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NON-EXISTENCE OF CHIRAL SPIN STATES IN FRUSTRATED ANTIFERROMAGNETS

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ABSTRACT

It is shown that for the Heisenberg antiferromagnet with nn and nnn couplings J and J', Wilson loops of statistical gauge fields are real by virtue of reflection positivity. This excludes the occurrence of $T-$ and $P-$ violating chiral-spin liquid states for most J' 's. The result also holds in the presence of pair-hopping away from half-filling.

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The discovery of high-temperature superconductivity has led to a great resurgence of interest in the properties of 2-dimensional spin-$\frac{1}{2}$ quantum antiferromagnets, and in particular the long-standing problem of the ground state. Though convincing arguments[1,2], but no rigorous proof, for Néel order at $T = 0$ exist in the case of the nn model on a square lattice, the situation is much less clear for other types of lattices or the addition of extra interactions, *e.g.* frustration. A variety of disordered ground states have been proposed[2]. They include RVB states,[3] dimer liquids (short range RVB)[4], dimer solids (Peirls states)[5−7], and flux states[5]. Another intriguing possibility are states with T- and P-invariance violation: the KL state[8], and the chiral spin state[9] on a frustrated square lattice. These proposals were supported by a variety of mean-field calculations. One should, however, be suspicious of such approximations. The spin Hamiltonians in question are equivalent[2] to strongly coupled lattice gauge theories (LGT). It is well known that mean-field approximations in gauge theory are, generally, unreliable even at a qualitative level [10].

In Ref. 9 a neat characterization of chiral spin states was provided in terms of Wilson loops of the statistical gauge field: in a T- and P-violating state, the expectation value of Wilson loops develops a non-trivial phase (imaginary part). Proving the existence of such states for reasonable model Hamiltonians is a necessary prerequisite for the physical realization of the anyon superconductivity scenario.

Now in a generic LTG of the usual sort, real-valuedness of the expectation of the Wilson loop (generally a complex operator) can be related to fundamental properties of the theory such as reflection positivity. One should, therefore, inquire whether such exact considerations place similar restrictions on expectations in the type of LGT encountered in the spin models.

In this paper we consider Heisenberg antiferromagnets with nn exchange J and next nn J' along plaquette diagonals, and show that expectations of Wilson loops are indeed always real by virtue of the reflection positivity properties of the theory. We first prove this for $J' \leq \frac{1}{2}J$ ($d = 2$), and then extend the result to much wider

ranges of (generally position-dependent) J''s. Extensions to some other types of frustration, as well as generalizations to $SU(N)$ gauge symmetry are also possible. Finally, we show that the result persists away from half-filling in the presence of hole hoping terms.

Consider the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on a hypercubic lattice Λ_s in d space dimension ($d \geq 2$):

$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J' \sum_{p=\langle ijk\ell \rangle} (\mathbf{S}_i \cdot \mathbf{S}_k + \mathbf{S}_j \cdot \mathbf{S}_\ell) \tag{1a}$$

with nn coupling J along each (oriented) bond $\langle ij \rangle$, and next nn coupling J' along the diagonals of every elementary (oriented) plaquette $\langle ijk\ell \rangle$. (1a) may also be written in the form:

$$H = \hat{J} \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J' \sum_{\langle ijk\ell \rangle} (\mathbf{S}_i + \mathbf{S}_\ell) \cdot (\mathbf{S}_j + \mathbf{S}_k) \tag{1b}$$

where $\hat{J} \equiv [J - 2(d-1)J']$. Both forms (1a) and (1b) will be useful in the following. We will employ a fermion representation of the spin operators $\mathbf{S}_i = \frac{1}{2}\, c^\dagger_{i\alpha} \sigma_{\alpha\beta} c_{i\beta}$ in terms of fermion operators $c^\dagger_{i\alpha}, c_{i\alpha}$ on site i with spin $\alpha = \pm 1$ and subject to the single occupancy constraint

$$c^\dagger_{i\alpha} c_{i\alpha} = 1 \tag{2}$$

at every site i. It will be convenient to employ a 2-component Nambu spinor notation: $\psi_{i1} \equiv c_{i1}$, $\psi_{i2} \equiv c^\dagger_{i-1}$. In terms of ψ_i the constraint (2) becomes $\psi^\dagger_i \sigma^3 \psi_i = 0$.

