## Ground State Properties of Antiferromagnetic Chains with Unrestricted Spin: Integer Spin Chains as Realisations of the O(3) Non-Linear Sigma Model

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A continuum limit treatment of planar spin chains with arbitrary S is presented. The difference between integer and half-integer spins is emphasised. While isotropic half-integer spin chains are gapless, and have power-law decay of correlations at T=0 with exponent  $\eta=1$ , integer spin systems have a singlet ground state with a gap for S=1 excitations and exponential decay of correlations. The easy-plane to easy-axis transition is described.

Note: this is a verbatim transcription of ILL preprint SP-81/95, which is cited in a number of places, but was rejected for publication in 1981, and remained unpublished in this original form, which gives somewhat different arguments for the central result as compared to the later paper finally published in Phys. Lett. 93A, 464 (1983); many thanks to Jenő Sólyom for preserving this historical document. The author's current address (November 2016) is: Department of Physics, Princeton University, Princeton NJ 08544-0708, USA.

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One dimensional quantum spin chains are currently the subject of much study. In this note, I outline some new results on axially-symmetric spin chains, without restrictions on S, that confirm and extend earlier results<sup>1,2</sup> restricted to spin  $S=\frac{1}{2}$ , and lead to an unexpected conclusion: while half-integral spin isotropic antiferromagnets have a gapless linear spin wave spectrum and power-law decay of ground state correlations  $\langle \vec{S}_n \cdot \vec{S}_0 \rangle \sim (-1)^n n^{-1}$ , integral spin system have a singlet ground state, with a gap for "massive" S=1 elementary excitations, and exponential decay of ground state correlations:  $\langle \vec{S}_n \cdot \vec{S}_0 \rangle$  $\sim (-1)^n n^{-\frac{1}{2}} \exp(-\kappa n)$ . Indeed, as will be outlined, the isotropic integer spin system can be related to the O(3)coupled rotor chain, or "non-linear sigma model"<sup>3</sup>, and thus to the 2D classical Heisenberg model. The role of quantum fluctuations controlled by  $S^{-1}$  is analogous to thermal fluctuations in the latter model.

I will discuss the XY-Heisenberg-Ising system, with all components of exchange antiferromagnetic: with  $\lambda \geq 0$ ,

$$H = |J| \sum_{n} \left( S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \lambda S_n^z S_{n+1}^z \right). \tag{1}$$

In the easy-plane limit ( $\lambda \ll 1$ ), a description in terms of quantum action-angle variables N,  $\phi$  (where  $[N, \exp(i\phi)] = \exp(i\phi)$ ) is appropriate:  $N_n = S + S_n^z$ ,  $S^+ = (-1)^n (S + S_n^z)^{\frac{1}{2}} \exp(i\phi_n)(S - S_n^z)^{\frac{1}{2}}$ . This representation, similar in spirit to the Holstein-Primakoff boson representation appropriate in the easy-axis limit, is exact<sup>4</sup>. The eigenvalues of  $N_n$  are integers. Physical states are restricted to the subspace  $0 \le N_n \le 2S$ .

It will prove useful to introduce a dual "angle" variable  $\theta_{n+\frac{1}{2}}$  defined on bonds, so  $2\pi S_n^z = \theta_{n+\frac{1}{2}} - \theta_{n-\frac{1}{2}}$ . In the limit of sufficiently strong easy-plane anisotropy,  $\phi_n$  will exhibit short-range order, and vary slowly along the chain. I will develop a continuum description in terms of fields  $\phi(x)$  and  $\theta(x)$ , where for lattice spacing a and  $x_n \equiv$ 

 $na, \phi_n \sim \phi(x_n)$ , and  $\Pi(x_n) = [\theta(x_{n+\frac{1}{2}}) - \theta(x_{n-\frac{1}{2}})]/2\pi a - S^z/L$  is conjugate to  $\phi(x_n)$ . This description is appropriate when zero-point fluctuations of  $\phi_n$  with respect to its neighbours are small compared to  $\pi$ . In this small-fluctuation regime, the locally-periodic character of  $\phi_n$  and the related discretisation of the spectrum of  $S_n^z$  are hidden.

