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LETTER TO THE EDITOR

SO(3) σ models of the two-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet

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Abstract. An SO(3) gauge theory of the spin-$\frac{1}{2}$ Heisenberg antiferromagnet (HA) on a two-dimensional square lattice is developed. The effective action Γ_{sc} of the system is described by an anisotropic SO(3) σ model supplemented by Berry's phase terms, featuring a possible instability of the regular Néel ground state. This problem is discussed in connection with the singlet nature of the ground state of the spin-$\frac{1}{2}$ HA and in terms of a generalised chiral SO(3)^2 σ model.

According to Haldane (1983) the first-order approximation to a semiclassical action Γ_{sc} of the spin-$\frac{1}{2}$ HA on a square lattice with Hamiltonian

$$H = J \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z) \tag{1}$$

represents an O(3) σ model

$$\tilde{\Gamma}_{sc} = \frac{1}{2f} \int d^3x \left(\frac{1}{c^2} (\partial_t \boldsymbol{n})^2 - (\nabla \boldsymbol{n})^2 \right). \tag{2}$$

Here $\boldsymbol{n} = (n^1, n^2, n^3)$ is a unit vector field, J and f are coupling constants and $c \sim J\hbar$. Additional terms to (2) taking account of finite spin s have been suggested in the form of Hopf's invariant by Wilczek and Zee (1983), and by Wen and Zee (1988) and Haldane (1988) in the form of Berry's (1984) phase term, where only the latter survives in perturbation theory. The correct expression for Γ_{sc} should be such that at $T = 0$ its ground state is non-degenerate corresponding to the spin singlet ground state of (1) (Lieb and Mattis 1962). Using (2) this is obviously hard to achieve, because its classical ground state at $T = 0$ is symmetry broken and has an ∞^2 degeneracy.

The approach described below is motivated by the observation that the dynamics described by (1) is invariant under gauge transformations SO(3) $\times$ SU(2) of coordinate and Hilbert space basis. The diagonal of this group $G_D \sim$ SO(3) corresponds to the subgroup $G \sim$ SO(3) of gauge transformations of the $\{\boldsymbol{n}\}$ field in (2). Accordingly if one applies to (2) $g \in G$ defined by

$$g : \boldsymbol{n} \to \boldsymbol{n}' = \mathbf{G} \cdot \boldsymbol{n} \qquad \mathbf{G} \in \mathrm{SO}(3) \tag{3}$$

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where $\mathbf{G}=\mathbf{G}(x)$, $x\equiv(\boldsymbol{r},t)$, one may also study $\tilde{\Gamma}_{sc}=\tilde{\Gamma}_{sc}(\{\mathbf{G}\},\{(d/dt)\mathbf{G}\})$. In this representation the dynamic variables of $\tilde{\Gamma}_{sc}$ are the sets $\{\mathbf{G}\}$ and $\{(d/dt)(\mathbf{G})\}$, whereas the $\{\boldsymbol{n}\}$ field may be gauge fixed by $\{\boldsymbol{n}_f\}$. The three-dimensional nature of SO(3)-space implies that one of its dimensions represents gauge degrees of freedom, which are fixed by those sets $\{g_f\}$, where $g_f=\{\mathbf{G}(x)\}$ satisfies

$$\boldsymbol{n}_f(x)=\mathbf{G}(x)\cdot\boldsymbol{n}_f(x). \tag{4}$$

Suppose that $\tilde{\Gamma}_{sc}\sim\Gamma_{sc}$ is derived from (1) in a two-step procedure. First apply $g\in G_D$ to (1) yielding

$$g:H\to H_g=H_g\left(\{\mathbf{G}\},\left\{\frac{d}{dt}G^{(1/2)}\right\};\{\mathbf{S}(x)\}\right) \tag{5}$$

where $G^{(1/2)}(x)$ is a spin-$\frac{1}{2}$ representation of $\mathbf{G}(x)$. In the second step $\{\mathbf{S}(x)\}$ is integrated out and yields

