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LETTER TO THE EDITOR

A novel non-linear σ-model for frustrated quantum antiferromagnets

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Abstract. A new continuum-limit effective action for the description of the low-temperature long-wavelength fluctuations about the classical Neél state is proposed for the triangular-net quantum Heisenberg antiferromagnet. It is found that the novel frustration field plays a dominant role in describing deviations from the classical state, which would appear to be unstable to quantum fluctuations.

The theoretical search for a model two-dimensional quantum Heisenberg antiferromagnet, which presents a spin-liquid quantum ground state and for which the Neél classical state is only metastable, is a central issue in many approaches to magnetically-induced high-temperature superconductivity [1].

Thus far, extensive investigations on the square-net nearest-neighbour antiferromagnet [2–4] have come to the conclusion that, at least for values of the parameter $c/|J|s^2$ ($J < 0$, the exchange parameter, s, the value of the quantum spin, c, the spin-wave velocity), less than a critical value, there is Neél long-range order at zero temperature and which are less spin-liquid ground state. Furthermore, also in contrast to the case of the linear chain [5], no topological phase term is present in the effective Hamiltonian to provide fermionic extended quasi-particle excitations [6] of the disordered ground state.

It has seemed evident, however, that the above conclusions are strongly dependent on the nature of the underlying lattice. Therefore, in this Letter I will extend the new and versatile path-integral approach developed in a previous article [4] to the case of the (fully frustrated) triangular-net Heisenberg antiferromagnet in order to obtain an effective (quantum) non-linear-σ-model (NLσM) Hamiltonian capable of providing a definite answer [7] to the problems of long-range order (LRO) and topological excitations in frustrated antiferromagnets. In Anderson's original proposal for the spin-liquid [8], frustration played a major role in destroying LRO; the present theory shows this may indeed be the case, and I expect that the conclusions drawn for the triangular net will carry through to less frustrated but more complicated lattice geometries. The approach presented here is quite novel, in that it should also apply to any value of the spin s; the only other published NLσM approach to this problem [9] suffers from the usual large-s limitations, uses a different unphysical SO(3) principal order parameter and leads to rather different conclusions. The principal order parameter used in the present work, the sublattice magnetisation $\boldsymbol{n}$, is found to be more amenable to NLσM calculations.

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Following the approach of our previous article [4], the partition function for the quantum spin Hamiltonian $\mathcal{H} = -\frac{1}{2}J\Sigma_{\langle i,j\rangle}\boldsymbol{S}_i \cdot \boldsymbol{S}_j$ (i, j nearest-neighbour sites of the triangular net) has the path-integral representation

$$\mathfrak{Z}(\beta) \simeq \int \mathfrak{D}\psi_i(\tau)\exp(-\mathcal{S}[\psi])$$

$$\mathcal{S} = \tfrac{1}{2}J\int_0^\beta \mathrm{d}\tau \sum_{\langle i,j\rangle} \boldsymbol{\psi}_i \cdot \boldsymbol{\psi}_j - s\int_0^\beta \mathrm{d}\tau \sum_i [|J||\boldsymbol{\Omega}_i| - \mathrm{i}\boldsymbol{A}(\boldsymbol{\Omega}_i)\cdot\partial_\tau\boldsymbol{\Omega}_i$$
$$- \frac{1}{|J|}M_{\alpha\beta}(\Omega_i)\partial_\tau\Omega_i^\alpha\partial_\tau\Omega_i^\beta + \ldots] \tag{1}$$

where $\boldsymbol{\Omega}_i = \Sigma_\delta\boldsymbol{\psi}_{i+\delta}$ entails the sum over all six first-neighbour-shell sites $\boldsymbol{\delta}$, $\boldsymbol{A}$ is Dirac's magnetic monopole potential, and $M_{\alpha\beta}(\boldsymbol{\Omega}) = (2|\boldsymbol{\Omega}|^3)^{-1}(\delta_{\alpha\beta} - \Omega_\alpha\Omega_\beta/|\boldsymbol{\Omega}|^2)$. The bosonic field $\boldsymbol{\psi}$ arises from a Hubbard–Strantonovitch transformation decoupling the spin operators for each infinitesimal 'time' slice, and can be interpreted as the local classical magnetic moment on site i. The only approximation involved in (1) is that the temperature is low, $\beta|J| \to \infty$, and that the typical time scale for the fluctuations of $\boldsymbol{\psi}_i(\tau)$ is large enough to justify the expansion in powers of time-derivatives of this field. For the linear-chain and square-net problems, the above approach has reproduced [4] the known [2, 5] effective actions for arbitrary s. Next, I carry out an expansion in the field's spatial derivatives, but I must first choose a ground state and a suitable order parameter which have smooth variations from site to site. The physical nature of $\boldsymbol{\psi}$ in (1) imposes an expansion about the classical Neél state, with the well-known [8] canted 120° *planar configuration* on three sublattices. The natural order parameter is then the single sublattice magnetisation, and the resulting effective action can be used to analyse the stability of the classical state to quantum fluctuations.

