FLUX PHASES IN POLARIZED SPIN LIQUIDS

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Abstract

We study the Gutzwiller ansatz with a gauge field and arbitrary polarization as a trial wave function for the spin liquid state of the Heisenberg Hamiltonian in two dimensions. This wave function is evaluated exactly for a 4x4 cluster with periodic boundary conditions. The energy as a function of the gauge field and magnetization is calculated.

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After the first proposal by Anderson[1] that high Tc superconductivity in cuprate materials is a consequence of the spin liquid nature of these systems, there has been a lot of theoretical activity trying to give a good description of the spin liquid phase[2-5].

It is generally assumed that the undoped insulating state of the cuprate materials is well described by a Heisenberg antiferromagnetic model on a square lattice. In fact, antiferromagnetic order has been observed in the Cu-O planes of the ceramic materials, with spins 1/2 mainly located at the Cu sites[6]. The effect of doping is usually modeled by removing some of the spins, the dynamics of the holes being described by the so called t-J model[1,7].

Diagonalization of small clusters and some variational procedures suggest that the ground state of a Heisenberg model in 2D has long range order. Presumably, doping with holes destroys the antiferromagnetic order and stabilizes the spin liquid phase. However, the nature of the ground state of the 2D Heisenberg model is still an open problem and some authors consider the possibility that the system might not order even at T=0. In any case it is instructive to analyze the spin liquid phase for the undoped system. A good description of this phase could be used as a starting point to understand the more interesting case of doped systems.

Different approaches have been used to analyze this phase. On one hand, variational wave functions have been proposed: the

Resonating Valence Bond (RVB) state and Gutwiller-type wave functions[8]. On the other hand, mean field treatments of the model were first done by Baskaran et.al.[9] and later by Afflek and Marston[10], and independently by Kotliar[11], who found lower energy solutions by introducing gauge fields.

In this paper we present results for the Gutzwiller wave functions where the projection operator is treated exactly for a finite cluster. Our interest is to understand the properties of the Gutzwiller wave functions as compared with the mean field treatments. We consider the more general case of the Heisenberg model with an external magnetic field which polarizes the system in the z direction.

$$H_J = J \sum_{<i,j>} \mathbf{S}_i . \mathbf{S}_j - h \sum_i S_i^z \quad (1)$$

We first discuss the h=0 case (unpolarized spin liquid). The Gutzwiller wave function is defined as

$$| \psi > = P | \psi_0 > \quad (2)$$

where $| \psi_0 >$ is the wave function of N non-interacting electrons in a N sites lattice, and P is a projection operator which eliminates from $| \psi_0 >$ all configurations with doubly occupied sites. One possibility, perhaps the most appealing, is to take $| \psi_0 >$ as the ground state of the following tight-binding Hamiltonian

$$H_0 = -\sum_{<i,j>} \left[e^{i\phi_{ij}} C^{+}_{i\sigma} C_{j\sigma} + \text{h.c.} \right] \qquad (3)$$

where $C^{+}_{i\sigma}$ creates an electron with spin σ at site i. The phases ϕ_{ij} are variational parameters, i.e. the expectation value $\langle\psi|H_J|\psi\rangle$ is minimized with respect to these phases. The Hamiltonian H_0 describes non-interacting electrons in a magnetic field (gauge field) which must be distinguished from the real polarization field h. The flux phase states correspond to phases such that the gauge field per plaquette is spatially constant in modulus. Later we will discuss other possibilities which lead to the Peierls state obtained in Ref. 10. In a mean field treatment, the flux phase state is at least a local minimum of the total energy[10,11]. We will show that if the projection procedure involved in Eq.(2) is carried out exactly, it is likely an absolute minimum.

Tight binding electrons in an external field are described by Hamiltonian (3) where the phases are $\phi_{ij} = 2\pi\int_i^j \mathbf{A}.d\mathbf{l}$, and $\mathbf{A}$ is the potential vector associated with the gauge field. For a uniform field the spectrum is the well known Hofstadter spectrum[12]. For commensurate fields of the type $\phi=(p/q)\phi_0$, where ϕ is the flux per plaquette, ϕ_0 is the quantum flux and p and q are integers, the energy spectrum consists of q bands (labeled by n) and the energy corresponding to Hamiltonian (3) is given by

$$E_0 = \sum_{nk\sigma}^{occ} E^{n}_{k\sigma} , \qquad (4)$$

where $E^n_{k\sigma}$ are eigenvalues of H_0.