$$\Gamma_{sc}\left(\{G\},\left\{\frac{d}{dt}\mathbf{G}\right\}\right) \tag{6}$$

where Γ_{sc} can also be expressed in terms of $\{G^{(1/2)}\}$ and $\{(d/dt)G^{(1/2)}\}$. If Γ_{sc} has anything to do with $\tilde{\Gamma}_{sc}$, a trace of the expectation value of the spin field $\{\mathbf{S}(x)\}$ under the rotational motion enforced by g should be observable in Γ_{sc} in the form of the field $\{\boldsymbol{n}_f(x)\}$. This field (if it exists) will play for Γ_{sc} the role of a gauge field, i.e. Γ_{sc} should prove invariant under the set $\{g_f\}$ satisfying (4). However, on account of the singlet nature of the ground state of H, the field $\{\boldsymbol{n}\}\sim\{\boldsymbol{n}_f\}$ is supposed to vanish. Accordingly $\tilde{\Gamma}_{sc}$ cannot be derived from (6) in a rigorous fashion, and the physical situation is similar as in polarisable media, i.e. 'electric' and 'magnetic' momenta corresponding to non-vanishing $\{\boldsymbol{n}\}$ fields may be induced by chiral fields, but decay after turn-off. For $s\to\infty$ the situation is qualitatively different, because symmetry-broken states leading to (2) may be long lived.

In the following the derivation of Γ_{sc} will be sketched and for more details the reader is referred to Holz (1990a). A gauge transformation $g\in G_D$ of (1) is characterised by a set $\{\mathbb{R}^{(1/2)}\}$ with $\mathbb{R}^{(1/2)}\in SU(2)$, and the unitary transformation

$$U=\prod_{i=1}^{N}\mathbb{R}_i^{(1/2)} \tag{7}$$

implying

$$g:H\to H_g=U^\dagger HU-i\hbar U^\dagger\partial_t U.$$

Next on a regular Néel sublattice L_A one defines

$$\varepsilon_i=\begin{cases}-1 & i\in L_A\\ +1 & i\notin L_A\end{cases}$$

and

$$\mathbb{R}_i^{(1/2)}=R_i^{(1/2)}\{\tfrac{1}{2}(1-\varepsilon_i)R_x^{(1/2)}+\tfrac{1}{2}(1+\varepsilon_i)I^{(1/2)}\} \tag{8}$$

where $R_x^{(1/2)}$ represents a 180° rotation around the $\hat{x}$ axis. Using the representation

$$\boldsymbol{S}_i=\hbar\{\tfrac{1}{2}(a_i^\dagger+a_i)\boldsymbol{e}_x+\tfrac{1}{2}i(-a_i^\dagger+a_i)\boldsymbol{e}_y+(a_i^\dagger a_i-\tfrac{1}{2})\boldsymbol{e}_z\} \tag{9}$$

where

$$a_i a_i^\dagger + a_i^\dagger a_i = 1 \tag{10}$$

and for $i \neq j$ all commutators of the set $\{a_i;\, a_i^\dagger\}_{i=1,\dots,N}$ vanish, one obtains

$$g : \boldsymbol{S}_i \to \boldsymbol{S}_i' = \boldsymbol{S}_i \qquad (\boldsymbol{e}_1 \to \boldsymbol{e}_{j1}' = (\boldsymbol{R}_j^\dagger)_{1p}\boldsymbol{e}_p). \tag{11}$$

Inserting (11) into H_g yields

$$H_g = \frac{J\hbar^2}{4} \sum_{\langle i,j\rangle} R_{zz}^{(ji)} + H_g^{(1)} + H_g^{(2)} \tag{12}$$

where

$$H_g^{(1)} = \frac{J\hbar^2}{4} \sum_i \sum_{j\in nn_i} \left\{ \left[\mathrm{i}R_{zy}^{ji} + \varepsilon_i R_{zx}^{ji} - \frac{2}{J\hbar z}(\Theta_{i,t}^1 + \mathrm{i}\varepsilon_i \Theta_{i,t}^2) \right] a_i \right.$$
$$\left. + \frac{1}{2}\left(R_{zz}^{(ij)} - \frac{2\varepsilon_i}{J\hbar z}\Theta_{i,t}^3 \right)(a_i^\dagger a_i - a_i a_i^\dagger) + \text{HC} \right\} \tag{13a}$$

$$H_g^{(2)} = \frac{J\hbar^2}{4} \sum_{i,j\in nn_i} \{[\tfrac{1}{2}(R_{xx}^{(ji)} + R_{yy}^{(ji)}) - \mathrm{i}\varepsilon_i R_{xy}^{[ij]}]a_i a_j + [\tfrac{1}{2}(R_{xx}^{(ji)} - R_{yy}^{(ji)}) - \mathrm{i}\varepsilon_i R_{xy}^{(ij)}]a_i^\dagger a_j$$
$$+ 2(\mathrm{i}R_{yz}^{ji} + \varepsilon_i R_{xz}^{ji}) a_j^\dagger a_i^\dagger a_i - R_{zz}^{(ji)} a_i^\dagger a_i a_j^\dagger a_j + \text{HC}\}. \tag{13b}$$

