Nonlinear Field Theory of Large-Spin Heisenberg Antiferromagnets: Semiclassically Quantized Solitons of the One-Dimensional Easy-Axis Néel State

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The continuum field theory describing the low-energy dynamics of the large-spin one-dimensional Heisenberg antiferromagnet is found to be the O(3) nonlinear sigma model. When weak easy-axis anisotropy is present, soliton solutions of the equations of motion are obtained and semiclassically quantized. Integer and half-integer spin systems are distinguished.

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Nonlinear excitations in one-dimensional magnetic systems have received much theoretical attention in recent years, primarily ferromagnetic, easy-plane, or $S=\frac{1}{2}$ systems.[1] In this Letter, I describe a nonlinear field-theory approach to weakly uniaxially anisotropic *easy-axis antiferromagnets* with *large* spin. Classically, these have a doubly degenerate ground state with axially aligned Néel order; topological soliton excitations corresponding to movable domain walls separating the two possible ground-state configurations are described, and semiclassically quantized. The methods used also reveal the field theory describing the semiclassical *isotropic* Heisenberg antiferromagnet, providing an alternative derivation of the recent identification[2] (based on a quantum action-angle representation of spins) of this model with the O(3) nonlinear sigma model with coupling $g=2/\hbar S$ as $S\to\infty$. The quantization of magnetization carried by the easy-axis-model solitions also shows up an intrinsic difference between integer-spin and half-integer-spin systems, leading to quite different instabilities of the ordered ground state as the anisotropy vanishes, consistent with the predictions[2] of quite different low-energy physics of the isotropic ground state in the two cases.

I will consider the easy-axis model

$$H=|J|\sum_n[\vec{S}_n\cdot\vec{S}_{n+1}+\lambda S_n^z S_{n+1}^z+\mu(S_n^z)^2], \qquad (1)$$

with $S_n^2=\hbar^2S(S+1)$, and $\lambda>\mu$ so that the classical ground state is given by $\vec{S}_n=\hbar S(-1)^n\hat{u}$, $\hat{u}=\pm\hat{z}$. In the classical limit, the equations of motion have small-amplitude spin-wave solutions with the frequency-wave-number relation

$$\omega^2(q)=\omega_0^2+[\omega_1\sin(qa)]^2, \quad |q|<\tfrac{1}{2}\pi/a, \qquad (2)$$

where a is the lattice spacing, $\omega_1=2J\hbar S$, and $\omega_0=\omega_1(\lambda-\mu)^{1/2}(2+\lambda-\mu)^{1/2}$. I will specialize to the case of *weak* anisotropy $\omega_0/\omega_1\ll 1$, when long-wavelength properties may be studied in the continuum limit $a\to 0$, $\omega_1\to\infty$, $\omega_1 a=c$; the dispersion relation (2) then develops Lorentz invariance with limiting velocity c. The elementary collective excitations (magnons carrying $S^z=\pm\hbar$) are obtained by a semiclassical quantization of the spin waves (e.g., by a linearized Holstein-Primakoff approach); for (crystal) momentum $|P|\ll\frac{1}{2}\pi\hbar/a$, the magnon dispersion is

$$\epsilon(P)=[(\hbar\omega_0)^2+c^2P^2]^{1/2}, \quad 0<(\lambda-\mu)^{1/2}\ll 1. \qquad (3)$$

To study the soliton excitations, a fully nonlinear treatment of (1) is needed. Following Mikeska,[3] I use the classical angle-variable representation

$$\vec{S}_n=(-1)^n\hbar S(\sin\theta_n\cos\varphi_n, \sin\theta_n\sin\varphi_n, \cos\theta_n).$$

The classical equations of motion are easily obtained from (1) in terms of these variables by using the Poisson-bracket algebra $\{\varphi_n, S_{n'}^z\}=\delta_{nn'}$, $\dot{\varphi}_n=\{\varphi_n, H\}$, etc.:

$$\dot{\theta}_n=-\tfrac{1}{2}\omega_1(-1)^n\sum_\pm[\sin\theta_{n+1}\sin(\varphi_{n+1}-\varphi_n)], \qquad (4a)$$

$$\dot{\varphi}_n=-\tfrac{1}{2}\omega_1(-1)^n\sum_\pm[(1+\lambda)\cos\theta_{n\pm1}-\mu\cos\theta_n-\cot\theta_n\sin\theta_{n\pm1}\cos(\varphi_{n\pm1}-\varphi_n)]. \qquad (4b)$$

