived from a general formula for the ϑ functions,[19]

$$\sum_n\sum_m(-1)^{n+m+nm}\exp\{-\pi[\tfrac{1}{2}(\xi-n)^2+\tfrac{1}{2}(\eta-m)^2+i\xi m-i\eta n]\}=0 , \quad (16)$$

where ξ and η are arbitrary real variables. By taking the derivative with respect to ξ or η successively at $\xi=0$ and $\eta=0$, it follows that, for any non-negative integer k,

$$\sum_{(n,m)\in\text{lattice}}(-1)^{n+m+nm}z_j^k\exp(-\tfrac{1}{2}|z_j|^2)=0 . \quad (17)$$

Equation (15) follows immediately from Eq. (11) and Eq. (17) by expansion in powers of z_j. This proof requires that the summmations in (15) be extended to infinity and hence the wave function (11) is manifestly a singlet in the thermodynamical limit. For a finite-size system with N_0 sites, we cannot conclude that the total spin is strictly zero. It seems plausible to us that the expectation value of $S^2_{\rm tot}$ in such a finite system is of order unity rather than of order N_0, but we have no conclusive proof as yet.

The proof given above is identical to that for the Kalmeyer-Laughlin (KL) state on a triangular lattice,[20] since the KL wave function is identical to the present one if one views the triangular lattice as the square lattice with all diagonal bonds in one direction. Hence, we have explicitly demonstrated that their wave function is a singlet as well.

(2) The energy *per bond* of our wave function is actually equal to that of the KL wave function on the triangular lattice. This is true because one can regard the triangular lattice as the square lattice with all diagonal bonds in one direction. The value of $\langle\mathbf{S}_n\cdot\mathbf{S}_{n+1}\rangle$ obtained by KL is 0.32. We therefore conclude that the energy per bond of our wave function is 0.16, which is too high compared to that of the best estimate of Liang, Doucot, and Anderson.[5] The energy can probably be improved upon using the Hofstadter states, rather than using the Landau-level states.[13] We wish to emphasize that the wave function constructed here is not the ground state of the nearest-neighbor Heisenberg model. But one can imagine modifying the Hamiltonian in such a way that our wave function becomes its exact ground state. Hopefully, the modified Hamiltonian and the original one belong to the same universality class and hence they have similar correlation properties. In essence, what we have written down here is an explicit RVB wave function which behaves like a FQH state and is manifestly a spin singlet.

(3) Our wave function on the square lattice looks similar to the Kalmeyer-Laughlin state (1). As a matter of fact, one can also obtain the state (1) from our fermion-based mean-field state by Gutzwiller projection, instead of using the hard-core boson representation. The essential physics for both wave functions on the square lattice and triangular lattice is the same, namely they are both Gutzwiller projected Slater determinant. The projection plays an essential role. The mechanism for the spin-liquid state is independent of lattice type.

Some subtlety remains here. The magnetic flux needed for our construction of the FQH wave function arises from dynamical effect, and they are in effect generated spontaneously in the variational treatment. It is not obvious that the wave function (11) is real, and the translation symmetry by one lattice spacing is spontaneously broken in the spin-liquid state, namely the size of the unit cell is doubled.

Since we have one-half flux quantum per square, it is possible to construct a "magnetic" superlattice with basis vectors $\mathbf{b}_1=2\mathbf{a}_1$ and $\mathbf{b}_2=\mathbf{a}_2$ such that the "magnetic" flux through the unit cell built in $\mathbf{b}_1$ and $\mathbf{b}_2$ is exactly one flux quantum. It is well known that the "magnetic" translation operators defined by

$$T(\mathbf{b}_j)=\exp\left[\frac{i}{\hbar}(\mathbf{p}+\frac{e^*}{c}\mathbf{A})\cdot\mathbf{b}_j\right],\ \ j=1,2 , \quad (18)$$

satisfy the "non-Abelian" relation

$$T^n(\mathbf{b}_1)T^m(\mathbf{b}_2)=(-1)^{nm}T(n\mathbf{b}_1+m\mathbf{b}_2) . \quad (19)$$

The phase factor $(-1)^{nm}$ that appears here ensures the correct group multiplication, which is obviously related to the phase factor in our wave function. The exact physical interpretation of this phase factor is not yet clear to us at the moment.

