CONTINUUM DYNAMICS OF THE 1-D HEISENBERG ANTIFERROMAGNET: IDENTIFICATION WITH THE O(3) NONLINEAR SIGMA MODEL

F.D.M. HALDANE

Department of Physics, University of Southern California, Los Angeles, CA 90089-0484, USA

Received 10 June 1982 Revised manuscript received 21 November 1982

An action—angle representation of spin variables is used to relate the large-S Heisenberg antiferromagnet to the O(3) nonlinear sigma model quantum field theory, with precise equivalence for integral S. A variant theory is found for half-integral S. Dynamic mass generation by the Néel magnon is predicted.

In this note, I derive the continuum-limit dynamics of the one-dimensional Heisenberg antiferromagnetic spin chain in the semiclassical limit of large-but-finite S. In this limit, the model is found to be related to the O(3) nonlinear sigma model quantum field theory, with coupling $g = 2/[S(S+1)]^{1/2}$. This Lorentz-invariant field theory is perhaps more familiar in its euclidean form, which describes the statistical mechanics of the classical 2-D Heisenberg model at low temperatures; its spin field describes the Néel order-parameter field of the quantum spin chain. Two variants of the model (S integral or half-integral) are distinguished.

I will consider the spin-S quantum antiferromagnet, in units with $\hbar = 1$:

$$H^{\text{AF}} = |J| \sum_{n} S_n \cdot S_{n+1}. \tag{1}$$

It will also be useful to discuss the effect of uniaxial anisotropy terms of both on-site and exchange types:

$$H' = |J| \sum_{n} \lambda S_{n}^{z} S_{n+1}^{z} + \mu(S_{n}^{z})^{2}.$$
 (2)

The central feature of the treatment will be the use of quantum action-angle variables S_n^z , ϕ_n , where $[S_n^z]$, $\exp(i\phi_n) = \delta_{nn'} \exp(i\phi_n)$, for the description of spin variables:

$$S_n^+ = (S + S_n^z)^{1/2} \exp(i\phi_n)(S - S_n^z)^{1/2}.$$
 (3)

This representation is exact [and similar in spirit to the

Holstein—Primakoff boson representation: the preand post-factors decouple the physical sector of the enlarged Hilbert space ($|S_n^z| \leq S$) from the unphysical sector ($|S_n^z| > S$)]; it is similar to the representation used by Villain [1] to study the planar (XY) spin chain. Depending on whether S is integral or half-integral, the wavefunction has the local rotational symmetry $\Psi(\phi_n + 2\pi) = \pm \Psi(\phi_n)$, which gives rise to quantisation of S_n^z in integer steps. S_n^z and ϕ_n are thus constrained periodic action—angle rather than canonical coordinate—momentum variables. It may be seen that while (3) depends on S in only a quantitative fashion, there is a qualitative distinction between integral and half-integral S which controls the character (integer or half-integer) of the discrete spectrum of S_n^z .

In terms of these variables, (1) is given by

$$H^{\text{AF}} = |J| \sum_{n} \frac{1}{2} \left\{ P_{n,n+1} \exp\left[i(\phi_n - \phi_{n+1})\right] P_{n+1,n} \right\}$$

+ h.c.} +
$$S_n^z S_{n+1}^z$$
, (4)

$$P_{n,n'} = \{ [S - \frac{1}{2}(S_n^z - S_{n'}^z)]^2 - \frac{1}{4}(S_n^z + S_{n'}^z)^2 \}^{1/2}.$$
 (5)

In the classical ground state of (1), antiferromagnetic long-range order (Néel order) is present: $1 + \cos(\phi_n - \phi_{n+1}) = S_n^z + S_{n+1}^z = 0$. This suggests an expansion in powers of these quantities to derive an effective hamiltonian valid in the limit of large S and low temperature when short-range order is present. To proceed,

the following identity is useful: if $[X, \exp(i\phi)]$ = $\exp(i\phi)$, and $A(X + \frac{1}{2})B(X - \frac{1}{2}) = F(X^2 - \frac{1}{4})$, F(x) = $\sum_m \alpha_m x^m$, then $\frac{1}{2}[A(X) \exp(i\phi)B(X) + \text{h.c.}]$ = $\sum_m \alpha_m X^m \cos(\phi) X^m$. As an example of this algebra, the identification $X = S_n^z$, $\phi = \phi_n$ allows (3) to be recast as