Before presenting results for the exact evaluation of the Gutzwiller projector, we briefly comment some analytical approximations.

It has been shown that the Gutzwiller approximation in the present case renormalizes the expectation values in the folowing way[8]:

$$< S_i . S_j > \cong g < S_i / S_j >_0 \qquad (5)$$

where $<...>$ and $<...>_0$ indicate the expectation values taken with $|\psi>$ and $|\psi_0>$ respectively and the classical factor g is 4 for a half filled band, *i.e.* one electron per site.

In this approximation the variational energy is then given by

$$< H_J > = -\frac{3J}{16} E_0^2 , \qquad (6)$$

The energy of the spin liquid phase is therefore given by the square of the Hofstadter energy.

This approximation is equivalent to Affleck and Marston's mean field[10] which also gives a quadratic dependence of the energy on the uncorrelated Hofstadter energy.

Recently it has been shown that E_0, and consequently $<H_J>$, has cusplike minima for $\phi=n\phi_0/2$, where n is the particle density[12]. In the present case this corresponds to $\phi=\phi_0/2$. For fixed ϕ, the energy E_0 as a function of n has discontinuities in

its derivative due to the energy gaps induced by the field.

The change in the number of particles by doping introduces complications due to the dynamics of the holes. We can however polarize the system to have $N_\uparrow$ spin up particles and $N-N_\uparrow$ spin down particles. Due to the electron-hole symmetry of the square lattice, the contribution of the spin up and spin down particles is the same, and within the Gutzwiller approximation the total energy is given by the square of the Hofstadter energy of $2N_\uparrow$ particles moving in the gauge field. The total energy of the system as a function of the magnetization M for fixed ϕ then shows discontinuities in its derivative. The cusplike minima of the energy as a function of the flux and the discontinuities of its derivative as a function of the number of particles (or magnetization) are a consequence of the gaps in the Hofstadter spectrum. The question is whether these features in $\langle H_J \rangle$ are a consequence of the approximation [Eq.(5)] or intrinsic properties of the Gutzwiller wave function.

We study numerically the spin liquid phase by evaluating exactly the wave function [Eq.(2)] in a finite cluster. We generate the projected wave function with $N_\uparrow$ spin up electrons and $N_\downarrow=N-N_\uparrow$ spin down electrons in the following way. Starting with the fully polarized state ($S^z=N/2$) we first destroy $N-N_\uparrow$ electrons and then we create the $N-N_\uparrow$ spin down electrons. The restriction of no double occupancy imposed by the projector is taken into account by creating the spin down electrons in the coordinates of the spin up holes. Without loss of generality we consider $N_\uparrow \geq N/2$.

The wave function in the coordinate representation is therefore a function of the coordinates of the spin down electrons only and is given by

$$\psi(x_1,\ldots,x_{N_\downarrow}) = D^{*}(\phi_\nu(x_1))\; D(\phi_\mu(x_1)), \tag{7}$$

where $D(\phi_\nu(x_1))$ is the Slater determinant constructed with the non-interacting wave functions with quantum numbers ν. If we start with the ground state of the uncorrelated electrons the projected wave function takes the form

$$\psi(x_1,\ldots,x_{N_\downarrow}) = (-1)^{\eta}\; \left|D(\phi_\nu\;(x_i))\right|, \tag{8}$$

where $(-1)^{\eta}$ is the Marshall sign, with η the number of spin up electrons in a given sublattice. Note that in this case the Marshall sign appears not only in the S=0 state but in states with $S=S^z$, *i.e.* the minimum total spin compatible with the polarization considered.

It is worth noting that starting with the ground state of the uncorrelated system does not imply that the energy $\langle H_J\rangle$ is a minimum. This is not surprising since the variational energy is calculated using a Hamiltonian which is different from that of the uncorrelated system. We must therefore also minimize the energy with respect to the set of quantum numbers of the uncorrelated electrons.

If one starts with excited states of the uncorrelated problem, two situations can be clearly distinguished. *a)* All minority spins in doubly occupied one particle states (See Fig. 1a). In this case the wave function takes the form of a square of a determinant, as in Eq. (8); however, the set of quantum numbers ν do not necessarily correspond to the lowest energy one-particle states. Clearly these states have total spin $S=S^z$. *b)*Some minority spins in singly occupied one-particle states (See Fig. 1b.) In this case the wave function takes the more general form of a product of determinants, as in Eq. (7). In this type of states the total spin is not a good quantum number.