Here HC represents the Hermitian conjugate, z the coordination number of the lattice, nn_i the nearest neighbours to i and $\mathbf{R}^{ji} \equiv \mathbf{R}_j^t \cdot \mathbf{R}_i$. Furthermore

$$\mathbf{R}^{(ji)} = \tfrac{1}{2}(\mathbf{R}^{ji} + \mathbf{R}^{ij}) \qquad \mathbf{R}^{[ij]} = \tfrac{1}{2}(\mathbf{R}^{ij} - \mathbf{R}^{ji}) \tag{14, 15}$$

and the angular velocity vector $(\Theta_{,t}^1, \Theta_{,t}^2, \Theta_{,t}^3)$ in the body-fixed frame is obtained from the three Maurer–Cartan 1-forms of SO(3)-space

$$\Theta^a = -\hat{\Theta}^a\, \mathrm{d}\Theta - \sin\Theta\, \mathrm{d}\hat{\Theta}^a + (1-\cos\Theta)\varepsilon^{abc}\, \mathrm{d}\hat{\Theta}^b \hat{\Theta}^c \tag{16}$$

in the form $\Theta^a = \Theta_{,t}^a\, \mathrm{d}t$. Here ε^{abc} is the totally antisymmetric symbol in 3-space, and $\{\hat{\boldsymbol{\Theta}}, \Theta\}$ are coordinates in SO(3)-space. Using the notation

$$\Delta\Theta_i^a \equiv \Theta_i^a(d \to \boldsymbol{\delta}_{ji} \cdot \boldsymbol{\nabla}_i) \tag{17}$$

where $\boldsymbol{\delta}_{ji}$ is a nearest-neighbour vector all quantities in H_g can be expressed in terms of the components of (16) and their derivatives.

Γ_{sc} can now be derived via the effective Lagrangian $\mathscr{L}_{\mathrm{eff},g}(\tau)$, which is computed over the ground-state amplitude

$$\exp\left[\frac{\mathrm{i}}{\hbar}\int_{t'}^{t} \mathrm{d}\tau\, \mathscr{L}_{\mathrm{eff},g}(\tau)\right] = \langle\Phi_0|\hat{U}(t,t')|\Phi_0\rangle. \tag{18}$$

Here the evolution operator is defined as usual

$$\hat{U}(t,t') = T\exp\left(-\frac{\mathrm{i}}{\hbar}\int_{t'}^{t} \mathrm{d}\tau\, H_{g,I}(\tau)\right) \tag{19}$$

where T is the time-ordering operator and $H_{g,I}(\tau)$ is H_g transformed to the interaction picture. This is formulated in terms of a magnon representation, where (10) is accounted for by a hard-core repulsion

$$H_{\text{hc}} = \lambda_\infty \sum_{i=1}^{N} a_i^{\dagger 2} a_i^2. \tag{20}$$

Within the magnon approach $\mathcal{L}_{\text{eff},g}$ has been computed by Holz (1990b) and can formally be represented as

$$\begin{aligned}\mathcal{L}_{\text{eff},g} \simeq \mathcal{L}_0 + \frac{1}{2J} \int & \mathrm{d}^2 r \{k_a (\Theta^a_{,t})^2 + k_{ab} \Theta^a_{,t} \Theta^b_{,t} \Theta^a_{,p} \Theta^b_{,p}\} \\ & - \frac{J\hbar^2}{2} \int \mathrm{d}^2 r \{g_a (\Theta^a_{,p})^2 + g_{ab} \Theta^a_{,pp'} \Theta^b_{,pp'} + g^{cd}_{ab} \Theta^a_{,p} \Theta^b_{,p} \Theta^c_{,q} \Theta^d_{,q}\} \\ & - \frac{\hbar}{2} \sum_{i=1}^{N} \varepsilon_i (\gamma^c + b^c_{ab} \Theta^a_{,p} \Theta^b_{,p}) \Theta^c_{,t}.\end{aligned} \tag{21}$$

Here the notation

$$\Theta^a = \Theta^a_{,t}\, \mathrm{d}t + \Theta^a_{,p}\, \mathrm{d}x^p \qquad \Theta^a_{,pq} \equiv \partial_q \Theta^a_{,p} \tag{22}$$

has been used and summation convention is implied. The second and third terms of $\mathcal{L}_{\text{eff},g}$ represent kinetic and potential energy respectively, and the last term represents a Berry's phase term. In third-order perturbation theory a Chern–Simons term may form but vanishes identically as a consequence of the symmetry of the bare propagators. Within a similar approach this result has been derived earlier by Wen and Zee (1988).