To study the system (1)-(2) we work in a $(d+1)$-dimensional path integral formulation where the operators $\psi^\dagger_{i\alpha}, \psi_{i\alpha}$ become independent anticommuting Grassman variables denoted $\bar{\psi}_{i\alpha}, \psi_{i\alpha}$. Let $\Lambda = \Lambda_s \times \beta$ denote the $(d+1)$-dim box of time-like extension β in which the system is placed, and $n_\mu(x)$, $\mu = 0, 1, \cdots, d$, the coordinates of site $x = (\tau, i)$. We work directly in the (Euclidean) time continuum[11]

and are interested in the zero-temperature thermodynamic limit, *i.e.* $|\Lambda| \to \infty$ limit. Working first with H in the form (1b), we linearize the four-fermion $\hat{J}$-interaction by the introduction[12] of a 2×2 matrix field $\mathbf{U}_b$ defined on nn bonds $b =< i, i, +\hat{\mu} >, (\hat{\mu} \neq 0)$, and of the form

$$\mathbf{U}_b = \begin{pmatrix} \alpha_b & -\beta_b \\ -\bar{\beta}_b & -\bar{\alpha}_b \end{pmatrix} = i\rho_b U_b$$

with complex $\alpha_b, \beta_b \in \mathbf{C}, \rho_b \equiv (|\alpha_b|^2 + |\beta_b|)^{1/2} \in \mathbf{R}^+$, and U_b and element of $SU(2)$. A Lagrange multiplier A_i is also introduced to enforce the constraint (2) at every site i. The partition function may then be written in the form:

$$\begin{aligned} Z_\Lambda = \int \prod_x d\bar{\psi}_x d\psi_x dA_x \prod_{\tau,b} dU_b d\rho_b \rho_b \\ \cdot \exp\left(- \int_0^\beta d\tau L \right) \end{aligned} \tag{3}$$

where dU_b is Haar measure over $SU(2)$, and antiperiodic (periodic) boundary conditions for fermionic (bosonic) fields are imposed in all directions. The Lagrangian is

$$\begin{aligned} L(\tau) = & \sum_i \bar{\psi}_i \left(\frac{d}{d\tau} - i\mathbf{A}_i \right) \psi_i \\ & - \frac{1}{4} \sum_{\substack{nn \\ \langle ij \rangle}} i\gamma_{\langle ij \rangle} \left[\bar{\psi}_i \rho_{\langle ij \rangle} U_{\langle ij \rangle} \psi_j - \bar{\psi}_j \rho_{\langle ij \rangle} U^\dagger_{\langle ij \rangle} \psi_j \right] \\ & + \frac{J'}{8} \sum_{p=\langle ijk\ell \rangle} \mathrm{tr} \left[(\mathbf{\Psi}_i^\dagger \cdot \mathbf{\Psi}_i + \mathbf{\Psi}_\ell^\dagger \cdot \mathbf{\Psi}_\ell) \cdot (\mathbf{\Psi}_j^\dagger \cdot \mathbf{\Psi}_j + \mathbf{\Psi}_k \cdot \mathbf{\Psi}_k) \right] \\ & + (4\hat{J})^{-1} \sum_{\substack{nn \\ b}} \rho_b \rho_b \end{aligned} \tag{4}$$