$$S_n^x = \{S(S+1)\}^{1/2} \sum_m \alpha_m C_n^m \cos(\phi_n) C_n^m,$$

$$C_n = S_n^z / [S(S+1)]^{1/2},$$
 (6)

where $\Sigma_m \alpha_m x^m = (1-x)^{1/2}$. The expansion of (4) proceeds with $X = \frac{1}{2}(S_n^z - S_{n+1}^z)$, $\phi = (\phi_n - \phi_{n+1})$: up to terms of order $(S_n^z + S_{n+1}^z)^2 [1 + \cos(\phi_n - \phi_{n+1})]$, H^{AF} is given by

$$\begin{split} H^{\text{AF}} &\approx |J| \sum_{n} S(S+1) \cos(\phi_{n} - \phi_{n+1}) \\ &- \frac{1}{4} (S_{n}^{z} - S_{n+1}^{z}) [1 + \cos(\phi_{n} - \phi_{n+1})] (S_{n}^{z} - S_{n+1}^{z}) \\ &+ \frac{1}{8} (2S+1)^{2} (S_{n}^{z} + S_{n+1}^{z})^{2} [S(S+1) - \frac{1}{4} (S_{n}^{z} - S_{n+1}^{z})^{2}]^{-1}. \end{split}$$

Full nonlinearity in the azimuthal Néel parameter $(S_n^z - S_{n+1}^z)$ has been retained in (7). Notice how S only appears in the "quantum combinations" S(S+1) and 2S+1.

I now follow Villain's [1] approach to the planar model, by ignoring the local rotation symmetry, and treating ϕ_n and S_n^z as canonical (non-periodic) variables, so $[1+\cos(\phi_n-\phi_{n+1})]\approx \frac{1}{2}(\phi_{n+1}-\phi_n-\pi)^2$ when short-range order is present. The justification for this is based on the idea that the aligning field on a spin due to its neighbours suppresses fluctuations away from local alignment that are sufficiently large for the local rotation symmetry to be experienced. In fact, important features (such as the distinction between integral and half-integral spins) are lost by this approximation, and a more correct treatment that respects the local rotation symmetry when the Néel parameter is close to alignment with the z axis is necessary for a full discussion. Such a generalised treatment will be given elsewhere [2].

If ϕ_n and S_n^z are treated as canonical, Fourier-transformed canonical variables ϕ_a , L_a can be introduced:

$$\phi_n = n\pi + N_a^{-1/2} \sum_q e^{iqna} \phi_q,$$

$$S_n^z = N_a^{-1/2} \sum_q e^{-iqna} L_q,$$
 (8)

where N_a is the number of sites, and a is the lattice spacing. If an harmonic expansion about the Néel-ordered state with $S_n^z - S_{n+1}^z = (-1)^n \langle N^z \rangle$ is made, the excitation spectrum has dispersion $\omega_q = (2S+1) \times |J\sin(qa)|$, independent of $\langle N^z \rangle$. The importance of fluctuations of modes near the two points $q \approx 0$ and $q \approx \pi/a$ can be seen. I now set up quasi-canonical "smeared" independent continuum fields $\phi(x)$, $\Omega(x)$, and their conjugate momentum densities L(x), $\Pi(x)$, respectively constructed from these two regions:

$$\phi(x) = N_a^{-1/2} \sum_{q \approx 0} e^{iqx} \phi_q$$

$$L(x) = a^{-1}N_a^{-1/2} \sum_{q \approx 0} e^{-iqx}L_q$$

$$\Omega(x) = [S(S+1)]^{-1/2} N_a^{-1/2} \sum_{q \approx 0} e^{-iqx} L_{q+\pi/a},$$

$$\Pi(x) = -a^{-1} \left[S(S+1) \right]^{1/2} N_a^{-1/2} \sum_{q \approx 0} e^{iqx} \phi_{q+\pi/a}. (9)$$

