CHIRALITY ORDERING OF CHIRAL SPIN LIQUIDS

D. M. Gaitonde

Institute of Physics, Sachivalaya Marg, Bhubaneswar 751005, India

Dileep P. Jatkar* and Sumathi Rao† ‡

Tata Institute of Fundamental Research, Homi Bhabha Road, Bombay 400005, India

ABSTRACT

We study the effect of introducing a weak antiferromagnetic interplanar exchange coupling in the two dimensional frustrated Heisenberg model. We show that a ferromagnetic(FM) ordering of chirality - i.e., same chirality on adjacent planes - is energetically favoured, thus leading to bulk violation of the discrete symmetries parity($P$) and time reversal($T$).

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Prefitem
Ever since the discovery of high $T_c$ superconductors [1] and the observation of their layered nature, it has been conjectured [2–4] that these materials are described by a ground state that explicitly violates the discrete symmetries parity ($P$) and time-reversal ($T$) macroscopically. Theoretical interest in these ideas began with the work of Kalmeyer and Laughlin [4], who (approximately) mapped the Heisenberg model on a triangular lattice, to a bosonic FQHE problem at filling fraction $\nu = 1/2$, with semionic excitations. An apparently very different line of investigation was initiated by Affleck-Marston [5] and Kotliar [6], who introduced the notion of ‘flux phases’. Working with a frustrated Heisenberg model on a square lattice, Wen, Wilczek and Zee [7] generalised the ‘half-flux’ phase of Affleck-Marston to a ‘quarter-flux’ phase which they called the chiral spin liquid ($CSL$). They found that this state explicitly violated $P$ and $T$ macroscopically and in the low energy long wavelength limit, its effective action led to semionic statistics, thus corroborating the Kalmeyer-Laughlin picture. More recently, Laughlin and Zou [8] have shown that the Gutzwiller projected $CSL$ state is identical to the Kalmeyer-Laughlin state, paving the way to a three dimensional generalisation of the physics underlying the FQHE. The concept of flux phases has also been extended to the doped situation and generalised flux phases have been shown to be plausible ground states of the doped $t$-$J$ model [9]. On the experimental front, many novel experiments were both suggested [10] and performed [11] to look for $P$ and $T$ violation, which appeared to be a robust prediction of all anyonic theories. But the experimental situation remains confused in the face of conflicting evidence.

Much of the earlier theoretical work was confined to studies of single planes. But lately, there have been several attempts to extend flux phase ideas to the fully three dimensional situation [12]. However, it is also of both theoretical and experimental importance to incorporate weak three dimensionality -i.e.,- to study the effect of weak interlayer couplings -in planar phenomena. We focus on this particular aspect in this letter. We study the effect of a weak antiferromagnetic interlayer spin-spin coupling (well motivated by neutron scattering studies [13]) on two dimensional $CSL$ ground states. By perturbatively computing the correction
to the ground state energy, we show that a FM ordering of chirality on adjacent planes is preferred. Our work is close in spirit, but somewhat complementary to the work of Rojo and Canright [14], who studied the ordering of anyons on adjacent planes when a static scalar potential is introduced between them. But our work studies the ordering of the ground states of a microscopic model - the frustrated Heisenberg model - whereas the starting point of their work involves a gas of anyons. The two calculations, therefore, cannot be directly compared, since it is not yet possible to explicitly derive a gas of anyons from the frustrated Heisenberg model or any other microscopic model.

Let us consider $2p$ planes, each of which has a spin $S = 1/2$ sitting on the sites of a square lattice, with Heisenberg antiferromagnetic interactions between all nearest neighbours within each plane. The ground state of this model is well known to be Neel ordered. However, one of the important effects of doping this model with mobile holes is to induce frustrating interactions [15], which cause an instability towards generalised flux phases. Qualitative features of these phases are captured by the CSL states of the frustrated Heisenberg ($J-J'$) model given by

$$H_0 = J \sum_{a=1}^{2p} \sum_{<i,j> \in n.n} S_i^a \cdot S_j^a + J' \sum_{a=1}^{2p} \sum_{<i,j> \in n.n.n} S_i^a \cdot S_j^a$$  \hspace{1cm} (1)$$