In (4) $\mathbf{A}_i \equiv \sigma^3 A_i$, and $\mathbf{\Psi}_i$ denotes the 2×2 matrix

$$\mathbf{\Psi}_i \equiv \begin{pmatrix} \psi_1 & \bar{\psi}_2 \\ \psi_2 & -\bar{\psi}_1 \end{pmatrix} \qquad \text{, with} \qquad \mathbf{\Psi}^\dagger_{i\alpha\beta} \equiv \bar{\mathbf{\Psi}}_{i\beta\alpha}.$$

A sign factor $\gamma_{\langle ij \rangle} = \pm 1$ can be arbitrarily chosen on each nn bond $\langle ij \rangle$ (see below). It is straightforward to verify by integration over $\mathbf{U}_b, A_i$ that (3) is indeed the partition function of the system (1b)-(2). The action in (3) is invariant under the gauge transformation $\psi_x \to h_x \psi_x$, $\bar{\psi}_x \to \bar{\psi}_x h_x^\dagger$, $U_{\langle x,y \rangle} \to h_x U_{\langle xy \rangle} h_y^\dagger$, $\mathbf{A}_i \to h_x[\mathbf{A}_i + i\frac{d}{d\tau}]h_x^\dagger$, with $h_x = e^{i\sigma^3 \omega_x} \in U(1)$. (4) is now seen to be the action of an $SU(2)$ gauge theory in a particular gauge, *i.e.* a (partially fixed) temporal-axial gauge where the "time-like" gauge field $\mathbf{A}_x$ has been gauge-rotated into the σ^3-generated $U(1)$ subgroup. Indeed note that all but the first term in (4) are actually invariant with $h_x \in SU(2)$, and recall that the Faddeev-Popov gauge-fixing ghost determinant decouples in axial gauges. Thus a gauge transformation of integration variables in (3) undoes the gauge fixing, and restores the full local $SU(2)$ invariance, *i.e.* invariance with $h_x \in SU(2)$, and $\mathbf{A}_x \equiv \sigma^a A_x^a$ now a general element of the $SU(2)$ Lie algebra. The argument in the rest of the paper does not depend on the presence or absence of such gauge fixings.

The sign factors γ_b in (4) have been left unspecified. We take

$$\gamma_{\langle x, x+\hat{\mu} \rangle} = (-1)^{\sum_{\nu > \mu} n_\nu(x)} \qquad , \mu \neq 0 \tag{5}$$

Clearly a redefinition of γ_b's amounts to a shift of U_b's by an element of Z_2, which by the invariance of the Haar measure leaves the path integral unaffected. The choice (5), however, will be shown to correspond to a choice of path integral variables preserving manifest reflection positivity. We thus end up with a lattice gauge theory of "staggered" fermions[13] in the strong coupling limit (no gauge field plaquette term).

Let π_μ denote any d-dim hyperplane in Λ perpendicular to the $\hat{\mu}$-direction, and lying between lattice sites, *i.e.* bisecting bonds. We only consider "time-like"

planes, *i.e.* $\hat{\mu} \neq 0$. π_μ decomposes Λ into two equal subsets Λ_+ and Λ_-.[14] Recall that reflection positivity[15,16] (RP) for reflection Θ about π_μ (where $\Theta(\Lambda_+) = \Lambda_-$) is the statement that

$$\langle F\Theta(F)\rangle_\Lambda \geq 0$$

for any observable F whose support is contained entirely in Λ_+. A standard trick[16] for discussing reflections about planes between sites is to introduce redundant "half-bond" variables for gauge fields by writing:

$$U_{\langle ij\rangle} \equiv w_{i,\langle ij\rangle} w^\dagger_{j,\langle ji\rangle} \qquad ,$$

and replacing $dU_{\langle ij\rangle}$ by $dw_{i,\langle ij\rangle} dw_{j,\langle ij\rangle}$ in (3). Reflections through a plane $\pi_{\mu\neq 0}$ without sites are now defined for the various fields by the rules:

