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Commensurate-flux-phase state of the $t$-$J$ model

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We propose a variational approach for the study of chiral flux-phase states. We present a class of variational wave functions of the generalized Laughlin-type. The generalization consists of the introduction of Gutzwiller projections and of a fictitious magnetic field. We classify antiferromagnetic chiral flux-phase states and evaluate analytically the corresponding expectation values of the $t$-$J$ Hamiltonian at any value of filling. There are two types of chiral flux-phase states: commensurate and fractional. We have found that the minimal energy has a commensurate-flux-phase state for which the value of the flux of the orbital magnetic field equals the filling.

An understanding of the mechanism of high-temperature superconductivity may perhaps come from improved studies of the ground-state properties of the $t$-$J$ model\cite{1} and of its excitations. The ground state of this model may be generated by fermions which condense on a two-dimensional lattice and carry spontaneous orbital currents.\cite{2,3} In Refs. 4 and 5, the Kalmeyer-Laughlin state\cite{5} has been generalized to include the case of the square lattice. It has been also shown that fractional quantum Hall state is equivalent to the resonating-valence-bond (RVB) state.\cite{6} This picture may be suitably described by introducing the so-called flux-phase states which break the discrete translational symmetry and parity of the lattice.\cite{7,8,9} In order to describe flux-phase states, in Ref. 10 an explicit singlet wave function has been proposed, which is a Gutzwiller projection of the Slater determinant of the noninteracting wave function, describing fermions in a uniform magnetic flux (the so-called commensurate flux phase (CFP)). Some additional interesting ideas about the construction of the wave function describing flux-phase states in a Hubbard Hamiltonian with large $U$ have been presented in Ref. 5, where the Gutzwiller projection is carried out on appropriate Jastrow functions, rather than on determinants as in Ref. 10.

In Ref. 11 it has been shown within a renormalized mean-field theory\cite{12} that the exchange energy is minimized in CFP states, when the fictitious flux exactly equals the filling. As we will show below in the framework of our approach, this result can be reproduced by direct variational estimation of the expectation value of the exchange energy. In Ref. 13 a CFP state on a finite 4X4 cluster with two holes has been investigated and a qualitative agreement with renormalized mean-field theory was obtained. In particular, the magnetic energy exhibits an absolute minimum when the flux exactly equals the filling. However, these results are not completely consistent with the ones obtained in Ref. 14 by means of Monte Carlo calculations. In Ref. 14 it has been shown that the flux phase has lower energies than the energy in the usual Gutzwiller wave function for certain ranges of electron density near half filling and coupling $J/t \sim 1$.

Our analysis is based on the assumption that the ground-state correlations and excitations of the model are due to the presence of a spontaneous gauge field which connects our approach with Laughlin’s treatment of the fractional quantum Hall effect\cite{15} and Kalmeyer-Laughlin state at half filling.\cite{2,3,5} Following Ref. 5, we choose a many-body wave function as a Gutzwiller projection of the generalized Laughlin function matched, for simplicity, to a two-dimensional square $L \times L$ lattice. Following Ref. 16, we impose periodic boundary conditions on the phase of a one-body density matrix, and by this way we obtain the flux quantization that gives us a classification of chiral flux-phase states. The flux per plaquette, consisting of the flux of the orbital and of the fictitious magnetic fields, is quantized and may carry either integer multiples of an elementary quantum $\Phi_\varepsilon$, i.e., a flux $\Phi_n = n\Phi_\varepsilon$, with $n = 0, 1, 2, \ldots$, or fractional portions of size $\Phi_n = \{ n/L \} \Phi_\varepsilon$ or $\{ n/(L+2) \} \Phi_\varepsilon$, with $n = 1, 2, \ldots$, except such $n$ for which the ratios $n/L,n/(L+2)$ become integers. We call the states with fractional quantum numbers as fractional chiral flux states. These states, indeed, break the lattice symmetries, parity $P$, translation $T$, charge conjugation $C$, and the composite symmetries except the CPT symmetry, which is still conserved. The existence of such states in antiferromagnets have been predicted in Ref. 9.