which is also an interesting model in its own right. We shall use this model as our starting point. In Eq.(1), $i$ is the two dimensional site index common to all the planes and the index $a$ identifies each plane. As argued in Ref.[7], the CSL state, characterised by the order parameter $< S_i \cdot S_j \times S_k >$, where $i$, $j$ and $k$ are the vertices of an elementary triangle, is a local minimum of this model for sufficiently large $J'$. In fact for slightly modified Hamiltonians, it is a plausible ground state. It is this ground state which has anyonic excitations and motivates the study of a gas of anyons which forms the basis of theories of anyon superconductivity [16]. In this letter, we shall focus our attention on the mean field description of this CSL state.
We use a fermionic description for the spins given by

\[ S_{i}^{c,a} = \sum_{\alpha,\beta} c_{i\alpha}^{a} \sigma_{\alpha\beta} c_{i\beta} \quad \text{and} \quad S_{i}^{d,a} = \sum_{\alpha,\beta} d_{i\alpha}^{a} \sigma_{\alpha\beta} d_{i\beta}, \]

where we have distinguished alternate planes by the nomenclature of the fermions as \( c \) and \( d \) planes. Also, for clarity and brevity of notation, we shall henceforth drop the index \( a \) and the summation over \( a \) which now goes from 1 to \( p \), since odd and even planes have been distinguished. In terms of the fermions, the Hamiltonian \( H_{0} \) can be rewritten, after a Fierz transformation followed by a Hubbard-Stratanovich transformation as

\[ H_{0} = \sum_{\{i,j\},\alpha} [\chi_{ij}^{c} c_{i\alpha}^{\dagger} c_{j\alpha} + \chi_{ij}^{d} d_{i\alpha}^{\dagger} d_{j\alpha} + h.c.] + \sum_{i,\alpha} [a_{0i}^{c}(c_{i\alpha}^{\dagger} c_{i\alpha} - 1) + a_{0i}^{d}(d_{i\alpha}^{\dagger} d_{i\alpha} - 1)] \]

\[ + \frac{2}{J} \sum_{\langle i,j \rangle \in \text{n.n.}} \chi_{ij}^{c,d} \chi_{ij}^{c,d} + \frac{2}{J'} \sum_{\langle i,j \rangle \in \text{n.n.n}} \chi_{ij}^{c,d} \chi_{ij}^{c,d}, \]

where \( \chi_{ij}^{c,d} \) are the Hubbard-Stratanovich fields. The notation \( \{i,j\} \) in the first summation stands for summation over both nearest and next nearest neighbours.

Following WWZ [7], we introduce the mean field ansatz for the chiral spin liquid state for both the \( c \) and \( d \) planes. For the nearest neighbour links,

\[ \langle \chi_{i,i+\hat{x}}^{c,d} \rangle = g e^{i\pi/4} \quad \text{and} \quad \langle \chi_{i,i+\hat{y}}^{c,d} \rangle = g e^{-i\pi/4} \]

where \( i \) here, is a site on the odd sublattice. However, for the diagonal links, the WWZ ansatz admits a two-fold degeneracy corresponding to the two possible chiralities - i.e., the flux through each elementary plaquette, which is now a triangle, could either be positive or negative. Since we wish to study the ordering of chiralities on different planes, we allow for independent chiralities on the two planes. Thus, the n.n.n links are described by

\[ \langle \chi_{i,i-\hat{x}+\hat{y}} \rangle = \delta_i f_{i}^{c,d} \quad \text{and} \quad \langle \chi_{i,i-\hat{x}-\hat{y}} \rangle = -\delta_i f_{i}^{c,d} \]

where \( \delta_i = (+(-)1 \) for \( i \) belonging to the even (odd) sublattice. \( f_{i}^{c} = f_{i}^{d} \) implies that the chiralities on the adjacent \( c \) and \( d \) planes are the same (FM ordering) and
$f^c = -f^d$ implies an AFM ordering. In the absence of any interplanar coupling, the two possibilities obviously remain degenerate. Finally, for the Lagrange multiplier fields we have

$$\langle a_{0i}^c \rangle = \langle a_{0i}^d \rangle = 0,$$

so that the fermions are no longer subject to the ‘no double occupancy’ constraint at each site. The constraint is now enforced only on the average.