Noting that periodic boundary conditions allow the field  $\phi(x)$  to increase by  $2\pi$  times an integer J around the ring of length L, the fields  $\theta(x)$  and  $\phi(x)$  can be represented as

$$\theta(x) = \theta_0 + 2\pi S^z x / L - i \sum_q \alpha_q^+ e^{iqx} \operatorname{sgn}(q) (b_q^{\dagger} + b_{-q}),$$

$$\phi(x) = \phi_0 + 2\pi J x / L - i \sum_q \alpha_q^- e^{iqx} (b_q^{\dagger} - b_{-q}), \qquad (2)$$

where  $\alpha_q^{\pm} = (2L\sin(\frac{1}{2}|q|a)/\pi a)^{-\frac{1}{2}}\exp(\pm\varphi(q))$ , and  $\varphi(q)$  is a free Bogoliubov transformation parameter.  $b_q^{\dagger}$  are boson creation operators labelled by  $q = 2\pi n/L$ ,  $q \neq 0$ ,  $|q| < \pi/a$ .  $\phi_0$  is the global spin angle conjugate to total azimuthal spin  $S^z$ ; similarly,  $\theta_0$  is the angle conjugate to the action-type variable J.

The momentum operator P is given by

$$P = (\pi + 2\pi J/L)(S^z + SL/a)/a + \sum_{q} q b_q^{\dagger} b_q.$$
 (3)

The first term provides a global rotation of  $\phi_0$  by  $\pi + 2\pi J/L$ . This is required in addition to a shift of the pattern of fluctuations for a translation of the spin configuration by one lattice spacing.

The representation of  $S_n^z$  in a way that reflects its discrete spectrum is crucial. The conserved magnetisation density can be regarded as residing in a fluid of "magnon" excitations about the fully-aligned state  $S_n^z = -S$ , each magnon carrying  $S^z = +1$ . As n increases,

 $\theta_{n+\frac{1}{2}}+2\pi S(n+\frac{1}{2})$  increases monotonically by  $2\pi$  each time such a magnon is passed. In the continuum field description, the magnons will be taken to be located at the points where  $\theta(x)+2\pi Sx/a$  is an integer multiple of  $2\pi$ . The magnon density operator is thus a sum of unit-weight delta-functions:  $\rho(x)=$ 

$$\sum_{n} \delta[\theta(x) + 2\pi Sx/a - 2n\pi] [\nabla \theta(x) + 2\pi S/a].$$

This can be written as  $\rho(x) = S/a + (2\pi)^{-1} \nabla \tilde{\theta}(x)$ ,

$$\tilde{\theta}(x) = \theta(x) + \sum_{m \ge 1} 2\sin[m\theta(x) + 2\pi mSx/a)]/m. \quad (4)$$

The spin operator  $S_n^z$  is then given by the integrated magnon density in the unit cell  $x_{n-\frac{1}{2}} \leq x \leq x_{n+\frac{1}{2}}$ ; this immediately gives  $\theta_{n+\frac{1}{2}} = \tilde{\theta}(x_{n+\frac{1}{2}})$ .  $S_n^z$  given in terms of the operators  $\theta_{n+\frac{1}{2}}$  constructed out of the continuum fields  $\theta(x)$  has the required discrete spectrum. For calculation of long-distance correlations, a gradient expansion in  $\theta(x)$  can be used to obtain an approximate local form for  $S_n^z$ . This form depends on whether S is integral or half-integral through the term  $2\pi m Sx/a$  in (4). For integral S,

$$S_n^z \sim a[S^z/L + \Pi(x_n)]\{1 + \sum_{m>1} 2\cos[m\theta(x_n)]\};$$
 (5)

for half-integral S, an oscillatory term is present:  $S_n^z \sim S_{n1}^z + (-1)^n S_{n2}^z$ , where

$$S_{n1}^z \ = \ a[S^z/L + \Pi(x_n)]\{1 + \sum_{m \geq 1} 2\cos[2m\theta(x_n)]\},$$

$$S_{n2}^{z} = \frac{1}{\pi} \sum_{m>0} 2\sin[(2m+1)\theta(x_n)]/(2m+1).$$
 (6)

If, following Villain<sup>4</sup>, the long-wavelength approximation  $S_n^z \sim a[S^z/L + \Pi(x_n)]$  is made, linearisation of (1) in  $S_n^z$  and  $(\phi_{n+1} - \phi_n)$  when  $\lambda < 1$  leads to the effective Hamiltonian

$$H = \sum_{q} \omega(q) b_{q}^{\dagger} b_{q} + (\pi v_{s}/L) [\eta(S^{z})^{2} + \bar{\eta}J^{2}],$$
 (7)