These have quasi-canonical commutation relations (CCRs) $[\phi(x), L(x')] = [\Omega(x), \Pi(x')] = i\delta(x - x')$ where the "delta function" $\delta(x)$ is actually "smeared" on a length scale $\xi \gtrsim a$. Then

$$\phi_n \approx n\pi + \phi(x) - a(-1)^n [S(S+1)]^{-1/2} \Pi(x),$$

$$S_n^z \approx aL(x) + (-1)^n [S(S+1)]^{1/2} \Omega(x),$$

$$\phi_{n+1} - \phi_n - \pi \approx a \, \nabla \phi(x) - 2a(-1)^n \left[S(S+1) \right]^{-1/2} \Pi(x),$$

$$S_n^z + S_{n+1}^z \approx 2aL(x) + a(-1)^n [S(S+1)]^{1/2} \nabla \Omega(x),$$

$$S_{n+1}^z - S_n^z \approx 2(-1)^n [S(S+1)]^{1/2} \Omega(x)$$

(the $q \approx 0$ term $a^2 \nabla L(x)$ has been omitted in this last expression since it is the gradient of a quantity small compared to $[S(S+1)]^{1/2}\Omega(x)$). $\Omega(x)$ is the azimuthal component of the normalised Néel order-parameter field, and $\phi(x)$ is its azimuthal angle. Substitution of the above expressions into (7) gives the continuum

form of the hamiltonian: as $S \to \infty$, two quantities $g_1 = (2S+1)/[S(S+1)]$ and $g_2 = 4/(2S+1)$ may both, to order $O(1/S^3)$, be replaced by their algebraic mean $g = (g_1g_2)^{1/2} = 2/[S(S+1)]^{1/2}$, and to this order

$$H^{\rm AF} \to \frac{1}{2} c \int \! \mathrm{d}x \, g [\Pi (1-\Omega^2) \, \Pi + (1-\Omega^2)^{-1} L^2]$$

$$+g^{-1}[(1-\Omega^2)^{-1}(\nabla\Omega)^2+(1-\Omega^2)(\nabla\phi)^2],$$
 (10)

where c is the velocity (2S+1)|J|a. The field $\Omega(x)$ is constrained to satisfy $\Omega^2(x) < 1$. In terms of these variables the continuum form (10) is singular if $\Omega(x) \to \pm 1$, and the regularisation around this singularity is controlled by the "smearing length" ξ – and by whether the underlying discrete lattice spins are integral or half integral [2]. If the implicit "smearing" of the CCRs is ignored, (10) (in addition to O(3) rotational invariance) exhibits Lorentz invariance with "light" velocity c, and conformal or scale invariance: if $x \to \Lambda x$, $c \to \Lambda c$, $\Pi \to \Lambda^{-1}\Pi$, and $L \to \Lambda^{-1}L$ then H^{AF} (10) and the CCRs are unchanged.

The continuum form of the generators of global rotations can be obtained from (6): by expanding to lowest order in L (or equivalently, taking $S \rightarrow \infty$ with the fields fixed), I obtain

$$S^x = \frac{1}{2} \int dx \ [\Pi(1 - \Omega^2)^{1/2} \sin(\phi)$$

$$-L\Omega(1-\Omega^2)^{-1/2}\cos(\phi) + \text{h.c.l.}$$

$$S^y = \frac{1}{2} \int dx \left[-\Pi(1 - \Omega^2)^{1/2} \cos(\phi) \right]$$

$$-L\Omega(1-\Omega^2)^{-1/2}\sin(\phi) + \text{h.c.}$$
,

$$S^z = \int dx L. \tag{11}$$

The continuum form of the lattice translation operator $T = \exp(iaP)$, where P is the crystal momentum (defined modulo $2\pi/a$) is easily obtained:

$$P = P_0 + (\pi/a) \int \mathrm{d}x \{ L + \frac{1}{2} a \Pi^2 + \frac{1}{2} a^{-1} \Omega^2 \}$$

$$+\frac{1}{2}\int \mathrm{d}x \left\{ \Pi \nabla \Omega + L \nabla \phi + \text{h.c.} \right\} . \tag{12}$$

