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Nonlinear sigma model approach to quantum spin chains

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Abstract : We introduce and motivate the study of quantum spin chains on a one-dimensional lattice We classify the varieties of methods that have been used to study these models into three categories, (a) exact methods to study specific models (b) field theories to describe fluctuations about the classical ordered phases and (c) numerical methods We then discuss the $J_1-J_2-\delta$ model in some detail and end with a few comments on open problems

1. Introduction ·

We start with the definition of a spin chain [1,2] as a spin model on a one-dimensional lattice — *e.g.*,

$$H = J_1 \sum_{nn} S_i \cdot S_j + J_2 \sum_{nn} (S_i \cdot S_j)^2 + J_3 \sum_{nnn} S_i \cdot S_j + \cdots \quad (1)$$

Here, i, j represent the sites on a lattice and the notation nn (= < i, j>) stands for nearest neighbour, nnn stands for next nearest neighbour and so on. The spins are Heisenberg spins satisfying $[S_i^a, S_i^b] = i\varepsilon^{abc} S_i^c$ and not classically commuting variables, and hence it is a quantum spin chain. We would like to find the ground state and excitation spectrum of these models.

But why are we interested in these models ? Spin systems as models of magnetic materials have been used for many years [3] because there exist large classes of materials where the electron stays localised and magnetic properties reside in the individual atoms — *i.e.*, one has localised moments which can be modelled by the spins.

But more specifically, there are several reasons for studying one-dimensional quantum spin chain. The first is simply that there really exist materials that behave like one-dimensional antiferromagnets [4, 5]. CsNiCl$_3$ is one of them, because the ratio between the intra-chain coupling and inter-chain coupling in this material is 0.018. Another compound which is even more

markedly one-dimensional is NENP (Ni($C_2H_8N_2)_2(NO_2)ClO_4$) where the ratio is of the order 10^{-4}. In both these materials, a gap in the excitation spectrum was found although translational symmetry remained unbroken. This was an experimental verification of a conjecture by Haldane [1, 2, 6] that $S = 1$ Heisenberg antiferromagnets should have a gap in the spectrum (unlike $S = 1/2$) and would not break translational symmetry (unlike dimers). More recently, even more exotic compounds which are quasione-dimensional and can be modelled by unusual spin chains (sawtooth spin chains) with missing bonds *viz.*

$$H = J \Sigma_i S_i \cdot S_{i+1} + J/2 \Sigma_i (1+(-1)^i) S_i \cdot S_{i+2} \quad \text{have been found [7].}$$

The second reason is that there exist exact solutions of some toy models, which can then be used as a check or testing ground for new analytical or numerical methods. Finally, quantum antiferromagnets in higher dimensions have become particularly prominent in the last few years in the context of high T_c superconductors. It is hoped that some of the methods to solve quantum spin chains may have generalisation to higher dimensions.

2. Varieties of approaches to solve quantum spin chains

In this section, we will discuss the various methods that have been used to 'solve' models of quantum spin chains.

I. *Spin-wave theory :*

In higher dimensions, the standard way to proceed is to start with the classical ground state and then use spin-wave theory. We first try to apply that method to the one-dimensional spin models here. Let us start with the simplest spin-chain, the Heisenberg antiferromagnet (*HAFM*)

$$H = J \sum S_i S_{i+1}.$$ (2)

Here, i runs over the sites on the one-dimensional lattice. If the spins were classical vectors, then

$$H = JS^2 \sum \cos(\theta_i - \theta_{i+1})$$ (3)

which is obviously minimum when $\cos(\theta_i' - \theta_{i+1}) = -1$ $\Rightarrow (\theta_i - \theta_{i+1}) = \pi$.