where  $\eta = \bar{\eta}^{-1} = \exp[-2\varphi(0)]$ ,  $\exp[2\varphi(q)] = 2\pi S[2 + 2\lambda\cos(qa)]^{\frac{1}{2}}$ . The spin-wave spectrum is linear as  $q \to 0$ :  $\omega(q) \sim v_s|q|$ ;  $\omega(q) = 2JS\sin(\frac{1}{2}|q|a)[2 + 2\lambda\cos(qa)]^{-\frac{1}{2}}$  note the soft mode at the Brillouin zone edge  $q = \pi/a \equiv \frac{1}{2}G$ . The linearisation is valid for large S, when nonlinear zero-point fluctuations are suppressed; however, for general S, provided such fluctuations do not lead to breakdown of the short-range order of  $\phi_n$ , a renormalisation procedure should yield an effective Hamiltonian of form (7), but with renormalised parameters  $\varphi(q)$ ,  $\omega(q)$ . This viewpoint has been advanced in Ref.(5), and is supported by studies of exactly-soluble models. The state described by (7) may be called a "spin fluid" state. The

magnon current  $j=(2\pi)^{-1}(d\theta_0/dt)=\bar{\eta}v_s(J/L)$  is conserved at low energies.

Correlation functions are easily evaluated in the fluid state. The momentum associated with the current excitation  $\Delta J=1$  is  $SG+2\pi S^z/L$ . When  $S^z\neq 0$ , harmonics of this wavevector appear in the correlations through sine and cosine terms in (5) and (6). However, I will describe only the case  $S^z=0$ .

For integer spins, the current excitation carries momentum 0 (mod. G). However, oscillatory terms with exponential decay constant  $\kappa_0$  (where  $\omega(\frac{1}{2}G+i\kappa_0)=0$ ) are still present, due to the soft-mode in the spin-density fluctuation spectrum at the Brillouin zone edge; these arise from the branch cut in  $\exp(2\varphi(q))$  at complex q. In the linearised approximation,  $\cosh(\kappa_0)=1/\lambda$ . For  $n\gg 1$ ,  $\langle S_n^z S_0^z \rangle \sim A(-1)^n n^{-\frac{1}{2}} \exp(-\kappa_0 n) + \bar{\eta}(2\pi n)^{-2}(1+Bn^{-\bar{\eta}})$ ,  $\langle S_n^+ S_0^- \rangle \sim C(-1)^n n^{-\eta} + Dn^{-\frac{3}{2}} \exp(-\kappa_0 n)$ , where A - D are constants depending on short-wavelength structure.

For half-integral spins, the current excitation carries momentum  $\frac{1}{2}G$ , and controls oscillatory behaviour, masking the soft mode. For  $n\gg 1$ ,  $\langle S_n^zS_0^z\rangle\sim A(-1)^nn^{-\bar{\eta}}+\bar{\eta}(2\pi n)^{-2}(1+Bn^{-4\bar{\eta}}),$   $\langle S_n^+S_0^-\rangle\sim Cn^{-\eta}[(-1)^n+Dn^{-\bar{\eta}}].$  These expressions agree with the  $S=\frac{1}{2}$  results previously obtained with the various fermion representations  $^{1,2}$ .

If the full forms (5), (6) for  $S_n^z$  are used, terms involving  $\cos(m\theta(x_n))$  are seen to be present in the Hamiltonian. These terms can be regarded as Umklapp terms, as they allow destruction of current quanta. When  $S^z=0$ , individual current quanta can be destroyed in integral spin systems (by a  $2\pi$  rotation of a spin), while in half-integral spin systems, they can only be destroyed in pairs (by a local  $4\pi$  rotation). The long-wavelength fluctuation part of the Hamiltonian has the form (8), with  $c=v_s/4\pi$ :

$$H = c \int dx \left[ \bar{\eta} (\nabla \phi)^2 + \eta (\nabla \theta)^2 + \sum_{m} \gamma_m \cos(m\theta) \right]. \quad (8)$$

Since  $(2\pi)^{-1}\nabla\phi$  is conjugate to  $\theta$ , this is easily recognised to be of sine-Gordon type<sup>6</sup>, with coupling parameters  $\beta_m^2 = 2\pi m^2 \bar{\eta}$ . The fluid state is only stable if  $\beta_m^2 > 8\pi$ , i.e.,  $\eta < \frac{1}{4}m^2$ . In the fluid state, fluctuations of  $\nabla\phi(x)$  are small compared to the conjugate fluctuations of  $\theta(x)$ . As  $\lambda$  increases,  $\eta$  and the fluctuations of  $\nabla\phi(x)$  increase, while those of  $\theta(x)$  decrease. Eventually, the fluctuations of  $\theta(x)$  are too small to prevent pinning by the cosine potential, and those of  $\nabla\phi(x)$  are sufficiently large that the local periodicity of  $\phi_n$  is restored.