The last term in (12) is just the generator of transla-

tions of the continuum fields, the second term produces the additional discrete transformation $\phi \to \phi + \pi$, $\Omega \to -\Omega$, $\Pi \to -\Pi$, that accompanies translation by one lattice spacing, and P_0 is an additional term present only in the case of half-integral spins:

$$P_0 = (\pi/a)(\frac{1}{2}N_a + J), \quad J = (2\pi)^{-1} \int dx \ \nabla \phi. \tag{13}$$

Alternatively, this term can be included in the other two by the replacement $L \to L + \frac{1}{2}a^{-1}$ when S is half integral. It arises because $\exp\left[i\alpha(S_n^z + \frac{1}{2})\right]$ rather than $\exp(i\alpha S_n^z)$ is the appropriate form of the local spin angle rotation operator to use in constructing T, to compensate the sign change accompanying 2π rotations of half-integral spins. The term P_0 exposes the essential difference between integer- and half-integer-spin antiferromagnets in zero field: in the latter case, after a singular event at some point in space-time where $\Omega(x,t)=\pm 1$, when the angle field winding number J changes by ± 1 , an extra crystal momentum π/a remains to be radiated away and reabsorbed at a second singular event [2].

In the continuum limit, the anisotropy term (2) becomes

$$H' = \frac{1}{2}c\int dx \ \{\gamma_1[gL^2 + g^{-1}(\nabla\Omega)^2] + \gamma_2g^{-1}\Omega^2\},\tag{14}$$

where $\gamma_1 = \frac{1}{2}(\mu + \lambda)$, $\gamma_2 = 2(\mu - \lambda)/a^2$; it is seen that two distinct couplings are still required to describe uniaxial anisotropy. γ_1 is dimensionless (stability requires $\gamma_1 > -1$) and also breaks Lorentz invariance, causing the "light velocity" to become Ω dependent. γ_2 has dimensions (length)⁻², and breaks conformal invariance.

I now make the identification of the nonlinear field theory (10) with the O(3) nonlinear sigma model, more usually described in lagrangian form, with manifestly Lorentz, conformally and O(3) rotationally invariant action

$$\mathcal{S} = \frac{1}{2}g^{-1} \iint dx dt (c^{-1}\hat{\boldsymbol{\Omega}} \cdot \hat{\boldsymbol{\Omega}} - c \nabla \boldsymbol{\Omega} \cdot \nabla \boldsymbol{\Omega}),$$

$$\mathbf{\Omega} \cdot \mathbf{\Omega} = 1. \tag{15}$$

This field theory may be understood as the continuum limit of the (quantum) "antiferromagnetic" rotator chain, described by the hamiltonian

$$H^{R} = (c/a) \sum_{n} (\frac{1}{2}gL_{n} \cdot L_{n} + g^{-1}\Omega_{n} \cdot \Omega_{n+1}),$$
 (16)

where Ω_n and L_n are rotator coordinate and angular momentum variables: $L_n \times L_n = \mathrm{i} L_n$, $L_n \times \Omega_n + \Omega_n \times L_n = 2\mathrm{i} \Omega_n$, $\Omega_n \times \Omega_n = 0$, $L_n \cdot \Omega_n = 0$, $\Omega_n \cdot \Omega_n = 1$. There are *two* independent pairs of conjugate variables per site, in contrast to the spin chain, with one pair per site. Unlike the spin chain, the "antiferromagnetic" rotator chain (16) is trivially equivalent to the "ferromagnetic" variant by the canonical transformation $\Omega_n \to (-1)^n \Omega_n$.

It is useful to introduce the representation

$$\Omega_{n} = ((1 - \Omega_{n}^{2})^{1/2} \cos(\phi_{n}), (1 - \Omega_{n}^{2})^{1/2} \sin(\phi_{n}), \Omega_{n}),
L_{n}^{x} = \Pi_{n} (1 - \Omega_{n}^{2})^{1/2} \sin(\phi_{n})
- L_{n} \Omega_{n} (1 - \Omega_{n}^{2})^{-1/2} \cos(\phi_{n}),
L_{n}^{y} = -\Pi_{n} (1 - \Omega_{n}^{2})^{1/2} \cos(\phi_{n})
- L_{n} \Omega_{n} (1 - \Omega_{n}^{2})^{-1/2} \sin(\phi_{n}),
L_{n}^{z} = L_{n},$$
(17)