We concentrate on the study of the standard two-dimensional $t$-$J$ model

$$H = -t \sum_{\langle i,j \rangle \sigma} a_{i\sigma}^\dagger a_{j\sigma} + J \sum_{\langle i,j \rangle} S_i S_j , \quad (1)$$

with the electron hopping-integral $t$, and Heisenberg constant $J$. This strength factor measures the exchange interaction between electrons on neighboring lattice sites. The Gutzwiller projected operator

$$a_{i\sigma}^\dagger = c_{i\sigma}^\dagger (1 - n_i - \sigma) , \quad (2)$$

where $c_{i\sigma}^\dagger (c_{i\sigma})$ creates (destroys) a fermion with spin projection $\sigma = + \text{ or } -$ at a lattice site $i, n_{i\sigma}$ is the occupation number operator $a_{i\sigma}^\dagger a_{i\sigma}$, and the operator $S_i$ is the
spin operator. The summations in Eq. (1) extend over the lattice sites \(i\) and \(j\) of the \(i-J\) model. The operator \(P_G(i)\) is the usual Gutzwiller projector: 
\[ P_G(i) = 1 - n_i^+ n_i^- \]
wer the associated next-nearest sites \(j\).

The microscopic treatment of the fractional quantum Hall effect by Laughlin provides a fruitful prescription for tailoring a set of correlated wave functions which may approximately describe the ground state and excited states of the \(i-J\) Model (1). We assume the occurrence of a spontaneous gauge field which generates the correlations presented in the state of the \(i-J\) Model, and which accounts for the orbital currents on the lattice. Exploiting this concept, we are led to the ansatz,

\[
\Psi_{\text{mq}}(z_1^+, z_2^+; \ldots, z_N^+; z_1^-, z_2^-, \ldots, z_N^-) = N_{\text{mq}} \prod_{i<j}^{N} (z_i^+ - z_j^+) \prod_{i<j}^{N} (z_i^- - z_j^-)^m P_G(i) \Psi(z_1^+) \Psi(z_2^-),
\]

for an approximate representation of the ground state and excited states of the \(i-J\) model. The functions \(\Psi_{\text{mq}}\) depend on the coordinates \(z_j = x_j + iy_j\) of lattice site \(j\) and specify the location of a fermion with a given spin projection. The operator \(P_G(i)\) is the usual Gutzwiller projector:

\[ P_G(i) = 1 - n_i^+ n_i^- \]

The function \(\Psi(z)\) is the single-particle wave function:

\[
\Psi(z) = \exp \left( -\frac{|z|^2}{4l_0^2} - \frac{\phi_B}{2i} - \frac{\phi_B}{4} \right),
\]

wherein \(l_0\) characterizes the effect of a spontaneous magnetic field inducing orbital currents on the lattice. The additional \(\phi_B/4\) is associated with a fictitious magnetic field \(B\) given by \(\phi_B = 2\int A ds\), where the gauge \(A = (y, x, 0)\) \(B\) is used. Expression (2) generalizes the familiar Laughlin form of the wave function. The factor \(N_{\text{mq}}\) normalizes the function (2) to unity. For ensuring the complete antisymmetry of ansatz (3), the exponents \(l\) and \(m\) must be odd integers, and the parameters \(q, l_0, B\) are trial parameters. The Hamiltonian (1) may describe the dynamics of \(N_+\) electrons with spin projection \(\sigma = +\) and \(N_-\) electrons with \(\sigma = -\). For simplicity, we limit ourselves to a study of the important case where \(N_- = N_+ \approx N\).