In view of the above considerations, a good candidate for a smooth order parameter field is the variable $\boldsymbol{n}_i(\tau)$, defined via

$$\boldsymbol{\psi}_i(\tau) = s\mathcal{R}_i[\boldsymbol{u}]\boldsymbol{n}_i(\tau).$$

The 3×3 matrix $\mathcal{R}_i$ takes into account the canted configuration of the ground state spins on each sublattice, as it is generated by a uniform field $\boldsymbol{n}$; in other words, $\mathcal{R}$ must include planar rotations by an angle 0, $+2\pi/3$, $-2\pi/3$ for the sites of the three sublattices A, B, C, respectively. (Mixing with the chiral state (0, $-2\pi/3$, $+2\pi/3$) is neglected here, as this entails higher energy excitations.) It is convenient at this point to break explicitly the O(3) rotation symmetry of the spin Hamiltonian and choose a particular plane for the Neél configuration; the full symmetry will be restored, non-linearly as usual [10], by a term proportional to $-\ln(1-(n^3)^2)$, where n^3 is the off-plane component, in the effective action. $\mathcal{R}$ then has the form

$$\mathcal{R}_i[\boldsymbol{u}] = \begin{pmatrix} \cos\theta_{[i]} & -\sin\theta_{[i]} & 0 \\ \sin\theta_{[i]} & \cos\theta_{[i]} & 0 \\ 0 & 0 & (-1)^{\varphi_i[\boldsymbol{u}]} \end{pmatrix} \tag{2}$$

where $\theta_{[i]} = 0$, $+2\pi/3$, $-2\pi/3$ according to whether $[i]$ = A, B, C. The $\mathcal{R}^{33}$ matrix element embodies the frustration content of each particular $\boldsymbol{\psi}$-configuration. True