In conclusion, we have shown that the KL quantum Hall wave-function approach can be extended to the square lattice, and we have constructed a wave function for the flux RVB state on the square lattice. Furthermore, the remarkable phase of the wave function explicitly constructed here (intuited by Laughlin) is shown in this work to be precisely that which makes the FQH wave function a spin singlet and hence acceptable as an RVB wave function.

ACKNOWLEDGMENTS

We thank Phil Anderson for many stimulating discussions and for encouragement throughout the work. We also benefited from discussions with G. Baskaran, T. Hsu, R. Laughlin, S. Liang, and J. Wheatley. Conversations with M. Kvale and B. J. Marston were also very helpful. This work was supported in part by the National Science Foundation (NSF) Grant No. DMR-8518163.

---

*Present address: Department of Physics, Stanford University, Stanford, CA 94305.

†Present address: CRTBT-CNRS,BP 166X, 38042 Grenoble Cedex, France.

‡On leave from Tata Institute of Fundamental Research, Bombay.

[1]V. Kalmeyer and R. B. Laughlin, Phys. Rev. Lett. **59**, 2095 (1987).

[2]P. W. Anderson, Mater. Res. Bull. **8**, 153 (1973); Science **235**, 1196 (1987).

[3]S. Kivelson, D. S. Rokhsar, and J. P. Sethna, Phys. Rev. B **35**, 8865 (1987); P. W. Anderson, G. Baskaran, Z. Zou, and T. Hsu, Phys. Rev. Lett. **58**, 2790 (1987).

[4]E. Mele, (unpublished).

[5]S. Liang, B. Doucot, and P. W. Anderson, Phys. Rev. Lett. **61**, 365 (1988); I. D. Reger and A. P. Young, Phys. Rev. B **37**, 5493 (1988); **37**, 5978 (1988); M. K. Gross, E. S. Velasco, and E. Siggia (unpublished).

[6]I. Affleck and B. J. Marston, Phys. Rev. B **37**, 3774 (1988).

[7]G. Kotliar, Phys. Rev. B **37**, 3664 (1988).

[8]I. Affleck, Z. Zou, T. Hsu, and P. W. Anderson, Phys. Rev. B **38**, 745 (1988).

[9]G. Baskaran and P. W. Anderson, Phys. Rev. B **37**, 580 (1988).

[10]G. Baskaran, A. Zou, and P. W. Anderson, Solid State Commun. **63**, 973 (1987); A. Ruckenstein, P. Hirschfeld, and J. Appel, Phys. Rev. B **36**, 857 (1988).

[11]F. C. Zhang, C. Gros, T. M. Rice, and H. Shiba, Supercond. Sci. Technol. **1**, 36 (1988).

[12]D. R. Hofstadter, Phys. Rev. B **14**, 2239 (1976).

[13]Anderson and Shastry have recently succeeded in constructing a singlet many-body wave function on the basis of the eigenstates of the Hofstadter model, though the wave function is not in a Jastrow form.

[14]R. Laughlin, Phys. Rev. Lett. **60**, 2677 (1988); (private communication).

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

[16]B. S. Shastry, Phys. Rev. Lett. **60**, 639 (1988).

[17]W. Marshall, Proc. R. Soc. London, Ser. A **232**, 48 (1958).

[18]P. W. Anderson, Phys. Rev. **112**, 1900 (1958).

[19]A. M. Perelomov, Theor. Math. Phys. (USSR) **6**, 156 (1971); M. Boon and J. Zak, J. Math. Phys (N.Y.) **22**(5), 1096 (1981); D. J. Thouless, J. Phys. C **17**, L325 (1984).

[20]Formally the proof can be carried out similarly, with the identity (16) replaced by a general sum rule on a Von Neumann lattice given in Ref. (17).