In Fig. 2 we show the energy $E_J = \langle J \sum_{<ij>} \mathbf{S}_i \mathbf{S}_j \rangle$ as a function of $M=(N_\uparrow - N_\downarrow)/2$, for different values of the gauge flux. The expectation value is calculated using the exactly projected wave function for a square 4x4 cluster with periodic boundary conditions. Each point corresponds to the minimum energy obtained by varying the set of one particle quantum numbers. The minimization is carried out by searching only among the set of states with total spin $S=S^z$.

We see in Fig. 2 that the energy as a function of magnetization has kinks as predicted by the Gutzwiller approximation: For $\phi/\phi_0=0$, the curve obtained is smooth. For $\phi/\phi_0=1/4$ we observe well defined kinks for $M=0, \pm 4$. Finally, for $\phi/\phi_0=1/2$ there is only one well defined kink for $M=0$. In the last case the curve presents a rather noisy structure which could be

due to a lack of precision in the minimization procedure or to finite size effects.

Comparing the three curves obtained we find that for low magnetization the best energy corresponds to $\phi=\phi_0/2$. For intermediate magnetizations the energy is minimized with $\phi=\phi_0/4$, and finally the highly polarized states correspond to $\phi=0$.

In our finite cluster with periodic boundary conditions, the allowed values of the gauge fields are only those mentioned above. Other values of the gauge field are not compatible with the periodic boundary conditions. In the thermodynamic limit one expects the flux to change continuously from $\phi_0/2$ to zero as the magnetization increases from zero to N/2. From the Gutzwiller approximation and the discussion given in Ref. 13 one obtains that the optimum flux is $\phi=(1-2M/N)\phi_0/2$.

In Fig. 3 we present the energy of our finite cluster as a function of the magnetization indicating the regions in which each flux is stable. For the sake of comparison we also present the energy corresponding to an RVB wave function with nearest neighbor singlets. This trial wave function is constructed as a superposition of all possible dimer configurations with equal weights.

The energies of the exactly projected Gutzwiller wave function for different gauge fields and magnetizations, and also the energy of the RVB state for our 4x4 cluster are presented in Table 1.

Note that for the Hamiltonian considered the RVB state has always lower energy; however for the magnetizations corresponding to a spin projection per site s^z= 0, 1/4 and 1/2, the energy of the Gutzwiller ansatz is very close to that of the RVB. These are precisely the situations in which the gauge field fits correctly for our cluster size. In the thermodynamic limit we expect the two energies to be very close for every magnetization. Although the RVB has lower energy for the case studied, for a generalized Heisenberg Hamiltonian the flux phase states could be stabilized.

It was shown by Affleck and Marston and also by Kotliar that in the mean field approach the flux phase corresponding to S^z=0 and $\phi=\phi_0/2$ are not absolute minima. They showed that there is another state, the so called Peierls state, which is lower in energy. In our treatment the Peierls state can be obtained using an uncorreladed Hamiltonian H_0 in which every site is connected via a hopping matrix element with only one of its four neighbors. In this case the uncorrelated wave funtion $|\psi_0>$ is a direct product of dimer wave functions and the projection procedure is straightforward. The energy per site of the projected Peierls state is -3J/8 . This energy is higher than the one corresponding to the exactly projected flux phase state, which in our 4x4 cluster we found to be -0.653J per site.

In summary, we have studied the flux phase states for a polarized spin liquid. We evaluated exactly the Gutzwiller wave funtion with a gauge field and arbitrary polarization for a finite cluster. Our results show that:

i) Within the limitations of our finite size calculation, the energy is minimized for a gauge flux per plaquette $\phi=(1-2M/N)\phi_0/2$, as predicted by mean field treatments.

ii) For fixed gauge flux, the energy as a function of the magnetization presents discontinuities in the derivative. These features are therefore an intrinsic property of the Gutzwiller ansatz rather than a consequence of the approximate schemes previously used.

iii) The flux phase states have lower energy than the Peierls state if the projector in the Gutzwiller ansatz is carried out exactly.