Hence, the classical ground state (*Neel* state) is given by

$$|s,-s,s,-s,...\rangle = |\uparrow, \downarrow, \uparrow, \downarrow,...\rangle.$$ (4)

Note that this is not an eigenstate of the Hamiltonian, because terms in the Hamiltonian flips nearest neighbour spins. However, for very large spins

$$\left[S_i^a, S_i^b \right] = \varepsilon_{abc} S_i^c = O(S) << O(S^2).$$ (5)

Hence, in the limit, $S \to \infty$ the *Neel* state must be the ground state. By perturbing about the *Neel* state, we can get the results for large but finite spin. This perturbation theory is called the spin-wave theory and is done using the Holstein-Primakoff transformation [3], which is given by

$$S_i^z = S - a_i^\dagger a_i, \quad S_i^z = -S + b_i^\dagger b_i,$$

$$S_i^+ = \sqrt{2S} \left(1 - \frac{a_i^\dagger a_i}{2S} \right)^{1/2} a_i, \quad S_i^+ = \sqrt{2S} b_i^\dagger \left(1 - \frac{b_i^\dagger b_i}{2S} \right)^{1/2}$$

$$S_i^- = \sqrt{2S} a_i^\dagger \left(1 - \frac{a_i^\dagger a_i}{2S} \right)^{1/2}, \quad S_i^- = \sqrt{2S} \left(1 - \frac{b_i^\dagger b_i}{2S} \right)^{1/2} b_i$$ (6)

for the A and B sub-lattices, which are denoted as $i \in A$ when i is even and $i \in B$ when i is odd or *vice-versa*. We can easily check that the spins satisfy the spin algebra when the a_i, b_i and their conjugates satisfy bosonic commutation relations. Note that in the A sublattice, the absence of any bosons in a state implies that it has the maximum spin and for the B sub-lattice, the absence of any bosonic excitation implies minimum spin. In the large S limit, the awkward square-root term can be dropped

and the spin raising and lowering operators can be approximated merely as

$$S_i^+ \to \sqrt{2S} a_i^\dagger, \quad S_i^- \to \sqrt{2S} a_i,$$

$$S_i^+ \to \sqrt{2S} b_i^\dagger, \quad S_i^- \to \sqrt{2S} b_i$$ (7)

on the A and B sub-lattices. In fact, we can develop a systematic $1/S$ expansion by expanding the square-root term, with the above terms being the first in the expansion. But in this review, we will stop with the first term. Next, we write the Hamiltonian in terms of these bosons (using the above approximation) as

$$H = J \sum_{<i,j>} \left[-S^2 + S\left(a_i^\dagger a_i + b_j^\dagger b_j + a_i b_j + a_i^\dagger b_j^\dagger \right) \right].$$ (8)

After going to momentum space and performing a Boguliobov transformation, we get

$$H = \sum_{k \in RBZ} E_k \left(c_k^\dagger c_k + d_k^\dagger d_k \right)$$ (9)

with $E_k = 2JS \sin$ c_k and d_k are rerelated to the Fourier transforms of the a_i and b_i fields as $c_k = u_k a_k - u_k b_k^\dagger$ and $d_k = u_k b_{-k} - v_k a_k^\dagger$, with $u_k = \cosh \theta_k$ and $v_k = \sinh \theta_k$ and furthermore, $\coth 2\theta_k = -\cos k$. As $k \to 0$, $E_k \to 2JS|k|$ which implies that the c and d bosons, which are the spin-wave modes, are massless and relativistic modes with spin-wave velocity given by $v_s = 2JS$. This in fact, gives us a clue that a relativistic field theory description of the spin-wave modes might be possible.

We can also understand more physically why there are two massless spin-wave modes. The *Neel* state breaks the SO (3) symmetry of the spin variables down to $SO(2)$ (rotations about the S^z axis). The spin-waves are the Goldstone modes of this spontaneous symmetry break down. (Choosing a direction for the *Neel* state (ground state) spontaneously breaks the $SO(3)$ spin symmetry to the Hamiltonian down to $SO(2)$).

Spin-wave theory works quite well for three dimensional magnets, but in low dimensions, spin-wave theory has problems due to quantum fluctuations. Let us calculate the reduction in the sub-lattice magnetisation due to quantum fluctuations (in arbitrary dimensions). This can be done by computing the expectation value of $\langle S_i^z \rangle$.

$$\langle S_i^z \rangle = \langle S - a_i^\dagger a_i \rangle = S - \left\langle \sum_k a_k^\dagger a_k \right\rangle.$$ (10)