Notice that the mean field ansatz for the CSL state divides the square lattice on each plane into two sublattices. Thus, we may take the spatial Fourier transformations separately for the odd and even sublattices, with respect to a 2-d wave vector $\mathbf{k}$ which now runs over the reduced Brillouin zone (RBZ). Hence, the momentum space mean field Hamiltonian is given by

$$H_{MF} = \sum_{\mathbf{k} \in RBZ, \alpha} \left[ \psi_{k\alpha}^{c\dagger} h_{k\alpha}^c \psi_{k\alpha}^c + \psi_{k\alpha}^{d\dagger} h_{k\alpha}^d \psi_{k\alpha}^d \right]$$

where $\psi_{k\alpha}^c = (c_{k\alpha}^o, c_{k\alpha}^e)$ and $\psi_{k\alpha}^d = (d_{k\alpha}^o, d_{k\alpha}^e)$, $o$ and $e$ stand for odd and even respectively and

$$h_{k}^{c,d} = \begin{pmatrix}
\epsilon_{k}^{c,d} & \Delta_{k} \\
\Delta_{k}^* & -\epsilon_{k}^{c,d}
\end{pmatrix} = \begin{pmatrix}
2f^{c,d} [\cos(k_x + k_y) - \cos(k_x - k_y)] & 2g[-i \cos(k_x) + \cos(k_y)] \\
2g[i \cos(k_x) + \cos(k_y)] & -2f^{c,d} [\cos(k_x + k_y) - \cos(k_x - k_y)]
\end{pmatrix}$$

This Hamiltonian can be diagonalised by a unitary transformation yielding

$$h_{k,\text{diag}}^{c,d} = \begin{pmatrix}
-E_k^{c,d} & 0 \\
0 & E_k^{c,d}
\end{pmatrix}$$

with $E_k^{c,d} = (|\Delta_k|^2 + (\epsilon_k^{c,d})^2)^{1/2}$ in terms of the transformed variables ($\gamma_{k\alpha}^V, \gamma_{k\alpha}^C$) and ($\eta_{k\alpha}^V, \eta_{k\alpha}^C$) for the valence band(V) and conduction band(C) fermions in the $c$
and $d$ planes respectively. The ground state has the valence band completely filled in both the planes and its energy, in terms of the mean field variables, is given by

$$E_{0}^{MF} = \frac{2}{J} \sum_{i \in \text{odd}} \sum_{j(i) \in \text{n.n}} g^2 + \frac{2}{J'} \sum_{i \in \text{odd}} \sum_{j(i) \in \text{n.n.n}} f^2 - 2 \sum_{k \in \text{RBZ}} E_k.$$  \hspace{1cm} (10)

In the absence of any interplanar coupling, the FM and AFM orderings of chirality remain degenerate. To lift the degeneracy, we introduce a weak interlayer Heisenberg antiferromagnetic coupling given by

$$H_{\text{int}} = J'' \sum_i S^c_i \cdot S^d_i$$ \hspace{1cm} (11)

where $S^c_i$ and $S^d_i$ refer to the spins on the $c$ and $d$ planes respectively. Such an interaction is particularly appropriate for the copper oxide systems and leads to 3-d Neel ordering in the undoped insulating phase. $J''$ has been estimated from neutron scattering experiments [13], to be about five orders of magnitude less than the in-plane coupling $J$. We treat $H_{\text{int}}$ as a static perturbing potential between the two species of fermions on adjacent planes. This is accomplished by taking momentum space Fourier transformations with respect to a 2-d wave vector. Thus, despite the extension of the problem into the third dimension, inter-layer particle transfers are avoided and the essential layered nature of the original problem is retained. The relative weakness of $J''$ with respect to $J$ justifies this approach.