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TABLE 1

M	$E(\phi_0/2)$	$E(\phi_0/4)$	$E(0)$	E_{RVB}
0	-0.5723	-0.6031	-0.6530	-0.6686
1	-0.5560	-0.5483	-0.5799	-0.6499
2	-0.4980	-0.4782	-0.4977	-0.5875
3	-0.4020	-0.4081	-0.4152	-0.4870
4	-0.2890	-0.3183	-0.2721	-0.3502
5	-0.1420	-0.1212	-0.1214	-0.1788
6	0.0469	0.0838	0.0711	0.0224
7	0.2500	0.2917	0.2500	0.2500
8	0.5000	0.5000	0.5000	0.5000

FIGURE CAPTIONS

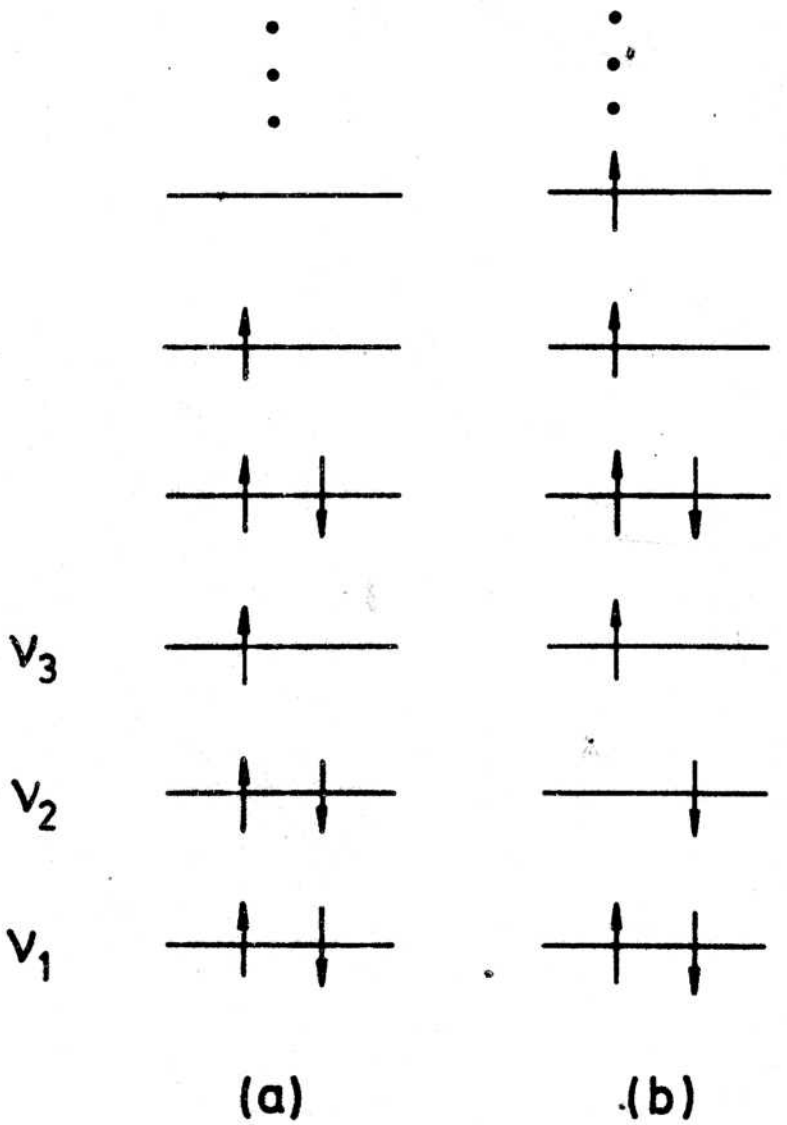
Figure 1.-Scheme of level occupancy for the one particle uncorrelated problem. (a) All minority spins in double occupied states ($S=S^z$). (b) Some minority spins in singly occupied states.