For integer spins, the m=1 process is present.  $\eta$  reaches its limiting value of  $\frac{1}{4}$  at some critical value  $\lambda_{c1} < 1$ , at which the correlations still have easy-plane character. For  $\lambda > \lambda_{c1}$ ,  $\theta(x_n)$  is pinned to values 0 (mod.  $2\pi$ ), and  $2\pi$  fluctuations of  $\phi_n$  are important. The resulting state may be described as a pinned spin-density wave with the same periodicity as the lattice, so no broken symmetry is present. Its excitations are "topological solitons" where  $\theta(x)$  slips by  $2\pi$  (one magnon), carrying  $S^z = \pm 1$ , and intrinsic momentum  $\frac{1}{2}G$  (from (3)). Predicted<sup>7</sup> correlations in

the singlet ground state phase with  $\lambda > \lambda_{c1}$  decay as  $\langle S_n^z S_0^z \rangle \sim A(-1)^n n^{-\frac{1}{2}} \exp(-\kappa_0 n) + n^{-2} [B \exp(-2\kappa_0 n)] + C \exp(-2\kappa_1 n)], \ \langle S_n^+ S_0^- \rangle \sim D(-1)^n n^{-\frac{1}{2}} \exp(-\kappa_1 n) + E n^{-2} \exp(-(\kappa_0 + \kappa_1) n), \text{ where } \kappa_1 \text{ is the decay constant associated with the } S^Z = \pm 1 \text{ soliton dispersion } \varepsilon_1(q)$ :  $\epsilon_1(\frac{1}{2}G + i\kappa_1) = 0.$ 

As  $\lambda$  increases, the soliton gap increases, while that of the soft mode decreases. At the isotropic point  $\lambda = 1$ ,  $\kappa_0$  $= \kappa_1$ , and the soft mode excitation forms a triplet with the  $S^z = \pm 1$  soliton excitation. The soft mode excitation has the lower energy for  $\lambda > 1$ , and its gap vanishes at a second critical point  $\lambda_{c2} > 1$ , signalling the instability against the doubly-degenerate Ising-Néel state. Though detailed justification cannot be given here, I note the critical behaviour can be identified with that of the singletdoublet transition in the " $(\phi)^4$ " field theory or 2-D Ising model, just as critical behaviour at  $\lambda_{c1}$  is related to that of the 2-D XY model.  $\kappa_0$  vanishes when  $\lambda = \lambda_{c2}$ , and predicted<sup>7</sup> correlations decay as  $\langle S_n^z S_0^z \rangle \sim A(-1)^n n^{-\frac{1}{4}} +$  $Bn^{-\frac{3}{2}}, \langle S_n^+ S_0^- \rangle \sim n^{-\frac{1}{2}} \exp(-\kappa_1 n) (C(-1)^n + Dn^{-\frac{5}{4}}).$  In the doublet Néel state when  $\lambda > \lambda_{c2}$ , the  $S^z = 0$  excitations again develop a gap, and can now be identified as pairs of solitons of the Néel state (which correspond to configurations like [+-+0-+-], and carry no magnetisation in the integral-spin case). Predicted<sup>7</sup> correlations now decay as  $\langle S_n^z S_0^z \rangle \sim (-1)^n \{A + n^{-2} [B \exp(-2\kappa_0 n) + n] \}$  $C \exp(-2\kappa_1 n)$ ] +  $n^{-1}$ [ $D \exp(-2\kappa_0 n) + E \exp(-2\kappa_1 n)$ ],  $\langle S_n^+ S_0^- \rangle \sim n^{-\frac{1}{2}} \exp(-\kappa_1 n) [(-1)^n F + G n^{-1}].$  As  $\lambda$  increases above  $\lambda_{c2}$  the excitation energy and associated decay constant  $\kappa_0$  of the  $S^z=0$  Néel solitons rapidly become larger than the corresponding quantities for the  $S^z$  $=\pm 1$  excitations, now identified as the Néel magnons.