Using different values for \(l\) and \(m\), one can describe the total hierarchy of anion states proposed in Refs. 17–19. For simplicity, we choose \(l = m = 1\) and \(q = 0\). At first, let us put \(B = 0\). For our choice, the expectation value of the Hamiltonian (1) is estimated analytically and is equal to

\[
E = -t \left( \frac{r}{2(1-r/2)} \right) \sum_{\langle i,j \rangle} n_\sigma(i,j) + J \left( \frac{r^2}{16(1-r/2)^2} \right) \sum_{\langle i,j \rangle} \left[ g_+(i,j) + g_-(i,j) \right]
\]

\[
-4n_+(i,j)n_-(j,i)-2 \right),
\]

where \(r\) is the filling \(\rho = 2N/L^2\), which gives the number

\[
F(x) = \begin{cases} 
L & \text{for } x = n\pi, \quad n = 0, 1, 2, \ldots \\
0 & \text{for } x = \left[ \frac{n}{L} + k \right] \pi, \quad n = 0, 1, 2, \ldots, L-1; k = 1, 2, \ldots \\
-(1 + \cos 2x) & \text{for } x_n \text{ otherwise.}
\end{cases}
\]

of fermions per lattice site. Equation (4) involves the one-body density-matrix \(n_\sigma(i,j)\) and the two-body density-matrix elements \(g_\sigma(i,j)\). The matrix elements are defined by the conventional multidimensional integrals over the probability distribution associated with the chosen many-body wave function. In the thermodynamic limit \(N \to \infty\), density \(\rho \) kept constant they are suitably normalized by \(n_\sigma(i,i) = 1\) and \(g_\sigma(i,j) \to 1\) as \(|z_i - z_j| \to \infty\) and have a form:

\[
n_\sigma(i,j) = \exp \left( \frac{1}{4l_0^2} (2z_i z_j^* - |z_i|^2 - |z_j|^2) \right),
\]

\[
g_\sigma(z_i, z_j) = 1 - \exp \left( -\frac{1}{2l_0^2} |z_i - z_j|^2 \right).
\]

Inserting Eqs. (5) and (6) into Eq. (4), and performing the lattice summations, we arrive at the energy expression

\[
E(x) = -4t \frac{\rho(1-\rho)}{2(1-\rho/2)} LF(x) - J \frac{3\rho^2}{2(1-\rho/2)^2} L^2 \exp(-2x).
\]

For convenience, the magnetic length \(l_0\) of the spontaneous gauge field is measured by the dimensionless quantity \(x = a^2/4l_0^2\) where the length \(a\) is the lattice constant of the square \(L \times L\) lattice. The function \(F(x)\) is defined by

\[
F(x) = \exp(-x) \sum_{l=1}^{L} \cos(2lx).
\]

It was Yang who first recognized that the imposition of periodic boundary conditions on a one-body density matrix appropriately matched to the square lattice, requires a quantization of flux. In our case, the flux corresponds to the field parameter \(x\). As the result we have:

\[
x_n = n\pi \quad \text{and} \quad x_n = n\pi \quad \text{for} \quad x_n = \frac{n}{L} + 2, \ldots
\]

with \(n = 0, 1, 2, \ldots\). For the discrete quanta (9), function (8) is split into three lines:
The explicit form of flux quantization depends, of course, on the actual choice of lattice symmetry. However, replacing the square lattice by a triangular one, for example, does not affect the classification of the energies and states into those with integer or fractional quantum numbers [see formula (10)]. For the square lattice adopted here, the energies of the first branch of $x$ [see first line in (10)] are negative and increase with increasing integer quantum number $n$. As $n \to \infty$, the energy vanishes. The second branch of $x$ [see second line in (10)] describes the energies of states which correspond to fractional quantum number.

The nature of the constructed quantum states may be further elucidated by following Affleck and Marston. To do this, we evaluate the expectation values of the valence-bond operator $\chi_{ij} = a_{i+} a_{j-}$ with respect to wave functions of type (4), specialized to $I = m = 1$ and $q = 0$. These expectation values are just given by the one-body density matrix (5) which we may decompose according to

$$
\langle \Psi | \chi_{ij} | \Psi \rangle = n (x_i, y_i) = R_{ij} e^{i \theta_{ij}} .
$$