where Π_n and L_n are the conjugate momentum variables to Ω_n and ϕ_n . L_n , ϕ_n are again periodic action—angle variables; Π_n , Ω_n are nonperiodic, but subject to the constraint $\Omega_n^2 \leq 1$. In terms of these variables, (16) becomes

$$\begin{split} H^{\mathrm{R}} &= (c/a) \sum_{n} \frac{1}{2} g \big[\Pi_{n} (1 - \Omega_{n}^{2}) \Pi_{n} + (1 - \Omega_{n}^{2})^{-1} L_{n}^{2} \big] \\ &+ g^{-1} \big[\Omega_{n} \Omega_{n+1} \\ &+ (1 - \Omega_{n}^{2})^{1/2} (1 - \Omega_{n+1}^{2})^{1/2} \cos(\phi_{n} - \phi_{n+1}) \big]. \end{split}$$

In the classical limit, g=0, Néel order $\Omega_n+\Omega_{n+1}=1+\cos(\phi_n-\phi_{n+1})=0$ is present in the ground state of (18). A linearisation in these variables, again making the expansion $\cos(\phi_n-\phi_{n+1})\approx -1+\frac{1}{2}(\phi_{n+1}-\phi_n-\pi)^2$, is easily developed, as in the case of the spin chain. A harmonic treatment of fluctuations about the Néel-ordered state with $\Omega_n=(-1)^n\langle\Omega\rangle$ gives the dispersion relations $\omega_q=2(c/a)|\sin(\frac{1}{2}qa)|$ (for the L_n,ϕ_n excitations) and $\omega_q=2(c/a)|\cos(\frac{1}{2}qa)|$ (for the Π_n,Ω_n excitations), independent of $\langle\Omega\rangle$. There are thus again

two important sets of low-energy modes, one set with $q \approx 0$ and one set with $q \approx \pi/a$. Then $L_n \approx aL(x)$, $\phi_n \approx n\pi + \phi(x)$, where L(x) and $\phi(x)$ are "smeared" quasicanonical fields constructed from $q \approx 0$ modes, and $\Omega_n \approx (-1)^n \Omega(x)$, $\Pi_n \approx (-1)^n a\Pi(x)$, where $\Omega(x)$ and $\Pi(x)$ derive from the $q \approx \pi/a$ modes. The continuum field theory thus derived from (18) is easily seen to be exactly as given by (10), (12), and (13) (of course without the half-integral-spin term P_0 in the generator of lattice translations, and with the *integer*-spin type of regularisation).

Even though the lattice form of the rotator chain has in total twice as many degrees of freedom as the lattice form of the spin chain, it is thus seen to have the same number of low-energy degrees of freedom, so the continuum limits of the two models, derived with the assumption of short-range order, can be equivalent. I now discuss some implications of this equivalence.

Classical dynamics. The classical equations of motion of the sigma model are exactly integrable [3], and an infinite set of constants of the motion can be found (though solitons do not occur). Thus (as is also the case with the classical Heisenberg ferromagnet [4]), the classical dynamics of the Heisenberg antiferromagnet become integrable in a continuum limit.

Quantum excitations: dynamical mass generation. In the harmonic treatment of excitations about the Néel-ordered state, two gapless modes are found. If easy-axis anisotropy $(\gamma_2 < 0)$ is present, both modes remain degenerate, and develop a gap, becoming the $S^z = \pm 1$ harmonic Néel magnon (transverse staggered spin-density fluctuation). If easy-plane anisotropy (γ_2 >0) is present, only one mode develops a gap, becoming the $S^z = 0$ longitudinal staggered spin-density fluctuation. However, it is well known that the gapless ordered state of the isotropic sigma model is marginally unstable with respect to the implicit breaking of conformal invariance by the "smearing" of the CCRs; this is seen both in perturbative treatments (the "2 + ϵ " expansion [5]) and non-perturbative ones (the "instanton" expansion [6]): the effective coupling grows according to the scaling equation $d(g/2\pi)/d(\ln \xi)$ = $(g/2\pi)^2 + (g/2\pi)^3$..., indicating a characteristic crossover length scale that diverges as $(\xi g) \exp(2\pi/g)$ as g \rightarrow 0 — for the spin model, this implies a crossover length κ^{-1} (in units of the lattice spacing) that diverges as $\sim S^{-1} \exp(\pi S)$ as $S \to \infty$. The non-perturbative treatment [6] proceeds by a projective-coordinate mapping of the sigma model onto a two-dimensional euclidean field theory; coordinate singularities at spacetime events $\Omega(x,t)=\pm 1$ are represented as "instanton-quarks" and "antiquarks". When fluctuations are taken into account, this "quark gas" behaves like a 2-D Coulomb gas in the plasma phase, with screening length κ^{-1} .