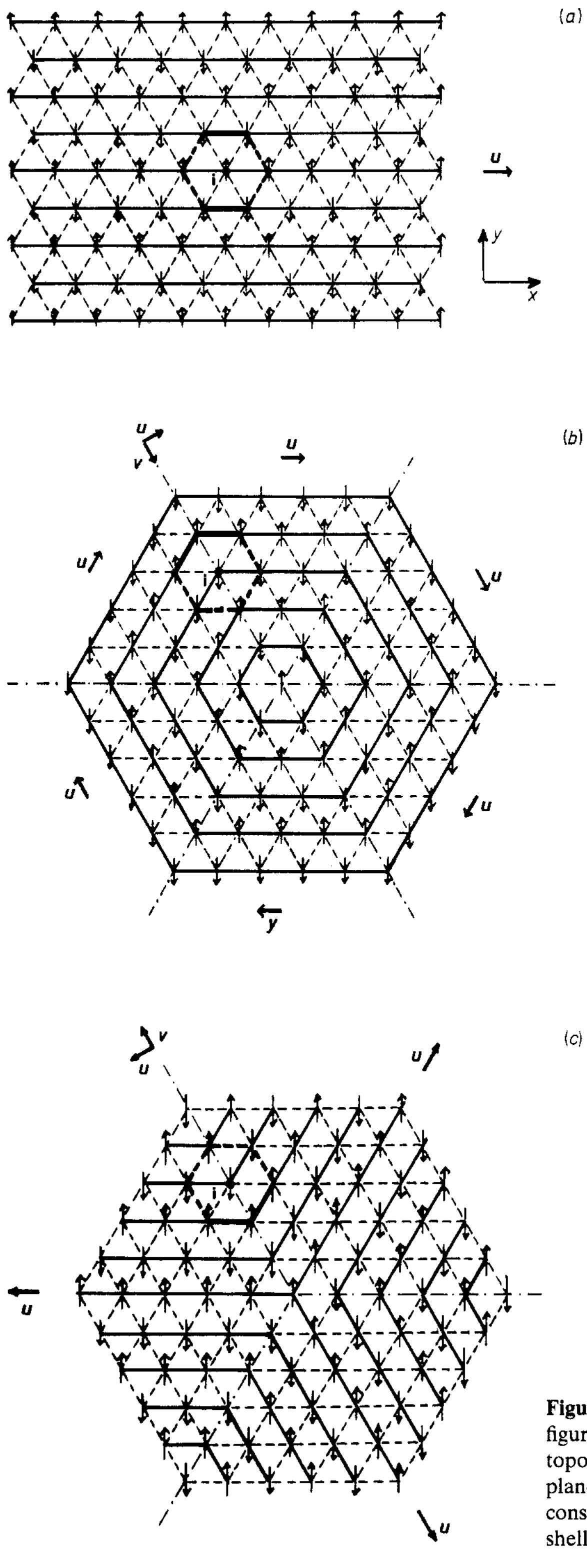

Figure 1. Examples of frustration field configurations relevant to this work. (*a*) flat, (*b*), (*c*) topological configurations. Arrows indicate off-plane spin component orientation, full lines the constant frustration field lines, first-neighbour-shells the nearest-neighbour frustration balance.

frustration arises as soon as out-of-plane spin fluctuations are allowed, since it is not possible to arrange the directions of the ψ^3 components in such a way that all bonds on each elementary plaquette are antiferromagnetically satisfied. Viewing the problem of arranging the $\pm$ directions of ψ_i^3—so as to involve only low-lying excitations of the Neél state—in terms of the Wannier ground states [11] for the antiferromagnetic Ising model, I will take into consideration here only ψ_i^3-configurations such that no plaquette with three parallel orientations is allowed. There are infinitely many ways of achieving this; here, I will classify each configuration in terms of its *frustration field* $\boldsymbol{u}_i(\tau)$. $\boldsymbol{u}$ is a unit vector lying on the physical (x, y) triangular-net plane and defining at each site the local direction of nearest-neighbour bond frustration. I will neglect all those $\boldsymbol{u}$-field configurations where the direction of frustration is multi-valued, as I believe they form a set of zero measure and are unimportant for the purposes of this work. Figure 1 shows examples of frustration field configurations believed to be relevant to this work. The field $\varphi_i[\boldsymbol{u}]$ is integer-valued and is such that $(-1)^{\varphi_i}$ is $+1$ (or -1) along the frustration lines. Notice that in the present description of fluctuations about the classical state the spins on each elementary plaquette are permitted to have *completely* separate motion, Wannier restrictions apart, a feature clearly unallowed by fluctuations ruled by an SO(3) principal order parameter [9] (observe that the $(\boldsymbol{n},\boldsymbol{u})$ global order parameter space, however, remains isomorphic to SO(3)).

From the above discussion it is clear that the partition function becomes a functional integral over all the configurations of the fields $\boldsymbol{n}$ and $\boldsymbol{u}$:

$$\mathfrak{X}(\beta) \simeq \int \mathfrak{D}\boldsymbol{u} \int \mathfrak{D}\boldsymbol{n} \exp\{-\mathcal{S}_{\text{eff}}[\boldsymbol{n}, \boldsymbol{u}] + \mathrm{i}\mathcal{S}_{\mathrm{B}}[\boldsymbol{n}, \boldsymbol{u}]\}$$

where the imaginary part S_{B} of the action is the sum over all single-spin Berry phases induced by the low-frequency expansion in (1). In the remainder of this Letter I will derive the form of the real part S_{eff} of the continuum-limit action. For this purpose, I will consider $\boldsymbol{u}$-field configurations made up of infinite two-dimensional domains where $\boldsymbol{u}$ is uniform (such as those of figure 1), briefly commenting on the form the action takes along the (one-dimensional) boundaries of such domains, e.g. along the radii of configurations figure 1(b, c). Consider the flat configuration of figure 1(a), the frustration field being uniform along the x-direction so that $\varphi_i = i_y$. For any site i, the form (2) of $\mathfrak{R}_i$ and the single-valuedness of $\boldsymbol{u}$ ensure that $\mathfrak{R}_{i+\delta} = \mathfrak{R}_i\mathfrak{R}_\delta$, beside $\mathfrak{R}_i^T = \mathfrak{R}_i^{-1}$, so that $\boldsymbol{\Omega}_{i+\delta} = s\mathfrak{R}_i\Sigma_\delta\mathfrak{R}_\delta\boldsymbol{n}_{i+\delta}$. Expanding the smooth $\boldsymbol{n}$-field