The phase $\theta_{ij}$ has the simple form

$$
\theta_{ij} = \frac{1}{2l_0^2} (x_i y_j - x_j y_i) .
$$

Calculating the sum of these phases by going counter clockwise around an elementary plaquette of length $a$ of a square lattice, we find the flux $\Phi = a^2/l_0^2 = 4\pi$ for the enclosed spontaneous magnetic field. According to result (9), this flux is quantized into portions

$$
\Phi_n = \begin{cases} 
    n \Phi, & n = 0, 1, 2, \ldots \\
    \frac{n}{L+k} \Phi, & n = 0, 1, 2, \ldots, L-1 \\
    \frac{n}{L+2+k} \Phi, & n = 0, 1, 2, \ldots, L+1 ,
\end{cases}
$$

with integer $k$ and the elementary quantum $\Phi_e = 4\pi$. Consequently, we may define the ground state of the Hamiltonian (1) as a state of zero flux $\Phi_0 = 0$, or, equivalently, as a state with $l_0 \to \infty$. It means that the electrons are located outside the lattice. On the other hand, there is a Laughlin condition that the electrons should be located inside the lattice (see, for example, Refs. 15 and 2),

$$
4k N l_0^2 \leq L^2 a^2 ,
$$

where $k$ is the factor of the commensurability of electrons to the lattice. The value of $k$ depends on the symmetry of the lattice. Laughlin used the following value $k = \pi/2$ (Refs. 15 and 2). Whence in the limit of homogeneous distribution of electrons on the square $L \times L$ lattice, we obtain that

$$
2k \rho = \frac{a^2}{l_0^2} .
$$

This condition contradicts Eq. (10) from which it follows that the ground state corresponds to $a^2/l_0^2 = 0$. This contradiction can be removed by introducing the fictitious magnetic field $B$ into the system; we should consider the different values of $B$ in (2). This field adds to the one-body density matrix an additional phase

$$
\Phi_{ij} = 2\pi / \Phi_0 \int A_{ds} ;
$$

thus, instead of (9) we have here the same quantization of the total flux which is the sum of the orbital flux $a^2/l_0^2$ and the flux of the fictitious magnetic field $2\pi \Phi_B = 2\pi a^2 B$. Then for the orbital flux the relation (15) is true. The introduction of the fictitious magnetic field $B$ as a trial parameter gives the minimal energy which corresponds to the marginal extremum of the expectation value function $E(x)$. For the ground state we obtain the following formula:

$$
E_g = 4\pi \frac{\rho (1-\rho)}{1-\rho/2} L^2 \exp(-\rho k/2)
$$

$$
- \frac{\rho^2}{1-\rho/2} L^2 \exp(-\rho k) .
$$

Are their spins polarized or unpolarized? The question may be answered by evaluating the expectation values of the total spin components $M_x$ and $M_y$ parallel to the lattice plane and orthogonal to it, $M_z$. The component $M_x$, for example, is calculated by taking the sum

$$
M_x = \sum_{i\sigma} \langle \Psi | S_{i\sigma}^x | \Psi \rangle = \sum_i \langle \Psi | (a_{i+}^+ a_{i-} + a_{i-}^+ a_{i+}) | \Psi \rangle .
$$

The expectation value is given by the sum of diagonal elements of the one-body density matrix (5) which yields $M_x = M_y = M_z = 0$. Since the complete spin and its projection are equal to zero, we conclude that the fermions form an antiferromagnetic phase.

At the half filling, ($\rho = 1$), we have for the Heisenberg Hamiltonian the ground-state energy which is higher than Néel's state energy:

$$
E_g = -4 JL^2 \exp(-\pi/2) .
$$

Here $\langle S_i S_{i+1} \rangle = -0.313$, but for Néel's state $\langle S_i S_{i+1} \rangle = -0.333[14]$. At any value of the filling $\rho$, one can calculate the spin-spin correlator:

$$
\langle S_i S_{i+n} \rangle = -\frac{3\rho^2}{8(1-\rho/2)^2} \exp(-\rho kn^2) .
$$

