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Absence of instanton-induced spin-Peierls order in the flux phase

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The flux phase of the fermionic SU(n) quantum antiferromagnet is charge-conjugation and translationally invariant. It follows that instantons do not generate spin-Peierls order, in contrast to their behavior in other antiferromagnets that break these symmetries.

The large-n limit of a nearest-neighbor fermionic SU(n) quantum antiferromagnet on the square lattice has a locally (and probably globally) stable spin-liquid saddle point called the flux phase.[1] This state has no broken symmetries and exhibits gapless spin excitations at momenta $(0,\pi)$ and $(\pi,0)$ in accordance with a proposed two-dimensional generalization of the Lieb-Schultz-Mattis theorem.[2] It is important to establish whether the flux phase survives at finite n since if it does it would be a nontrivial example of a two-dimensional spin liquid. In a recent Letter[3] I discussed how the appearance of Néel order as n decreases from infinity down to sufficiently small values can be understood as a transition in which the fermions become massive and bind into massless mesons. These mesons are simply the gapless spin waves required by Goldstone's theorem. However, the role of topological excitations (instantons) remained unclear. In this Rapid Communication I show that instantons do not induce spin-Peierls order in the flux phase. This behavior contrasts with that of certain other quantum antiferromagnets which I review below.

Topological excitations can radically change the ground states of some quantum antiferromagnets. In one spatial dimension, the critical properties of spin chains are well described by nonlinear σ models with an additional Berry's phase term.[4] For half-integer spins, Berry's phase of smooth space-time configurations of the staggered spin equals $n\pi$ where n is the integer winding number of the configuration. The destructive interference between different configurations accounts for the existence of gapless spin excitations. In contrast, spin excitations in integer-spin chains generically have a nonzero gap because Berry's phase vanishes (modulo 2π) for all staggered spin configurations and the coupling constant of the pure nonlinear σ-model flows to large values at long length scales. This picture is borne out by exact solutions of spin-chain systems.[5,6]

On the two-dimensional square lattice, smooth space-time configurations of the staggered spin always have zero Berry's phase.[7,8] Haldane showed that nontrivial Berry's phases only arise if space-time singularities in the staggered spin (instantons) are permitted.[7] When the ground state is Néel ordered, pairs of instantons with opposite charge are strongly confined and do not contribute significantly to the partition function. If, on the other hand, the system is not Néel ordered (a possibility when frustrating interactions are included in the Hamiltonian) then instantons are deconfined and proliferate. The total charge must be zero to satisfy periodic boundary conditions, but Berry's phase in the half-integer spin case (specified below) can be either 0, $\pi/2$, π, or $3\pi/2$ depending on the locations and charges of the individual instantons. The existence of four possible phases suggests that the ground state will be fourfold degenerate. However, it was unclear from Haldane's approach exactly what the ground state would be since the σ model only makes sense if the staggered spin has at least quasi-long-range order. This assumption precludes the possibility of a detailed understanding of ground states with short-range spin-spin correlations.

Read and Sachdev addressed this problem by studying the compact U(1) gauge theory of a bosonic SU(n) antiferromagnet.[9] Unlike the σ model, this formulation of the problem[10] is exact and does not rely on the existence of long-range spin order. Indeed, the SU(n) model can be solved exactly in the large-n limit and on the square lattice exhibits a phase with no Néel order and no low-energy spin excitations. Instantons are deconfined in this massive phase and appear as U(1) monopoles in the phases of the Hubbard-Stratonovich fields that are introduced to factorize the four-boson interaction term. The effective action for these gauge fields contains the Berry's phase term (identical to the term Haldane found): $\theta_B=(\pi/2)\sum_{\mathbf{s}} q_{\mathbf{s}}\zeta_{\mathbf{s}}$ where $q_{\mathbf{s}}$ is the (integer) instanton charge (summed over all time) centered on site $\mathbf{s}$ of the dual lattice (the lattice formed by the centers of the squares) and $\zeta_{\mathbf{s}}$ is 0, 1, 2, or 3 depending on whether $\mathbf{s}$ is, respectively, an even-even, even-odd, odd-odd, or odd-even dual lattice site. Despite appearances, θ_B is actually invariant under a $\sqrt{2}$ diagonal translation of all instantons because $\sum_{\mathbf{s}} q_{\mathbf{s}}=0$. Another piece of the effective action couples the electric field on each link to the spin-Peierls order parameter $\langle \mathbf{S}_{\mathbf{x}}\cdot\mathbf{S}_{\mathbf{x}+\mathbf{e}}-\mathbf{S}_{\mathbf{x}}\cdot\mathbf{S}_{\mathbf{x}-\mathbf{e}}\rangle$ where $\mathbf{x}$ is a lattice site and $\mathbf{e}$ is a unit vector connecting neighboring sites.