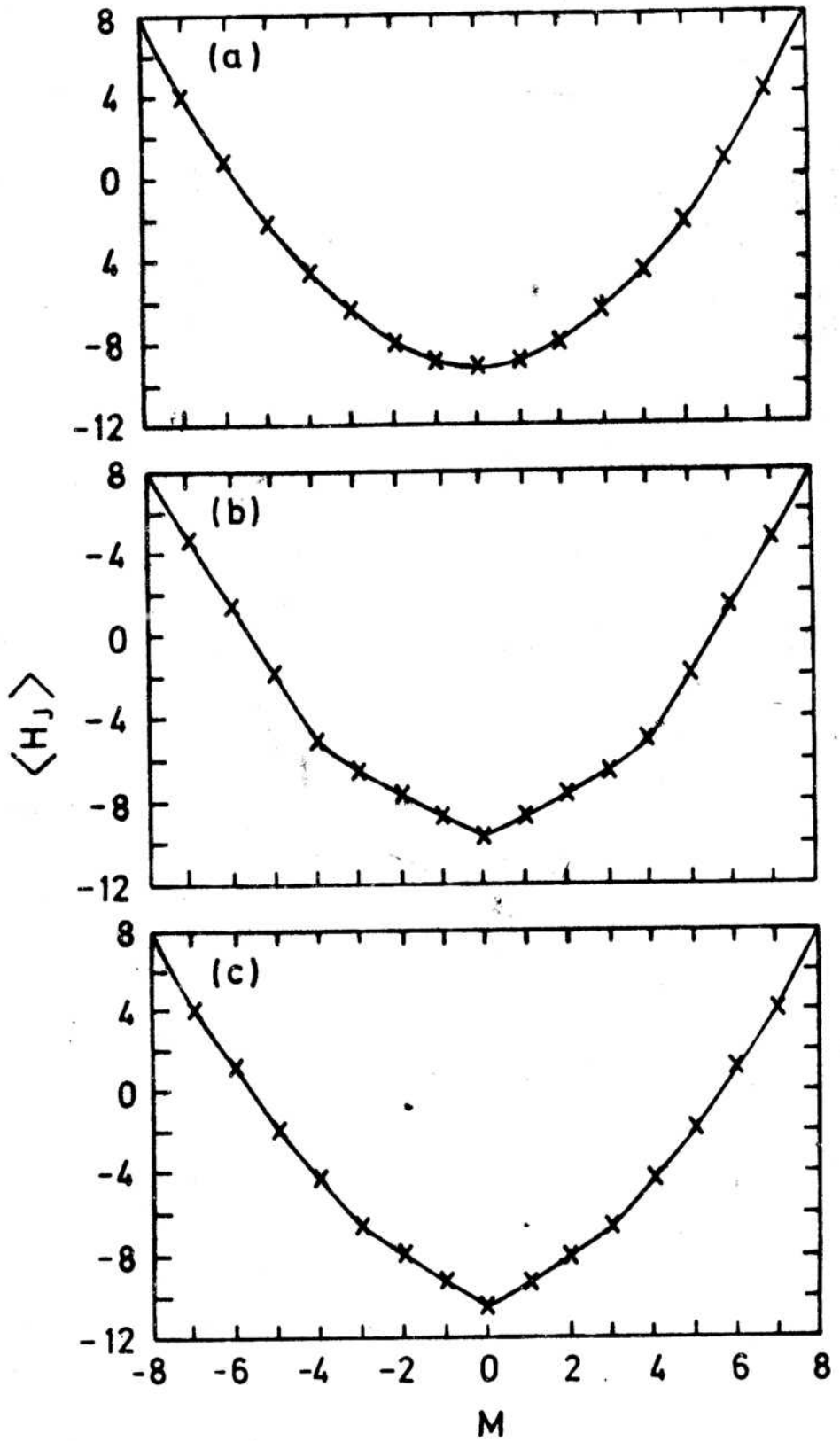
Figure 2.-Total enrgy E_J in units of J as a function of the magnetization M for the considered 4x4 cluster. Figures (a),(b) and (c) correspond to ϕ=0, 1/4 and 1/2 respectively.

Figure 3.- Energy E_J *vs.* magnetization as minimized with respect to the gauge flux values given in Fig.2 (crosses). The corresponding fluxes are also shown. For M=±2 the energy with ϕ=0 competes with that of ϕ=1/2 (see Table 1.) Dots indicate the energy of the polarized RVB state.

TABLE CAPTION

Table 1.- Energies per site in units of J for the exactly evaluated flux phases and RVB state for different magnetizations.


ν_3
ν_2
ν_1
(a)
(b)


(a)
(b)
(c)
8
4
0
-4
-8
-12
-8
-6
-4
-2
0
2
4
6
8
M
⟨H_J⟩

M
$\langle H_J \rangle$
0
-2
-4
-6
-8
-12
-8
-4
0
4
8
$\Phi=0$
$\Phi=\Phi_0/4$
$\Phi=\Phi_0/2$