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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Abstract

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 η = 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.

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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 restriction on S, that confirm and extend earlier results[1,2] restricted to spin $S = \frac{1}{2}$, and lead to an unexpected conclusion: while <u>half-integral spin</u> isotropic antiferromagnets have a gapless linear spin wave spectrum and <u>power-law decay</u> of ground state correlations $\langle \vec{S}_n \cdot \vec{S}_0 \rangle \sim (-1)^n n^{-1}$, <u>integral spin</u> systems have a singlet ground state, with a gap for "massive" $S = 1$ elementary excitations, and <u>exponential decay</u> 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"[3], and thus to the 2-D 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 $\lambda \geq 0$,

$$H = |J| \sum_n (S^x_n S^x_{n+1} + S^y_n S^y_{n+1} + \lambda S^z_n S^z_{n+1}) \quad . \tag{1}$$

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

It will prove useful to introduce a dual "angle" variable $\theta_{n+\frac{1}{2}}$ defined on bonds, so $2\pi S^z_n = \theta_{n+\frac{1}{2}} - \theta_{n-\frac{1}{2}}$. In the limit of sufficiently strong easy-plane anisotropy, ϕ_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 ϕ_n with respect to its neighbors are small compared to π. In this small-fluctuation regime, the locally periodic character of ϕ_n and the related discretisation of the spectrum of S^z_n are hidden.

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

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

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

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 $q = 2\pi n/L$, $q \neq 0$, $|q| < \pi/a$. ϕ_0 is the global spin angle conjugate to total azimuthal spin S^z; similarly, θ_0 is the angle conjugate to the action-type variable J.

The momentum operator P is given by

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

The first term provides a global rotation of ϕ_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^z_n 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 $S^z_n = -S$, each magnon carrying $S^z = +1$. As n increases, $\theta_{n+\frac{1}{2}} + 2\pi S(n+\frac{1}{2})$ increases monotonically by 2π 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 2π. The magnon density operator is thus a sum of unit-weight delta-functions: $\rho(x)$ =

$$\sum_n \delta\left[\theta(x) + 2\pi Sx/a - 2n\pi\right]\left[\nabla\theta(x) + 2\pi S/a\right] .$$

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

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

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 $2\pi mSx/a$ in (4). For integral S ,

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

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

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

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

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

$$H = \sum_q \omega(q) b_q^\dagger b_q + (\pi v_S/L)\left[\eta (S^z)^2 + \bar{\eta} J^2\right] \quad , \tag{7}$$

where $\eta = \bar{\eta}^{-1} = \exp\left[-2\varphi(0)\right]$, $\exp\left[2\varphi(q)\right] = 2\pi S\left[2 + 2\lambda\cos(q)\right]^{\frac{1}{2}}$. The spin-wave spectrum is linear as $q \to 0$: $\omega(q) \sim v_S|q|$; $\omega(q) = 2JS\sin(\frac{1}{2}|q|a)\left[2 + 2\lambda\cos(q)\right]^{-\frac{1}{2}}$ - 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 non-linear zero-point fluctuations are suppressed; however, for general S, provided such fluctuations do not lead to breakdown of the short-range order of ϕ_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 $j = (2\pi)^{-1}(d\theta_0/dt) \doteq \bar{\eta} v_S(J/L)$ 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 <u>integer</u> spins, the current excitation carries momentum 0 (mod. G). However, oscillatory terms with exponential decay constant κ_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 $n \gg 1$, $\langle S^z_n S^z_0 \rangle \sim A(-1)^n n^{-\frac{1}{2}}\exp(-\kappa_0 n) + \bar{\eta}(2\pi n)^{-2}(1+Bn^{-\bar{\eta}})$, $\langle S^+_n S^-_0\rangle \sim C(-1)^n n^{-\eta} + Dn^{-3/2}\exp(-\kappa_0 n)$, where A - D are constants depending on short-wavelength structure.