The Berry's phase depends on the charges and positions of the instantons because the bosonic SU(n) formulation of the nearest-neighbor antiferromagnet breaks translational and charge-conjugation symmetries. In particular, different representations of the SU(n) bosons (related by charge conjugation) are placed on the even and odd sites of the square lattice.[11] Thus, the Hamiltonian itself breaks translational and charge-conjugation symmetries and the massive phase should not be considered a true spin-liquid, even in the infinite n limit. At finite n, for SU(n) representations that are the analogues of the half-integer spin SU(2) representations, this $\sqrt{2}$ unit cell is spontaneously broken in the massive phase by the appearance of a nonzero density of positive and negative instantons that are oriented because of the Berry's phase term. A static electric field appears along particular links, which in turn induces spin-Peierls order in the form of a slight (exponentially small in n) enhancement of singlet correlations on one quarter of the links. These links form columns throughout the lattice, consistent with Haldane's hypothesis that the ground state should have a fourfold degeneracy. (An identical crystallization pattern was reported in a study of short-range resonating valence bonds.[12] In that model, an explicit background electric-field breaks translational and charge-conjugation invariance. Again the Berry's phase term appears, and instantons induce dimer ordering.)

In contrast, the *fermionic* SU(n) Hamiltonian does not break translational or charge-conjugation symmetries because the fermions on each lattice site are in the same (antisymmetric self-conjugate) representation of SU(n).[13] In the large-n limit, translational symmetry breaks spontaneously on a wide variety of lattices (including the square lattice) in the absence of biquadratic coupling.[14] But the inclusion of this term stabilizes the flux phase on the unfrustrated square lattice without altering the physical SU(2) Hamiltonian apart from a trivial renormalization of the usual bilinear spin-exchange constant. (See Ref. 1 for an extended discussion of this system.) The flux phase preserves all the symmetries of the original Hamiltonian: there is no Néel nor spin-Peierls order, and translational, time-reversal, reflection and charge-conjugation symmetries are preserved. Therefore, the Berry's phase of an instanton cannot depend on the sign of its charge or its position.

To illustrate this invariance with a simple calculation, consider the effect of charge-conjugation on the effective action for instantons. Both the bilinear (J) and biquadratic ($\tilde{J}$) interactions can be decomposed via Hubbard-Stratonovich transformations by introducing complex link fields $\chi_{\mathbf{xy}}$ and real link fields $\Phi_{\mathbf{xy}}$. The phases of the $\chi_{\mathbf{xy}}$ fields transform as spatial gauge fields under local U(1) transformations and the time component of the gauge field appears in the guise of a Lagrange multiplier field ($\phi_{\mathbf{x}}$) that enforces the local particle-number constraint ($n/2$ fermions live on each site, where n is an even integer). The effective action is now obtained by integrating out the Grassman fields $c_{\mathbf{x}}$ and $c_{\mathbf{x}}^*$:

$$\exp(-S_{\text{eff}}[\chi,\Phi,\phi]) = \int [dc^*][dc] \times \exp(-nS[\chi,\Phi,\phi,c^*,c])\,.$$