$$\begin{aligned}
&\Theta(zA) \equiv z^*\Theta(A),\ \Theta(AB) \equiv \Theta(B)\Theta(A) \\
&\Theta(w_{x,\langle xy\rangle}) \equiv w^*_{\theta(x),\langle\theta(x),\theta(y)\rangle} \\
&\Theta(\mathbf{A}_x) \equiv \mathbf{A}_{\theta(x)},\ \Theta(\rho_{\langle xy\rangle}) \equiv \rho_{\langle\theta(x),\theta(y)\rangle} \\
&\Theta(\psi_x) \equiv i\bar{\psi}_{\theta(x)}\Gamma(x,\Theta(x)) \\
&\Theta(\bar{\psi}_x) \equiv i\psi_{\theta(x)}\Gamma(x,\Theta(x))
\end{aligned} \tag{6}$$

where Θ is a reflection that takes site x to site $\Theta(x)$, z any complex number, and A, B arbitrary polynomials in the variables with support in Λ_+. $\Gamma(x,\Theta(x))$ denotes the product of the $\gamma_{\langle y,y+\hat{\mu}\rangle}$'s along the straight line path from site x to site $\Theta(x)$. The factor of i in (6) is a consequence of the i occurring in the second sum in (4), which is in turn a consequence of the antiferromagnetic nature of the couplings in (1). In terms of the original spins $\mathbf{S}_x$, (6) indeed translates into $\Theta(\mathbf{S}_x) = -\mathbf{S}_{\theta(x)}$, *i.e.* a "twisted" reflection appropriate for antiferromagnetic couplings.[15] Let us also note that the Θ-operation should **not** be confused with a parity transformation.[17]

Using (6) one may verify that the action can be written in the form

$$-\int_0^\beta L d\tau = A + \Theta(A) + \sum_a c_a(\rho_{b\cap\pi}) B_a \Theta(B_a) - \int_0^\beta d\tau \sum_b \rho_b^2/4\hat{J}$$

where A, B_a are observables with support in Λ_+, and c_a depend only on ρ_b's for

which $b \cap \pi \neq \emptyset$, and are all non-negative provided $\hat{J}, J' \geq 0$. By a standard argument[15,16], and recalling that $\rho_b \in \mathbf{R}^+$, this implies that the full measure (3) satisfies RP for any observable of the form $F = \sum_k a_k(\rho_{b\cap\pi})F_k$, where F_k's have support in Λ_+ and $a_k \geq 0$. In other words the expectation of $\langle F\Theta(F)\rangle$ for such an F can be shown to be of the form

$$\sum_a \int \prod_{b\cap\pi} d\rho_b \rho_b e^{-\int \rho_b^2/4\hat{J}} |f_a(\rho_{b\cap\pi})|^2 \geq 0$$

for some set of functions $f_a(\rho_{b\cap\pi})$, and hence real non-negative.

We now apply this result to expectations of space-like Wilson loops of the statistical gauge field $\gamma_b \mathbf{U}_b$ whose imaginary part has been shown to provide an order parameter for the occurrence of generalized (chiral) "flux states"[9]. Consider any rectangular loop C bisected by a plane π_μ without sites (this implies that the loop length along $\hat{\mu}$-direction is odd – otherwise the loop size is arbitrary). The single plaquette p is the simplest example of such a loop. Then

$$W[C] \equiv \langle \mathrm{tr} \prod_{b\epsilon C} \gamma_b \mathbf{U}_b \rangle = \gamma_C \langle \mathrm{tr} \prod_{b\epsilon C} \rho_b U_b \rangle \tag{7}$$

where $\gamma_C \equiv \prod_{b\epsilon C} \gamma_b = \pm 1$. But, as with any Wilson loop bisected by a plane, $\mathrm{tr}(\prod_{b\epsilon C} \rho_b U_b)$ can be written in the form[16] $(\prod_{b\cap\pi} \rho_b)(\sum_a F_a \Theta(F_a))$, where $F_a(\{U_b, \rho_b\})$ has support only in Λ_+. Hence (7) is real by RP, and of constant sign determined by γ_C; *e.g.* for the single plaquette $\gamma_p = -1$.