To make progress with these equations, I assume as in Ref. 3 that θ_n and φ_n vary *slowly* with n, with a *small* superimposed staggered-fluctuation component; this should be valid at low energies and weak anisotropy $\omega_0\ll c/a$:

$$\theta_n=\theta(x)+a(-1)^n\alpha(x), \quad \varphi_n=\varphi(x)+a(-1)^n\beta(x), \quad x=na. \qquad (5)$$

$\theta(x)$ and $\varphi(x)$ are slowly varying angle fields, while $\alpha(x)$ and $\beta(x)$ are small staggered-fluctuation fields, chosen to have dimensions of density. The variables on neighboring sites can be expressed through a gradient expansion about $x=na$. Full nonlinearity in the angle fields must be maintained, but (4a) and (4b) can be approximated by an expansion up to quadratic order in α, β, and ∇ (or alternatively, by taking the limit $a\to 0$ with α, β, ω_0, and c fixed). There is a second (dimensionless) anisotropy parameter $\gamma_1=\frac{1}{2}(\mu+\lambda)$ in addition to $\lambda-\mu\simeq\frac{1}{2}(\omega_0 a/c)^2$; for simplicity, I first specialize to the neighborhood of the isotropic model with $\gamma_1\simeq 0$, and drop terms involving γ_1. Each equation (4a) and (4b) yields *two* independent equations of motion (for the uniform and staggered parts), essentially Eqs. (2.11)–(2.14) of Ref. 3, but with minor corrections[3]:

$$\dot\theta/c=2\beta\sin\theta;\quad \dot\varphi/c=-2\alpha/\sin\theta;\quad (\dot\alpha\sin\theta)/c=-\tfrac{1}{2}\nabla(\sin^2\theta\,\nabla\varphi)-\alpha\beta\sin 2\theta;$$
$$(\dot\beta\sin\theta)/c=\tfrac{1}{2}\nabla^2\theta-\tfrac{1}{4}\sin 2\theta[(\omega_0/c)^2+(\nabla\varphi)^2-(2\alpha/\sin\theta)^2+4\beta^2]. \quad (6)$$

These simplify considerably when I introduce new density fields $L(x)=-2g^{-1}\alpha\sin\theta$, $\Pi_\theta(x)=2g^{-1}\beta\sin\theta$, where g is the coupling constant $2/\hbar S$ [more accurately,[2] $g=2/\hbar\{S(S+1)\}^{1/2}$]; $L(x)$ is the azimuthal spin density:

$$S^z\equiv\hbar S\textstyle\sum_n(-1)^n\cos\theta_n \xrightarrow{a\to 0} \int dx\,L. \quad (7)$$

The equations (6) become

$$\dot\theta=gc\Pi_\theta;\quad \dot\varphi=gcL/\sin^2\theta;\quad g\dot L/c=\nabla(\sin^2\theta\,\nabla\varphi);\quad g\dot\Pi_\theta/c=\nabla^2\theta-\tfrac{1}{2}\sin 2\theta[(\omega_0/c)^2+(\nabla\varphi)^2-(gL/\sin^2\theta)^2]. \quad (8)$$

These equations may now be recognized as deriving from the Hamiltonian

$$H=\tfrac{1}{2}c\int dx\big(g(\Pi_\theta^2+L^2/\sin^2\theta)+g^{-1}\{(\nabla\theta)^2+[(\nabla\varphi)^2+(\omega_0/c)^2]\sin^2\theta\}\big), \quad (9)$$

expressed in terms of independent canonical classical fields $\{\varphi(x),L(x')\}=\{\theta(x),\Pi_\theta(x')\}=\delta(x-x')$. The corresponding Lagrangian density is easily obtained; in terms of the unit-vector field $\vec\Omega(x,t)=(\sin\theta\times\cos\varphi,\sin\theta\sin\varphi,\cos\theta)$,

$$\mathcal{L}=\tfrac{1}{2}g^{-1}[c^{-1}|\partial_t\vec\Omega|^2-c|\nabla\vec\Omega|^2-(\omega_0^2/c^2)\Omega_\perp^2],\quad |\vec\Omega|^2=1, \quad (10)$$

where $\Omega_\perp^2\equiv(\Omega^x)^2+(\Omega^y)^2$. This is just the Lorentz-invariant *O(3) nonlinear sigma model*,[4] with additional easy-axis anisotropy.