In the fermionic representation,

$$H_{\text{int}} = \frac{J''}{2} \sum_{i,\alpha,\beta} c_{i\alpha}^\dagger c_{i\beta}^\dagger d_{i\beta}^\dagger d_{i\alpha}$$ \hspace{1cm} (12)

which, when Fourier transformed with respect to 2-d wave vectors, becomes

$$H_{\text{int}} = \frac{J''}{N} \sum_{k,k',q} \left[ c_{k+q\alpha}^\dagger c_{k\beta}^\dagger d_{k'\beta}^\dagger d_{k'\alpha} + c_{k+q\alpha}^\dagger c_{k\beta}^\dagger d_{k'\beta}^\dagger d_{k'\alpha} \right].$$ \hspace{1cm} (13)

Notice that a change in momentum in the $c$ plane is compensated by an opposite change in momentum in the $d$ plane. We now evaluate the total ground state
energy, treating $H_{int}$ as a perturbation, for the two cases of FM and AFM orderings of chirality. The unperturbed ground state is given by

$$|\text{Ground state}\rangle = \prod_{k, \alpha} V^{\dagger}_{k\alpha} |0\rangle \otimes \prod_{k, \alpha} V^{\dagger}_{k\alpha} |0\rangle$$

and the unperturbed ground state energy is given in Eq. (10). The FM ground state has $f^c = f = f^d$, whereas the AFM ground state has $f^c = f = -f^d$, so that the Boguliobov transformation coefficients and hence the definition of the transformed fermions $\eta_{k\alpha}^{V,C}$ differ in the two cases. It is now straightforward to rewrite $H_{int}$ in terms of the transformed fermions and compute $E_{FM} - E_{AFM}$.

At first order, we find that

$$E_{FM}^{(1)} - E_{AFM}^{(1)} = \frac{2J''}{N} \left( \sum_k \frac{\epsilon_k}{E_k} \right)^2 = 0,$$

since $\epsilon_k/E_k$ is odd under reflection about the $k_y$-axis and the summation over $k$ includes both positive and negative $k_x$. This result is easily understood, since at first order, the only term in $H_{int}$ that contributes involves no momentum transfer $q$ hence, the two planes are essentially independent and the degeneracy between FM and AFM orderings of chirality is not lifted. At second order too the degeneracy is not lifted. We find that

$$E_{FM}^{(2)} - E_{AFM}^{(2)} = \left( \frac{J''}{2N} \right)^2 \sum_{k,k',q} \frac{1}{E_k + E_{k'} + E_{k+q} + E_{k'-q}} \left( \frac{\epsilon_{k'-q}}{E_{k'-q}} \frac{\epsilon_{k'}}{E_{k'}} \right) \left( \frac{\epsilon_{k+q}}{E_{k+q}} \frac{\epsilon_k}{E_k} \right).$$

Making the changes $k \to k - q, q \to -q$, and $k' \to -k'$ successively in the dummy variables, and using $\epsilon_{-k} = \epsilon_k, \Delta_{-k} = \Delta_k$ and $E_{-k} = E_k$, we find that

$$E_{FM}^{(2)} - E_{AFM}^{(2)} = -(E_{FM}^{(2)} - E_{AFM}^{(2)}) = 0.$$

However, the third order contribution does lift the degeneracy and is given by

$$E_{FM}^{(3)} - E_{AFM}^{(3)} = E_A + E_B + E_C$$
where

\[
E_A = -\frac{J'^3}{N^3} \sum_{k,k',q,q'} \frac{(\epsilon_{k+q} + \epsilon_{k+q+q'} - \epsilon_k - \epsilon_{k'q}q)\epsilon_{k+q+q'}}{E_k + E_{k+q} + E_{k'} + E_{k'q}} \]

\[
\frac{\epsilon_{k'} + \epsilon_{k'-q'} - \epsilon_{k'-q} - \epsilon_{k'q} - \epsilon_{k'q}q}{E_k + E_{k+q} + E_{k'} + E_{k'-q}} - \frac{\epsilon_{k'q} + \epsilon_{k'-q'} - \epsilon_{k'} - \epsilon_{k'q}q}{4(E_k + E_{k+q} + E_{k'} + E_{k'-q})} \]

(19)

\[
E_B = -\frac{J'^3}{2N^3} \sum_{k,k',q,q'} \frac{1}{(E_k + E_{k+q} + E_{k'} + E_{k'-q})(E_k + E_{k+q} + E_{k'} + E_{k'-q})} \]

\[
(\epsilon_{k+q}\delta_{k+q} + \epsilon_{k'q}q + \delta_{k'q}q + \delta_{k'q}q + h.c.) + \epsilon_{k'}(\delta_{k+q} + \epsilon_{k'q}q + \delta_{k'q} + h.c.) + \epsilon_{k+q+q'}(\delta_{k+q} + \epsilon_{k'q}q + h.c.) \]