Thus our flux-phase state is a spin-spin short-range correlated state. On the other hand due to the periodical behavior of the flux phase of the one-body density matrix for the states constructed here, there is an off-diagonal long-range order, i.e., there is the strong long-range correlation in the flux phase. This state has not a minimal energy at half filling, but nevertheless it can play a role at the hole doping when $\rho < 1$. The other states associated with the first line of $x$ in (10) are generated by an orbital magnetic field with magnetic length $l_0 = a / 2\sqrt{\pi} n$ and are specified by flux quanta with integer quantum numbers, $\Phi_n = n \Phi_e$. For each of these states the introduction of the fictitious magnetic field gives the same ground-state energy as the state with $n = 0[16]$. The states with noninteger quantum numbers, identified also as fractional-flux-phase states, are characterized by an en-
ergy $E_{fr}$ higher than the ground-state energy (16),

$$E_{fr} = -\frac{J - \rho^2}{(1 - \rho/2)^2} L^2 \exp(-\rho k). \quad (20)$$

It is interesting to note that at half filling, $\rho = 1$, the energy of the fractional-flux-phase states coincides with (16).

The states, described in the present work, generate spontaneous currents and diamagnetic moments which, effectively, screen the electron-electron spin correlations. The magnetic length of the associated magnetic field plays the role of a Debye radius $l_D^2 \sim 1/\rho$. The excitations of the states obtained here will have this special "plasma" character, that is, they will have a gap which is proportional to the filling $\rho$ and long-range "special Langmuir wave condensate." It would be very interesting to determine the connection between this "magnetoplasmon" and spinons and holons.

The fractional-flux-phase states presented here break the discrete symmetries such as the parity $P$, translation $T$, charge conjugation $C$, and their double products. The $PCT$ symmetry is, however, conserved. We have classified and estimated the ground-state energy for the different flux-phase states which occur in the $t-J$ model. One can conclude that such fractional-flux-phase states have anion statistics, breaking $T$, $P$, and $C$ symmetries. In the limit $t \to 0$, the antiferromagnetic flux-phase states breaking such symmetries have been predicted by Wiegmann.

The present study gives the structure of flux-phase states and the relationship between the properties of the $t-J$ model and the mechanism of the generation of orbital current on the lattice. We are able to explore the structure of the ground state of the $t-J$ model by employing the concept of a spontaneous magnetic field which generates appropriate correlated many-body wave functions of the generalized Laughlin form in conjunction with the fictitious magnetic field added to Gutzwiller projections.

Our results are consistent with those obtained on the basis of the boson-vortex Skyrmion duality. According to such a duality-transformation approach, the fermion splits into a boson and a vortex. In the case considered in our paper ($l = m = 1$ and $q = 0$), we have for the state with minimal energy that each pair of hard-core bosons has one vortex of statistical flux (the flux of the orbital magnetic field) and one vortex of fictitious magnetic field $B$. Both vortices have one quantum of flux. On average, the statistical flux density cancels the fictitious magnetic flux density and the pairs of bosons condense. Such condensation acquires long-range phase coherence. According to Yang, it is due to periodic boundary conditions and, as a consequence, it is due to flux quantization [see (13)]. For the fractional-flux-phase states, the average statistical flux density does not cancel the fictitious magnetic flux density and, as a result, we have a fractional value of the total flux per elementary plaquette of the lattice. Such a fractional flux corresponds to uncompensative vortices. It means that these states describe excitations of the vortex-Skyrmion-type. But at half filling, $\rho = 1$, the energy of all the states coincides. Among these fractional-flux-phase states, there is one with a half quantum of the total flux per particle, which has been proposed by Mele. Using the different values for $l$, $m$, and $q$, one can also obtain the total hierarchy of possible anion states proposed in Refs. 17–19. This will be published elsewhere.

Thus the analysis permits the explicit construction of a type of possible excitation in a two-dimensional antiferromagnetic system, which we may attribute to fractional-flux-phase states and have an analogy with magnetoplasma waves. This may be particularly important for the analysis of cluster calculations or Monte Carlo calculations employing lattices of small or finite size.

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