If the analysis is repeated keeping the additional anisotropy term γ_1, the Hamiltonian (9) gains an extra term,

$$H'=\tfrac{1}{2}\gamma_1 c\int dx[gL^2+g^{-1}(\nabla\cos\theta)^2]. \quad (11)$$

This term breaks Lorentz invariance, causing a change in the collective-mode "light velocity" from c to $(1+\gamma_1)^{1/2}c$ if the system becomes *easy plane* [i.e., if ω_0^2 in (10) becomes negative]; stability requires $\gamma_1>-1$. This term will not be considered further here.

I now obtain *topological soliton* solutions of the equations of motion (8) by the device of minimizing the Hamiltonian (9) with respect to the fields at fixed values of the conserved quantities S^z (7) and momentum $P=\int dx(\Pi_\theta\nabla\theta+L\nabla\varphi)$, with the boundary condition $\cos\theta\to\pm\,\mathrm{sgn}(x)$ as $|x|\to\infty$. Lorentz invariance allows the moving finite-P solution to be obtained by a boost of the static $P=0$ soliton. I obtain $L=g^{-1}(\omega/c)\sin^2\theta$, $\varphi=\omega\tau$, $\theta=\theta(s)$, where $(s,\tau)=(1-v^2/c^2)^{-1/2}(x-vt,\ t-vx/c^2)$, and

$$\theta''=\tfrac{1}{2}[(\omega_0^2-\omega^2)/c^2]\sin 2\theta. \quad (12)$$

For $\omega^2<\omega_0^2$, (12) has soliton solutions $\cos\theta=\pm\tanh[(s-s_0)/R]$, where $c^2/R^2=\omega_0^2-\omega^2$. The total azimuthal spin carried by the soliton is found to be given by $\frac{1}{2}gS^z=\omega/(\omega_0^2-\omega^2)^{1/2}$. This variational procedure leads to the single-soliton solution, but cannot produce multisoliton solutions. When $\omega_0^2=0$, the equations of motion (8) derived from (9) or (10) are known to be *integrable.*[4] It is tempting to speculate that this may remain true when $\omega_0^2\neq 0$, allowing multisoliton generalizations of the single-soliton solution obtained here to be found. Somewhat fortuitously (as he studied a system with $\gamma_1\neq 0$, but omitted[3] certain terms involving γ_1), Mikeska[3] has previously obtained (12) with $\omega=0$ and its solution from an *Ansatz* for the $S^z=0$ soliton.

At this point, it is useful to introduce the *semiclassical quantization* of the allowed values of the internal precession frequency of the soliton: This simply means that S^z is quantized in *integer steps* $S^z=m\hbar$. The quantum number m can be used to parametrize the internal state of the soliton. The soliton energy-momentum relation obtained from (9) is then given by

$$E_m(P)=[(m^2+S^2)(\hbar\omega_0)^2+c^2P^2]^{1/2}\geq S\hbar\omega_0. \quad (13)$$

The soliton parameters are given by $v = \partial E/\partial P|_m$ and

$$R = (c/\omega_0)S^{-1}(m^2 + S^2)^{1/2},$$
$$\omega = \omega_0 m/(m^2 + S^2)^{1/2}. \tag{14}$$

In the semiclassical limit, the soliton energy gap is always much larger than that of the elementary magnon. The soliton rest energy may also be written as $E_m(0) = 2g^{-1}c/R + m\hbar\omega$; these terms can be interpreted as a basic defect configuration energy plus an internal kinetic energy. For $|m| \ll S$, $E_m(0) \simeq S\hbar\omega_0 + (\hbar\omega_0/S)m^2$; the kinetic energy can be interpreted as that of a free planar rotator with moment of inertia $I = (g\omega_0)^{-1}$. As $|m|$ increases, the defect configurational energy is decreased; for $|m| \gg S$, $\omega \to \omega_0$ and the rest energy can be interpreted in terms of $|m|$ magnons weakly bound to the defect in a loose bound state.