(20)

and

\[
E_C = \frac{J'^3}{8N^3} \sum_{k,k',q,q'} \frac{1}{(E_k + E_{k+q} + E_{k'} + E_{k'-q})(E_k + E_{k+q} + E_{k'} + E_{k'-q})} \]

\[
(\epsilon_{k+q}\delta_{k+q} + \epsilon_{k'q}q + \delta_{k'q}q + \delta_{k'q}q + h.c.) + \epsilon_{k'}(\delta_{k+q} + \epsilon_{k'q}q + \delta_{k'q} + h.c.) + \epsilon_{k+q+q'}(\delta_{k+q} + \epsilon_{k'q}q + h.c.) \]

(21)

(Here, \(\epsilon_k = \epsilon_k/E_k\) and \(\delta_k = \Delta_k/E_k\) for any momentum \(k\).) The \(k\)-summations in Eqs.(19), (20) and (21) were performed numerically using a Monte Carlo routine, for different values of \(J'/J\), with the corresponding values of \(f/J\) and \(g/J\) being obtained by minimising \(E_0\) in Eq.(10) with respect to \(f\) and \(g\). Our numerical results are tabulated below.
Thus, for any value of $J'/J$ for which the CSL state is a local minimum, and for $J'' > 0$, (which is the case for copper oxides), the FM ordering of chirality is energetically favoured. Notice that the energy difference is an extensive quantity and scales linearly with $N$. In fact, using typical values for $La_2CuO_4$, ($J = 1200^\circ K$ and $J'' = 0.03^\circ K$), and assuming $N \sim 10^{15}$, $E_{AFM} - E_{FM}$ ranges between $3.2^\circ K$ and $15.4^\circ K$ for $J'/J$ between 0.5 and 0.7. Thus, despite the weakness of the interlayer coupling, its potency is effectively increased by its extensivity. Hence, at low enough temperatures, the weak Heisenberg antiferromagnetic interlayer coupling has sufficient strength to tilt the scales in favour of a FM ordering of chirality.

In our calculation, we have completely ignored gauge field fluctuations - i.e., the phase fluctuations of the order parameter $\chi_{ij}$ and the fluctuations of the Lagrange multiplier field $a_{0i}$. These fluctuations could lead to a substantial contribution to the ground state energy. However, they cannot lift the degeneracy between the FM and AFM orderings of chirality, since they only act within each plane. Thus, as long as these fluctuations do not destabilise the mean field ground state, $E_{FM} - E_{AFM}$ and consequently, the ordering of chirality is determined only by the interplanar coupling.

\begin{table}
\begin{tabular}{cccc}
\hline
$J'/J$ & $f/J$ & $g/J$ & $(E_{FM}^{(3)} - E_{AFM}^{(3)})/J$ \\
\hline
0.50 & 0.015 & 0.23 & $-1.7 \times 10^{-4} N(J''/J)^3$ \\
0.55 & 0.024 & 0.24 & $-2.9 \times 10^{-4} N(J''/J)^3$ \\
0.60 & 0.035 & 0.24 & $-4.6 \times 10^{-4} N(J''/J)^3$ \\
0.65 & 0.046 & 0.23 & $-6.8 \times 10^{-4} N(J''/J)^3$ \\
0.70 & 0.060 & 0.23 & $-8.2 \times 10^{-4} N(J''/J)^3$ \\
\hline
\end{tabular}
\end{table}
We have worked within the framework of the $J-J'$ model, which is a limiting case of the $t$-$t'$-$J$-$J'$ model. However, we expect the qualitative aspects of our result - i.e., the tendency towards FM ordering of chirality - to be valid even for the generalised flux phases of the doped $t$-$J$ model, at least for low doping. Notice that our result suggests that bulk $P$ and $T$ violation is an inescapable consequence of CSL ground states of models that are relevant to high $T_c$ superconductors. Moreover, despite the controversy regarding the observation of local $P$ and $T$ violation, bulk $P$ and $T$ violation has certainly been ruled out in the cuprate compounds [11]. Hence, our calculation disfavours models with CSL ground states as candidates to describe the doped Mott insulating phases of the copper oxides.

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