$W[C]$ is, of course, $SU(2)$ gauge invariant. Expectations of gauge-dependent quantities will, by Elitzur's theorem, vanish unless computed after a gauge has been fixed. One may, for example, consider $U(1)$-gauge invariant expectations in the axial gauge:

$$\widetilde{W}[C] = \langle \mathrm{tr} \prod_{b\epsilon C} \gamma_b \frac{1}{2}(1 - \sigma^3)\mathbf{U}_b \rangle \tag{8}$$

Noting that, by the equations of motion for (4), the composite field $\mathbf{U}_b$ is given in

terms of the original variables by

$$(2\hat{J})^{-1}\gamma_{\langle ij\rangle}\mathbf{U}_{\langle ij\rangle} = \begin{pmatrix} -\bar{c}_{j\alpha}c_{i\alpha} & \epsilon_{\alpha\beta}c_{i\alpha}c_{j\beta} \\ -\epsilon_{\alpha\beta}\bar{c}_{j\alpha}\bar{c}_{i\beta} & \bar{c}_{i\alpha}c_{j\alpha} \end{pmatrix} \quad ,$$

one sees that $\widetilde{W}[C]$ is the expectation of the product of $\chi_{\langle x,x+\hat{\mu}\rangle} \equiv (\bar{c}_{x\alpha}c_{x+\hat{\mu},\alpha})$ around the loop C. $\widetilde{W}[C]$ are in fact the Wilson loops that have customarily been considered in the literature, in particular various mean-field calculations of disordered ground states[2]. The RP argument goes through unaltered for $\widetilde{W}[C]$; which hence is shown to be real.

As with all such RP arguments, this result holds uniformly in the volume $|\Lambda|$; in particular, it holds for all β, and in fact goes through directly in the infinite volume limit. It also holds with ψ_i coupled to an external uniform statistical field U_b^{ext}.[18] We conclude that all rectangular Wilson loops bisected by a time-like plane are real for $J, \hat{J} \geq 0$, *i.e.* $0 < J' \leq \frac{1}{2}J$ $(d = 2)$.

We now consider various generalizations of this result. First, the condition $J' \leq \frac{1}{2}J$ can be considerably relaxed, since it originates in the use of (1b) for H which is actually needed **only** for those p's bisected by the plane π. For p's not intersected by π, we may revert to the use of (1a) which results into no such restriction on J'. Furthermore, by linearizing both the nn and next nn interactions in (1a) we may consider Wilson loops of other than rectangular shape. Consider a loop C symmetric about a time-like plane π but otherwise arbitrary. Let Λ_o denote the set of bonds b and plaquettes p intersected by π. We write H in a hybrid form where (1a) is used for all $b, p \notin \Lambda_o$, and (1b) for all $b, p \in \Lambda_o$, and also generalize to space-dependent couplings $J_{\langle ij\rangle}, J'_p$. By introducing $\mathbf{U}_{\langle ij\rangle}$ for both nn and next nn site pairs $\langle ij\rangle \notin \Lambda_o$, one obtains a straightforward generalization of (4) with shifted couplings

$$\hat{J}_{\langle ij\rangle} \equiv (J_{\langle ij\rangle} - \sum_{p\ni\langle ij\rangle} J'_p) \qquad \text{only for } \langle ij\rangle \in \Lambda_o.$$

RP for reflections about π is maintained provided that $J_b = J_{\theta(b)}, J'_p = J'_{\theta(p)}$, and

for next nn $\langle ij \rangle \notin \Lambda_o$ we take

$$\gamma_{\langle x, x+\hat{\mu}\pm\hat{\nu}\rangle} = (-1)^{\sum_{\lambda>0} n_\lambda(x)} \tag{9}$$

as the analog of (5). It again follows that $W[C]$ is real if $\hat{J}_b \geq 0$. One thus obtains a large class of systems with various patterns of space-dependent couplings for which loops symmetric about a given plane, but otherwise of arbitrary shape and size probing all Λ_s are proven not to develop a non-trivial phase.