$\mathcal{L}_{\text{eff},g}$ suffers under at least three defects.

(i) It is not invariant under the chiral transformations

$$\mathbf{R}(x) \to \mathbf{A} \cdot \mathbf{R}(x) \cdot \mathbf{B}' \qquad \mathbf{A}, \mathbf{B} \in \mathrm{SO}(3) \times \mathrm{SO}(3). \tag{23}$$

More precisely it is invariant under $\mathbf{A}$ (left invariance) but not under $\mathbf{B}$ (gauge transformation). This is a consequence of the symmetry-broken ground state.

(ii) The coefficients $\{g_a\}$ are not necessarily all positive, at least in low-order perturbation theory. If true it signals an instability of the regular Néel sublattice L_A.

(iii) Some of the coefficients in $\mathcal{L}_{\text{eff},g}$ (e.g. $\{k_a\}$) suffer under infrared infinities.

From this various conclusions can be drawn.

(*a*) Non-existence of a Chern–Simons term may be an artifact of perturbation theory, which fails due to (iii). Consequently use of a renormalised (by the chiral field) propagator of lower symmetry may change this result.

(*b*) L_A has to be modified by means of a dynamic network of phase boundaries. This will partially restore the rotational symmetry, broken by the imposition of L_A.

(*c*) For $\{g_a\} < 0$ defects classified by the homotopy groups $\pi_1(\mathrm{SO}(3)) = Z_2$ and $\pi_3(\mathrm{SO}(3)) = Z$ will form abundantly and restructure the Néel ground state.

(*d*) The use of a renormalised propagator based on the harmonic part of H_g will feature for generic gauges $\{\mathbb{R}^{(1/2)}\}$ negative mass for certain domains of the 2-space. This leads to an abundant production of magnons and in this way to a decay of the Néel ground state. Presumably this is the physical origin of $\{g_a\} < 0$.

(*e*) A computation of the new ground state of Γ_{sc} requires that the saddle point (trajectory) is sought in complex SO(3)-space. That is obtained by replacing the chiral vector $\Theta\hat{\mathbf{\Theta}}$ by a complex quantity $\Theta(\mathrm{e}^{\mathrm{i}\varphi a}\hat{\Theta}^a)$, i.e. SO(3) is replaced by SO(3, 1), which can be formally considered as two coupled SO(3)-spaces.

From this I conclude tentatively that Γ_{sc} is represented by two SO(3) fields, $\{\mathbf{R}_\sigma\}_{\sigma=1,2}$ reflecting the two earlier Néel sublattices and being described by a Lorentz invariant action postulated to be of the form

$$\Gamma_{sc} \sim \frac{1}{4}\sum_{\sigma,\sigma'}\frac{1}{f_{\sigma\sigma'}}\int d^3x\,\eta^{\mu\nu}\,\mathrm{trace}(\partial_\mu \mathbf{R}'_\sigma \partial_\nu \mathbf{R}_{\sigma'})$$
$$+\frac{1}{2}\sum_{\sigma,\sigma'}\frac{1}{g_{\sigma\sigma'}}\int d^3x\left[\frac{1}{c^2}(E^a_{\sigma,1}E^a_{\sigma',1}+E^a_{\sigma,2}E^a_{\sigma',2})-B^a_\sigma B^a_{\sigma'}\right]$$
$$+\sum_{\sigma,\sigma'}\frac{\vartheta_{\sigma\sigma'}}{8\pi^2}\int \Theta^1_{(\sigma}\wedge\Theta^2_{\sigma'}\wedge\Theta^3_{\sigma')} \tag{24}$$

where

$$E^a_{\sigma,q} \equiv (\Theta^a_{\sigma,tq}-\Theta^a_{\sigma,qt}) \qquad q=x,y$$
$$B^a_\sigma \equiv \Theta^a_{\sigma,xy}-\Theta^a_{\sigma,yx} \tag{25}$$