$$\boldsymbol{n}_{i+\delta} = \boldsymbol{n}_i + \delta^a\partial_a\boldsymbol{n}_i + \tfrac{1}{2}\delta^a\delta^b\partial_a\partial_b\boldsymbol{n}_i + \ldots$$

then summing over all six first-neighbour $\boldsymbol{\delta}$s and rescaling $n^3 \to \frac{2}{3}n^3$, one finds

$$\boldsymbol{\Omega}_i = -3s\mathfrak{R}_i\left\{1 + \frac{a^2}{4}\begin{pmatrix} \boldsymbol{\nabla}^2 & 0 & 0 \\ 0 & \boldsymbol{\nabla}^2 & 0 \\ 0 & 0 & 3\partial_y^2 - \partial_x^2 \end{pmatrix} + \ldots\right\}\boldsymbol{n}_i.$$

The first two real terms of the lattice action of (1) become:

$$\tfrac{1}{2}J\int_0^\beta \mathrm{d}\tau \sum_{i,\delta} \boldsymbol{\psi}_i \cdot \boldsymbol{\psi}_{i+\delta} - s|J|\int_0^\beta \mathrm{d}\tau \sum_i |\boldsymbol{\Omega}_i|$$

$$= \frac{\sqrt{3}}{a^2}|J|s^2\int_0^\beta \mathrm{d}\tau\int \mathrm{d}x\mathrm{d}y\,(|\boldsymbol{n}| - 1)^2 + \frac{\sqrt{3}}{2}|J|s^2a^{-2}\int_0^\beta \mathrm{d}\tau\int \mathrm{d}x\mathrm{d}y\,(n^3)^2$$

$$+\frac{\sqrt{3}}{4}|J|s^2\int_0^\beta \mathrm{d}\tau \int \mathrm{d}x\mathrm{d}y\, \boldsymbol{n}$$
$$\times \begin{pmatrix} (1-2/|\boldsymbol{n}|)\boldsymbol{\nabla}^2 & 0 & 0 \\ 0 & (1-2/|\boldsymbol{n}|)\boldsymbol{\nabla}^2 & 0 \\ 0 & 0 & (1-4/3|\boldsymbol{n}|)(\frac{9}{2}\partial_y^2 - \frac{3}{2}\partial_x^2) \end{pmatrix} \boldsymbol{n} + \ldots \tag{3}$$

with the first integral giving the usual NLσM constraint $|\boldsymbol{n}| = 1$. The second-order term in the low-frequency expansion (1) then becomes:

$$\frac{s}{|J|}\int_0^\beta \mathrm{d}\tau \sum_i M_{\alpha\beta}(\boldsymbol{\Omega}_i)\partial_\tau \Omega_i^\alpha \partial_\tau \Omega_i^\beta = (3\sqrt{3}|J|a^2)^{-1}\int_0^\beta \mathrm{d}\tau \int \mathrm{d}x\mathrm{d}y\,(\partial_\tau \boldsymbol{n})^2 + \ldots \tag{4}$$

which gives the usual dynamics of the order parameter. Gathering the relevant terms of (3) and (4), one gets:

$$\mathcal{S}_{\mathrm{eff}}[\boldsymbol{n}, \boldsymbol{u} = x] = \frac{\sqrt{3}}{4}|J|s^2 \int_0^\beta \mathrm{d}\tau \int \mathrm{d}x\mathrm{d}y \Big[(\boldsymbol{\nabla}\boldsymbol{n}^{\parallel})^2 + \frac{1}{c^2}(\partial_\tau n^{\parallel})^2$$
$$+ 2a^{-2}(n^{\perp})^2 + \tfrac{3}{2}(\partial_y n^{\perp})^2 - \tfrac{1}{2}(\partial_x n^{\perp})^2 + \frac{1}{c^2}(\partial_\tau n^{\perp})2\Big] \tag{5}$$