Though we have not systematically investigated next nn couplings other than along plaquette diagonals, it is easy to see that similar considerations can be applied to other short range interactions.[19] An example where the above argument also goes through is the off-axis antiferrogmanetic exchange ($d = 2$) with $J_{\langle ij \rangle} \neq 0$ if $n_1(i) - n_1(j) = 1,\ n_2(i) - n_2(j) > 1$.

It should also be noted that various generalizations from $SU(2)$ to $SU(N)$ gauge symmetry[5,6] are also straightforward.

Finally, we consider relaxing the half-filling constraint (2) by adding to the Lagrangian (4) a mass term for $\mathbf{A}_i$. This then allows the introduction of hole hopping terms which have often been cited as a source of disorder favoring a spin liquid state. The Lagrangian (4) is correspondingly extended to[20]

$$\begin{aligned} L' = L - (\frac{t}{J}) \sum_{\substack{nn \\ \langle ij \rangle}} i\ \rho_{\langle ij \rangle} \left[\mathrm{tr}\frac{1}{2}(1+\sigma^3) U_{\langle ij \rangle} - \mathrm{tr}\frac{1}{2}(1+\sigma^3) U^\dagger_{\langle ij \rangle} \right] \\ + \mu \sum_u \mathrm{tr}\mathbf{A}_i^2 \end{aligned} \tag{10}$$

Integration over $\mathbf{U}_b$ now reproduces the Lagrangian for the sum of (1) plus a kinetic hole Hamiltonian

$$H_h = -t \sum_{\substack{nn \\ \langle ij \rangle}} \gamma_{\langle ij \rangle} [\bar{\psi}_i \sigma^3 \psi_j + \bar{\psi}_j \sigma^3 \psi_i] \tag{11}$$

Now L' preserves RP under reflections (6). Hence all Wilson loops (7)-(8) remain real also in the presence of hole hopping (11).

The violation of the single occupancy constraint (2) is proportional to μ. Note that in (10) the fermion concentration was not fixed to some particular value by an explicit chemical potential term. This is because, as is well-known, non-zero chemical potentials for fermions generally violate RP. This, however, should be of little consequence for our purposes here: by appropriately varying μ, expectations can receive contributions (of any relative amount) from all parts of the function space in (3), *i.e.* configurations at any filling.

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10. This is true even at large N unless one first manages to integrate out the gauge fields. An exception occurs in the presence of a large modulus Higgs

field (in unitary gauge) freezing bond variables along some group direction. This is not the case here.

11. A more careful definition of the path integral in terms of a latticized τ-direction can be given, and provides insight in the relation between fermion doubling, chiral symmetry breaking, and long-range order; but it is not really necessary for our argument.

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14. Note that with Λ wrapped around a torus ((anti)periodic b.c.) such a hyperplane actually consists of a pair of planes cutting the torus in two pieces.

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17. Thus, *e.g.*. , a P-transformation reverses the direction around a closed loop, but Θ does not.

18. $U_b^{\mathrm{ext}} \epsilon\, U(1)$ if the symmetry has been gauged fixed down to $U(1)$.

19. An argument (non-rigorous), not related to the methods employed in this paper,that a FQHE state cannot be the ground state of Heisenberg antiferromagnets with short range interactions was given in S. Yu. Khlebnikov, JETP Lett., 53, 88 (1991).

20. The $\mathbf{A}_i$-mass term, which mimics finite U in an underlying Hubbard model, actually preserves invariance under τ-independent gauge transformations. The hopping term appears to break all gauge invariance. Since the rest

of the Hamiltonian is gauge invariant, however, such breaking may, as always, be viewed as implicit gauge fixing – in this case, the unitary gauge of rotating a complex (slave boson) scalar field of constant modulus (absorbed in t) to unity.