Here the imaginary time action (setting $J=1$) is given by

$$S[\chi,\Phi,\phi,c^*,c] = \int d\tau \Bigg\{ \sum_{\mathbf{x}} \left[\tfrac{1}{2} c_{\mathbf{x}}^* \left(\frac{\partial}{\partial\tau} c_{\mathbf{x}} \right) - \frac{1}{2} \left(\frac{\partial}{\partial\tau} c_{\mathbf{x}}^* \right) c_{\mathbf{x}} + i\phi_{\mathbf{x}} (c_{\mathbf{x}}^* c_{\mathbf{x}} - \tfrac{1}{2}) \right] + \sum_{\langle\mathbf{xy}\rangle} [(1/\tilde{J})\Phi_{\mathbf{xy}}^2 + |\chi_{\mathbf{xy}}|^2 + (1-2i\Phi_{\mathbf{xy}})^{1/2} (\chi_{\mathbf{xy}} c_{\mathbf{y}}^* c_{\mathbf{x}} + \chi_{\mathbf{xy}}^* c_{\mathbf{x}}^* c_{\mathbf{y}})] \Bigg\}\,.$$

By choice of gauge, $\phi_{\mathbf{x}}$ can be set to zero. Also, $\Phi_{\mathbf{xy}}$ is equal to an imaginary constant at the flux saddle point. (The Φ_{xy} fields are gauge invariant.) Upon charge conjugating the fermions

$$c_{\mathbf{x}} \rightarrow \begin{cases} c_{\mathbf{x}}^*;\ \mathbf{x} \in \text{even sublattice}\,, \\ -c_{\mathbf{x}}^*;\ \mathbf{x} \in \text{odd sublattice}\,, \end{cases}$$

the effective action transforms as $S_{\text{eff}}[\chi,\Phi] \rightarrow S_{\text{eff}}[\chi^*,\Phi]$. Thus, the effective action for an instanton equals that of an anti-instanton, since the instanton charge is reversed when the $\chi_{\mathbf{xy}}$ fields are complex conjugated. (The $\chi_{\mathbf{xy}}$ fields can be chosen to be purely real at the flux-phase saddle point by a gauge transformation. Instantons then contribute an imaginary component to $\chi_{\mathbf{xy}}$ which changes sign under complex conjugation.) Berry's phase is just the imaginary part of the Euclidean effective action and is clearly invariant under the charge-conjugation operation. Instantons therefore do not induce a net electric field along particular links and no spin-Peierls ordering will occur.

The fact that the fermionic SU(n) and the bosonic SU(n) quantum antiferromagnets behave differently may seem paradoxical, since both versions describe the same two-dimensional nearest-neighbor square lattice spin-$\frac{1}{2}$ Heisenberg antiferromagnet at $n=2$. Actually, neither spin-liquid nor spin-Peierls behavior occurs in the physical SU(2) limit; instead, the ground state is Néel ordered. Dynamical processes are likely responsible for this long-range spin order.[3] But the absence of topologically induced spin-Peierls order in the fermionic SU(n) quantum antiferromagnet means that the flux phase remains a viable spin-liquid candidate for finite $n > 2$.

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[11]In fact, bosonic SU(n) generalizations of SU(2) models do not work on nonbipartite lattices, for systems with frustrating interactions, nor for t-J models of holes hopping in an antiferromagnetic background because some pairs of spins will be in the same representation and cannot be combined into the SU(n) singlet form needed to make a Hamiltonian with antiferromagnetic couplings. [This problem does not arise in the physical SU(2) case because the SU(2) representations are self-conjugate.] A different bosonic generalization, based on the symplectic group $Sp(n)$, does not break charge-conjugation or translational symmetries at the Hamiltonian level and works on frustrated and nonbipartite lattices [N. Read and S. Sachdev (unpublished)]. The global U(1) gauge symmetry breaks spontaneously at the saddle point and the bosons acquire opposite charges on two sublattices. The Berry's phase again depends on the positions of the instantons because of this sublattice structure.

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[13]Fermionic SU(n) generalizations of antiferromagnets are possible on all lattices and electronic degrees of freedom can be easily incorporated. These extensions work because spins have an electronic origin in itinerant models and electrons are fermions, not bosons.

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