and $\mathrm{diag}(\eta^{\mu\nu})=(1/c^2,-1,-1)$. The first term of (24) represents a generalised $SO(3)^2\sigma$ model, and a diagonal term is of the form

$$\Gamma^\sigma_{SO(3)} = \frac{1}{2f_{\sigma\sigma}}\int d^3x\left\{\left[\frac{1}{c^2}(\partial_t\Theta_\sigma)^2-(\nabla\Theta_\sigma)^2\right]+2(1-\cos\Theta_\sigma)\left[\frac{1}{c^2}(\partial_t\hat{\Theta}_\sigma)^2-(\nabla\hat{\Theta}_\sigma)^2\right]\right\}. \tag{26}$$

This is a composite O(2) and O(3) σ model. The second term in (24) depends only on curvatures, and the third term is of Wess–Zumino type (see e.g. Zakrzewski 1989), where brackets indicate symmetrisation. For the coupling constant and critical angles one may set

$$F_{11}=F_{22}>0 \qquad F_{12}=F_{21}>0 \qquad \text{for } F=f,g$$
$$\vartheta_{11}=\vartheta_{22}>0 \qquad \vartheta_{12}=\vartheta_{21}>0. \tag{27}$$

The chiral fields $\{\hat{\Theta}_\sigma,\Theta_\sigma\}_{\sigma=1,2}$ are supposed to act on the spin field in a Lorentz invariant fashion, yielding for fixed gauge field

$$n^a_\sigma(x)\sim A\Theta^{a\cdot\mu}_{\sigma,\mu\cdot}+B\varepsilon^{abc}(\Theta^b_{\sigma,\mu\mu'}-\Theta^b_{\sigma,\mu'\mu})(\Theta^{c\mu\mu'}_{\bar{\sigma},}-\Theta^{c\mu'\mu}_{\bar{\sigma},}) \qquad \begin{cases}\sigma=1,2\\ \bar{\sigma}=2,1.\end{cases} \tag{28}$$

The expectation values $\{\langle n^a_\sigma(x)\rangle\}$ are computed with respect to an invariant measure of $SO(3)^2$-space and (24), and vanish for $T\geq 0$. Alternatively the correlation functions

$$\langle n^a_\sigma(x)n^a_{\sigma'}(x')\rangle \tag{29}$$

do not vanish at $T=0$ for $|x-x'|\to\infty$. Due to f_{12}, $g_{12}>0$ smooth configuration will imply $\Theta^{a\cdot\mu}_{1,\mu\cdot}\sim-\Theta^{a\cdot\mu}_{2,\mu\cdot}$, and therefore (29) will reflect 'antiferromagnetic staggering'.

Disordering of the $SO(3)^2\sigma$ model requires, via (29), two types of processes, where the first restores SO(3) symmetry of the chiral fields and is reflected in exponential decay of (29). The second process restores part of the local symmetry lost by 'antiferromagnetic staggering'. It is driven by the dissociation of topological defects, which are generated as twins in the two chiral fields. Observe that for f_{12}, $g_{12}\to 0$ such twins are strongly coupled and (24) describes effectively an SO(3) σ model. Interaction between pairs of twins will follow the law $\log|\boldsymbol{r}-\boldsymbol{r}'|$ and between twins it will follow

$|\boldsymbol{r}_1 - \boldsymbol{r}_2|^2 \log|\boldsymbol{r}_1 - \boldsymbol{r}_2|$. For $T > 0$ the first law will be screened and the second law reduced to $\log|\boldsymbol{r}_1 - \boldsymbol{r}_2|$. Accordingly two types of phase transition can be expected within this model. The second transition corresponds roughly to a disordering of Néel sublattices in the O(3) σ model via a network of domain boundaries (see e.g. Holz 1989). It may lead to a non-analyticity in $\langle n_1^a(x) n_2^a(x) \rangle$.

In conclusion I suggest Γ_{sc} given by (24) as a semiclassical action for the spin-$\frac{1}{2}$ HA. Γ_{sc} can be considered as the closest relative to the O(3) σ model at least if one admits just one chiral SO(3) field. This implies that most of the ideas developed for the O(3) σ model in connection with high-T_c superconductivity may easily be generalised to the $SO(3)^{(2)}\sigma$ model.

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