The semiclassical quantization of the internal motion was described above rather loosely; the allowed discrete values of m were *not* specified, only their integer spacing. The action of the *time-reversal* operator $\overline{T}$ on spin wave functions is well known: They are eigenstates of $\overline{T}^2$ with $\overline{T}^2 \equiv (-1)^{2m} = (-1)^{2S} = \pm 1$. The soliton extended structure naturally involves an *odd* number of spins of the underlying magnetic chain: Its wave function must thus also have the eigenvalue $\overline{T}^2 = (-1)^{2S}$. I conclude that the allowed values of the soliton spin m are *integers* if the underlying spin chain has integer spin, and *half integers* if S is half integer. This conclusion can also be reached by considering the spin of an odd-membered ring of spins with periodic boundary conditions; such a structure necessarily contains a soliton.

The semiclassical pictures of the soliton and magnon described above will only be valid for *weak but finite* anisotropy, $S\exp(-\pi S) \ll (\lambda - \mu)^{1/2} \ll 1$. The origin of the lower bound is the well-known renormalization[5] of the coupling g of the *isotropic* O(3) nonlinear sigma model due to nonlinear zero-point fluctuations ("instantons"[6]). The model (9) with $\omega_0 = 0$ is apparently invariant under scale transformations (conformally invariant), and in a harmonic approximation, its collective magnon excitation is gapless. However, the nonlinear vacuum fluctuations dynamically break this symmetry: g is renormalized to strong coupling, and the collective mode develops a *finite* rest energy $\epsilon_0 = \xi^{-1}cg^{-1}\exp(-2\pi g^{-1}/\hbar)$, where $\xi \sim a$ is the ultraviolet cutoff length scale.[5] This nonlinear mechanism will only be suppressed by the anisotropy if $\hbar\omega_0 \gg \epsilon_0$, leading to the above condition on $(\lambda - \mu)^{1/2}$.

As the isotropic limit $\omega_0 \to 0$ is approached, these nonlinear effects mean that the renormalized soliton rest energy will eventually become *lower* than the renormalized magnon rest energy. The lowest-energy excitations are then the principal $m = 0$ or $m = \pm\frac{1}{2}$ solitons, depending on whether S is integer or half integer. In both cases, the eventual disappearance of Néel order in the ground state as the isotropic limit is approached will be signaled by an instability against pairs of the *order-destroying* topological soliton excitations, and *not* of the *order-preserving* collective magnon excitations, as might be misleadingly suggested by the results in the harmonic approximation. Similarly, it is the thermal excitation of solitons, not the thermal excitation of magnons, that disorders the system at any finite temperature.

The integer-spin case ($\overline{T}^2 = +1$) corresponds to the "standard" quantization of the O(3) sigma model, for example as a one-dimensional (1D) lattice of discrete O(3) rotators.[7] This quantization is directly related to the thermodynamics of the 2D classical Heisenberg model. The $m = 0$ soliton gap will vanish at a finite critical anisotropy $(\hbar\omega_0)_c \simeq \epsilon_0$, signaling a doublet-singlet transition of the Onsager/φ^4-field-theory type to the singlet ground state of the nearly isotropic model exhibited by the strong-coupling rotator version of the model.[7]

The half-integer–spin case ($\overline{T}^2 = -1$) corresponds to a nonstandard quantization of the sigma model, but the results from the $S = \frac{1}{2}$ model limit[8] serve as a guide to its behavior. The $m = \pm\frac{1}{2}$ soliton gap only vanishes at the isotropic point $\omega_0 = 0$, signaling a direct transition of the Kosterlitz-Thouless/$\beta^2 = 8\pi$–sine-Gordon–field-theory type to the gapless easy-plane state.

Recent numerical finite-size scaling studies of the $S = 1$ model[9] provide convincing evidence in favor of the "novel" prediction[10] of an isolated singlet disordered ground state in integer-spin 1D antiferromagnets with sufficiently weak anisotropy.

In conclusion, I note that while the discussion of topological defects of the easy-axis model was specifically one-dimensional in character, the derivation of an equivalence between the low-energy dynamics of the large-spin Heisenberg antiferromagnet and the O(3) nonlinear sigma model will be independent of dimension. The extension of the derivation to a d-dimensional hypercubic lattice is trivial; (10) is obtained with the replacement $|\nabla\vec{\Omega}|^2 \to \sum_i |\nabla^i \vec{\Omega}|^2$, with summation over $i = 1,\ldots,d$, and with the coupling given by $g = 2d^{1/2}a^{d-1}/\hbar S$.

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