where $c = 3|J|as/2$ is the spin-wave velocity and where $(\boldsymbol{n}^{\parallel}, n^{\perp}) = (n^1, n^2, n^3)$ with $\boldsymbol{n}^2 = 1$. It is straightforward to show that for a uniform frustration field direction chosen along the two other possible lattice directions the form of $\mathcal{S}_{\mathrm{eff}}$ is exactly the same, *provided* the reference frame (x, y) is rotated so that the x axis is always along the direction of $\boldsymbol{u}$. Thus, for the arbitrary $\boldsymbol{u}$-field configurations of interest, one concludes that

$$\mathcal{S}_{\mathrm{eff}}[\boldsymbol{n}, \boldsymbol{u}] = \frac{1}{2g_0}\int_0^{\beta c} \mathrm{d}t \int \mathrm{d}x\, \mathrm{d}y\, [(\partial_\mu \boldsymbol{n})^2 + m_0^2(n^3)^2 + \tfrac{1}{2}(\boldsymbol{v}\cdot\boldsymbol{\nabla}n^3)^2 - \tfrac{3}{2}(\boldsymbol{u}\cdot\boldsymbol{\nabla}n^3)^2] \tag{6}$$

where $g_0 = 2c/(\sqrt{3}|J|s^2)$ is the coupling constant of the resulting NLσM, $m_0^2 = 2a^{-2}$, and where $\boldsymbol{v}$ is a unit vector orthogonal to $\boldsymbol{u}$.

Hence, for a chosen Neél plane and flat frustration field configuration (e.g. (5)) one can seen that the resulting NLσM presents a number of new features, not merely a modification of g_0 as previously conjectured [3], all induced by frustration. (i) The Goldstone mode and linear dispersion relation remain associated with in-plane fluctuations of $\boldsymbol{n}^{\parallel}$. (ii) As soon as out-of-plane fluctuations occur, there is a restoring term proportional to $(n^3)^2$. (iii) While it costs energy to modulate in the direction for which nearest-neighbour bonds are antiferromagnetically satisfied ($\boldsymbol{v}$), it clearly pays to modulate along the direction of frustration ($\boldsymbol{u}$). To corroborate this physical interpretation, I will now give the form of the effective Lagrangian for those sites (on the radii of configurations (b) and (c) of figure 1 where the $\boldsymbol{u}$-field has the only possible change of direction (120°). I find for these sites

$$\mathcal{L} = (1/2g_0')[(\partial_\mu \boldsymbol{n}^{\parallel})^2 + m_0^2(n^3)^2 + 3(\boldsymbol{v}\cdot\boldsymbol{\nabla}n^3)^2 + (\partial_t n^3)^2]$$

where $\boldsymbol{v}$ is along the direction of the radius (hence $\boldsymbol{u}$ is orthogonal to it). This reflects the fact that along the $\boldsymbol{u}$-direction there is an exact balance between frustrated and unfrustrated bonds; thus it only costs energy to modulate along $\boldsymbol{v}$. Notice that these sites do not contribute to the full two-dimensional action, which remains of form (6).

Details of a full renormalisation group analysis of the LRO properties of the present NLσM, as well as of the model's symmetries and possible topological phases arising from the imaginary term $\mathcal{S}_B[\boldsymbol{n}, \boldsymbol{u}]$ (the latter clearly being sensitive to the topology of the $\boldsymbol{u}$-field itself) will be given elsewhere. Here, it suffices to say that a cursory look at the flat frustration form of $\mathcal{S}_{\rm eff}$, (5), indicates that at large distances there will be a crossover in both effective spin and spacetime dimensionalities, with the n^3-component and $\boldsymbol{u}$-direction being renormalised away at long wavelengths and small frequencies. This should result in quasi-XY, quasi-$(1+1)$-dimensional asymptotic behaviour, and thus in the destruction of the Neél LRO at large distances by quantum fluctuations. At short distances, however, the spins will be ordered, and the crossover may represent the first quantitative (albeit classical) description of the spin-liquid state, predicted [8] and perhaps observed [12] for the triangular systems.

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