For <u>half-integral</u> spins, the current excitation carries momentum $\frac{1}{2}G$, and controls oscillatory behaviour, masking the soft mode. For $n \gg 1$, $\langle S^z_n S^z_0 \rangle \sim A(-1)^n n^{-\bar{\eta}} + \bar{\eta}(2\pi n)^{-2}(1+Bn^{-4\bar{\eta}})$, $\langle S^+_n S^-_0 \rangle \sim Cn^{-\eta}[(-1)^n + Dn^{-\bar{\eta}}]$. 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^z_n 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 2π rotation of a spin), while in half-integral spin systems, they can only be destroyed in <u>pairs</u> (by a **local** 4π rotation). The long-wavelength fluctuation part of the Hamiltonian has the form (8), with $c = v_S/4\pi$:

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

Since $(2\pi)^{-1}\nabla\phi$ is conjugate to θ, this is easily recognised to be of sine-Gordon type[6], 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 λ increases, η 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 ϕ_n is restored.

For <u>integer spins</u>, the m=1 process is present. η 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. 2π), and 2π fluctuations of ϕ_n are important. The resulting state may be described as a pinned spin density wave with the <u>same</u> periodicity as the lattice, so no broken symmetry is present. Its excitations are "topological solitons" where $\theta(x)$ slips by 2π (one magnon), carrying $S^z = \pm 1$, and intrinsic momentum $\frac{1}{2}G$ (from (3)). Predicted[7] correlations in the <u>singlet ground state</u> phase with $\lambda > \lambda_{c1}$ decay as $\langle S^z_n S^z_0\rangle \sim A(-1)^n n^{-\frac{1}{2}}\exp(-\kappa_0 n) + n^{-2}\{B\exp(-2\kappa_0 n)+C\exp(-2\kappa_1 n)\}$, $\langle S^+_n S^-_0\rangle \sim D(-1)^n n^{-\frac{1}{2}}\exp(-\kappa_1 n) + En^{-2}\exp(-(\kappa_0+\kappa_1)n)$, where κ_1 is the decay constant associated with the $S^z = \pm 1$ soliton dispersion $\varepsilon_1(q)$: $\varepsilon_1(\frac{1}{2}G + i\kappa_1) = 0$.

As λ 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-Neel state. Though detailed justification cannot be given here, I note the critical behaviour can be identified with that of the singlet-doublet transition in the "(ϕ^4)" field theory or 2-D Ising model, just as critical behaviour at λ_{c1} is related to that of the 2-D XY model. κ_0 vanishes when $\lambda = \lambda_{c2}$, and predicted[7] correlations decay as $\langle S^z_n S^z_0\rangle \sim A(-1)^n n^{-\frac{1}{4}} + Bn^{-3/2}$, $\langle S^+_n S^-_0\rangle \sim n^{-\frac{1}{2}}\exp(-\kappa_1 n)(C(-1)^n + Dn^{-5/4})$

In the doublet Néel state when $\lambda > \lambda_{c2}$, The $S^z = 0$ excitations again develop a gap, and can now be identified as <u>pairs</u> of solitons of the Néel state (which correspond to configurations like [+-+0-+-], and carry <u>no</u> magnetisation in the integral-spin case). Predicted[7] correlations now decay as $\langle S^z_n S^z_0\rangle \sim (-1)^n\{A + n^{-2}[B\exp(-2\kappa_0 n) + C\exp(-2\kappa_1 n)]\} + n^{-1}[D\exp(-2\kappa_0 n)+E\exp(-2\kappa_1 n)]$, $\langle S^+_n S^-_0\rangle \sim n^{-\frac{1}{2}}\exp(-\kappa_1 n)[(-1)^n F + Gn^{-1}]$.

As λ increases above λ_{c2} the excitation energy and associated decay constant κ_0 of the $S^z = 0$ Neel solitons rapidly become larger than the correponding 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-integral spins. The m=1 Umklapp process is absent, and the m=2 process drives an instability against a doubly degenerate Néel-Ising density-wave state, where $\theta(x_n)$ alternates between 0 and π. 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 η at breakdown of the fluid state is $\eta = 1$, when the correlations are isotropic, hence the transition occurs at $\lambda = 1$. For $\lambda \gtrsim 1$, 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 $S^z = \pm\frac{1}{2}$ 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[1], 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[9].

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[3]. The rotor chain Hamiltonian is

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

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=1 elementary excitations for all non-zero g, and models the 2-D classical Heisenberg model with g playing the role of temperature[3]. 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., <u>integral</u> 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 λ_{c1} and λ_{c2} instabilities to the 2-D XY and Ising critical behavior, and justifies the discussion of the λ_{c2} instability given above.

References

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