The sigma model develops a mass gap $c\kappa$ ($\sim JS^2 \times \exp(-\pi S)$) as $S \to \infty$) for a triplet elementary excitation: this can be viewed as dynamical mass generation by the Néel magnon, driven by nonlinear zero-point fluctuations ("instantons"). The massive $S^z = 0$ longitudinal staggered spin-density fluctuation mode of the easy-plane system and the $S^z = \pm 1$ transverse modes of the easy-axis system remain massive in the isotropic limit, forming an S = 1 triplet carrying intrinsic crystal momentum π/a .

Ground-state properties. A full description of ground-state properties of the spin chain on length scales larger than the crossover length κ^{-1} requires a fuller treatment of the local rotation symmetry distinguishing the regularisation procedures of integer and half-integer spin systems when $\Omega \to \pm 1$. This is beyond the scope of this letter, but drawing on the study [2], I state briefly without derivation my conclusions:

(A) Integer S. This case is essentially identical to the rotator chain and the standard form of the sigma model. The ground state is an isolated singlet, and the massive S=1 Néel magnon is the only elementary excitation. The large-separation correlations have the Ornstein-Zernike form $\langle S_n \cdot S_0 \rangle \sim (-1)^n |n|^{-1/2} \times \exp(-\kappa |n|)$.

(B) Half-integer S. This case appears to correspond to a sigma model variant in which the euclidean field theory exhibits "instanton-quark" confinement: the "quarks" are paired into doubly charged or neutral entities by "strings", representing the propagators of the excess crystal momentum π/a generated by the change in winding number at the $\Omega=\pm 1$ singularities. This variant model would seem to involve spinor fields: the mapping from vector-spin to spinor variables is not fully defined without the specification of branch-cut coordinate singularities ("strings" joining pairs of "quarks") of the associated spinor gauge field. Fluctuations generate a string tension, with confinement length κ^{-1} . In the strong coupling limit, the doubly-charged strings behave as a marginally bound 2-D

Coulomb gas at the critical limit of the dielectric phase. The half-integer spin chain thus remains in the effectively harmonic phase, and (in addition to the massive Néel magnon) has gapless excitations that can be described in terms of massless $S=\frac{1}{2}$ entities, carrying crystal momentum $\pm\frac{1}{2}\pi/a$, created only in *pairs*. These give a universal *power-law* contribution $(\eta=1)$ that dominates the $\kappa|n| \gg 1$ correlations: $\langle S_n \cdot S_0 \rangle \sim (-1)^n |n|^{-1}$.

The strong-coupling limit of the half-integer S case is the soluble $S=\frac{1}{2}$ model [7], in which the massive S=1 Néel magnon is absent: I conclude that $\kappa\to\infty$ as $S\to\frac{1}{2}$. (The absence of S=1 elementary excitations was recently emphasised in ref. [8].) An explicitly rotationally invariant nonlinear continuum form of the $S=\frac{1}{2}$ model can be derived from the Hubbard chain [9]. The correspondence to a marginally bound 2-D Coulomb gas of doubly charged "instanton-quark" pairs follows from the results [9,10].

An exactly soluble generalised Heisenberg antiferromagnet with arbitrary S has recently been reported [11]; this model is gapless for all S, integer or half-integer. For $S > \frac{1}{2}$ it has additional couplings not present in the standard Heisenberg model: these apparently suppress the dynamic mass generation mechanism described here, making the soluble model unlike the standard model.

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