The transition from easy-plane to easy-axis system is simpler in the case of half-integer spin. The m=1 Umklapp process is absent, and the m=2 process drives an instability against a doubly-degenerate Néel-Ising densitywave state, where  $\theta(x_n)$  alternates between 0 and  $\pi$ . The solitons (configurations like  $[+-+\sigma-+-]$ ,  $\sigma=\pm\frac{1}{2}$ ) are created in pairs, and carry magnetisation  $S^z = \pm \frac{1}{2}$ . The critical value of  $\eta$  at breakdown of the fluid state is  $\eta = 1$ , when the correlations are isotropic, hence the transition occurs at  $\lambda = 1$ . For  $\lambda \geq 1$ , pairs of  $S^z = \pm \frac{1}{2}$  solitons are the lowest energy excitations, and a strong enough axial field will drive a second-order transition into a weakly incommensurate density wave state, which can be considered as a dilute fluid of  $S^z = +\frac{1}{2}$  solitons. The origin of the  $S^z = \pm 1$  Néel magnon excitations, which have much lower energy than the solitons at larger easy-axis anisotropies, is not yet clarified. In the strong anisotropy limit, the response to a magnetic field is a first-order "spin-flop" transition. It seems likely that the easy-axis Néel magnon is connected with the easy-plane zone-edge soft mode; it is not clear whether these excitations have a gap at  $\lambda=1$ , when the soliton gap vanishes.

The soluble  $S=\frac{1}{2}$  chain exhibits the m=2 Umklapp instability, which was overlooked in the earlier "fermion representation" treatment<sup>1</sup>, but first pointed out in Ref.(5). The details of the solution are in precise accord with the scaling theory of  $(8)^8$ . A feature special to  $S=\frac{1}{2}$  is the absence of the Néel magnon for  $\lambda>1$ , and the soft mode for  $\lambda<1$ . This can be attributed to the hard-core nature of the quantum of magnetisation. In the easy-axis case, a treatment in terms of fermion "disorder variables" (solitons) is more appropriate than a treatment using Holstein-Primakoff boson variables.

Finally, I note the similarity between the behaviour described here for the integral-spin antiferromagnetic chain and that of the O(3) rotor chain, or "non-linear sigma model", which can be related to the classical 2-D n=2 vector spin model<sup>3</sup>. The rotor chain Hamiltonian is

$$H = \sum_{n} \frac{1}{2} g L_n^2 + (\Omega_n^x \Omega_{n+1}^x + \Omega_n^y \Omega_{n+1}^y + \lambda \Omega_n^z \Omega_{n+1}^z)$$
 (9)

where  $\vec{L}_n \cdot \vec{\Omega}_n = 0$ ,  $\Omega_n^2 = 1$ , and the rotor commutation relations are  $\vec{L}_n \times \vec{L}_n = i\vec{L}_n, \frac{1}{2}(\vec{L}_n \times \vec{\Omega}_n + \vec{\Omega}_n \times \vec{L}_n) =$  $i\vec{\Omega}_n, \ \vec{\Omega}_n \times \vec{\Omega}_n = 0.$  In the isotropic case  $\lambda = 1$ , this model has a singlet ground state with a gap for L=1elementary excitations for all non-zero g, and models the 2-D classical Heisenberg model with g playing the role of temperature<sup>3</sup>. Consider now a spin chain with alternating ferromagnetic and antiferromagnetic exchange, H = $J\sum_{n}(-1)^{n}\vec{S}_{n}\cdot\vec{S}_{n+1}$ . This model has two spins per unit cell, and to study it, it is useful to decimate it by blocking the spins into pairs. If it is chosen to combine ferromagnetically coupled spins, it is easily seen that the resulting effective Hamiltonian is that of a spin 2S (i.e., integral spin) antiferromagnet. If antiferromagnetically coupled spins are combined, one can introduce new variables  $\vec{L}$  $= \vec{S}_1 + \vec{S}_2, \ \vec{\Omega} = (2S)^{-\frac{1}{2}} (\vec{S}_1 - \vec{S}_2).$  For large S these obey rotor-like commutation relations, and an effective rotor-chain Hamiltonian is obtained. The identification with (9) provides the connection of the  $\lambda_{c1}$  and  $\lambda_{c2}$  instabilities to the 2-D XY and Ising critical behaviour, and justifies the discussion of the  $\lambda_{c2}$  instability given above.

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- Hasslacher and A. Neveu, Phys. Rev. D **11**, 3424 (1975). <sup>7</sup> Power-law prefractors to exponential decay of correlations given here are to be regarded as *conjectures*, based on the assumption that an Ornstein-Zernike type of approach can be applied in the massive phases, and that these power-laws are coupling-independent. A factor  $n^{-\frac{1}{2}}$  is associated with each elementary excitation, with an extra  $n^{-1}$  due to a matrix element usually associated with a pair of excitations. The correlation functions predicted here agree with the  $\beta^2$
- =  $4\pi$  limit of the sine-Gordon theory, and the Holstein-Primakoff treatment of the easy-axis antiferromagnet. 2-D Ising model results have been taken into account in the predictions for behaviour of integer spins near  $\lambda_{c2}$ .
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- <sup>9</sup> F. D. M. Haldane, article in preparation.