In terms of the spin-wave modes, this can be rewritten as

$$\langle S_i^z \rangle = S - \sum_k \left[|u_k|^2 \langle c_k^\dagger c_k \rangle + u_k^* v_k \langle c_k^\dagger d_k^\dagger \rangle \right.$$

$$+|v_k|^2 \left\langle d_k^\dagger d_k \right\rangle + u_k v_k^* \left\langle c_k d_k \right\rangle + |v_k|^2 \right], \tag{11}$$

where the u_k and v_k have been defined before. All the expectation values are zero in the ground state and we are left with

$$S_i^z = S - \sum |u_k|^2 \sim S - \int \frac{d^d k}{(2\pi)^d} \frac{1}{k} \tag{12}$$

which is linearly divergent in one dimension and logarithmically divergent in two dimensions.

Hence, in one dimension, the *Neel* state is always destabilised by quantum corrections. This is just a manifestation of the familiar result that there is no long range order in one dimension (Mermin-Wagner theorem) or equivalently, that there is no spontaneous symmetry breakdown in 1+1 dimensions (Coleman's theorem). Both these theorems are a consequence of the infra-red divergences in the theory.

Other methods used in higher dimensions are fermionic and bosonic mean field theories. By substituting $S_i = \psi_i^\dagger \vec{\sigma} \psi$ [8] or $S_i = a_i^\dagger a_i$ [9] or $S_i^a = i\varepsilon^{abx} a_{ib}^\dagger a_{ic}$ [10] in the Hamiltonian, we get four fermion or four boson terms which can then be treated through appropriate mean field ansatz. But in one dimension, fluctuations beyond the mean field theory turn out to be infra-red divergent. Hence, specifically in one dimension, other methods are needed. We can divide them roughly into three categories. The first one involves the exact solution of some model Hamiltonians by sone ansatz wave-functions. For example,

Heisenberg AFM for S = 1/2 .

The Heisenberg AFM for $S = 1/2$ in one dimension has been solved using Bethe ansatz [11, 12]. The solution is hard to write down, but it is known that the ground state is unique and that there is no gap. Correlation functions fall off algebraically.

S = 1 model

The Hamiltonian is given by

$$H = \sum_i S_i \cdot S_{i+1} - \sum_i (S_i \cdot S_{i+1})^2. \tag{13}$$

For $S = 1$, this has a Bethe ansatz solution, which shows that the model has a unique ground state with no energy gap.

Models with valence bond ground states

— The Majumdar-Ghosh Hamiltonian is given by [13]

$$H = J \sum_i S_i S_{i+1} + J/2 \sum_i S_i S_{i+1} \tag{14}$$

For $S = 1/2$, the ground state is given in terms of valence bonds. There are two degenerate ground states given by

$$\frac{(\uparrow \downarrow - \downarrow \uparrow)}{\sqrt{2}}$$

There exists a gap in the spectrum and correlation functions have an exponential fall-off. Translational symmetry is broken.

The Hamiltonian for one of the Affleck-Kennedy-Lieb-Tasaki (AKLT) models [14] for $S = 1$ is given by

$$H = J \sum S_i S_{i+1} + J/3 \sum (S_i S_{i+1})^2. \tag{15}$$

This has a unique valence bond ground state found by considering each $S = 1$ to be built of a symmetrised product of $2s = 1/2$'s.

$$(\quad) \; (\quad) \; (\quad)$$

$$(\quad) \; = \text{symmetrisation}$$

The ground sate is formed by symmetrizing after forming the singlets. Here, again, it was found that there exists a gap in the spectrum.

Besides all those explicit exact solutions of specific moels, there is another exact statement that can be proven in general. That is the Lieb-Schultz-Mattis *LSM* theorem [15]. This theorem proves that teh 1/2 integer spin chain either has massless excitations or degenerate ground states corresponding to spontaneously broken parity.

To prove this, let us start with a chain of length L obeying periodic boundary conditions. Let us call its ground state $|\psi_0\rangle$ and assume that this state is rotationally invariant and an even eigenstate of parity. Now construct a new state $|\psi_1\rangle = U|\psi_0\rangle$ where

$$U = e^{(i\pi/L)\sum_{j=-l}^{l}(j+1)S_j^z} \tag{16}$$

i.e. every site from $-l$ to $+l$ is rotated about the z axis through angles $i\pi/l, 2i\pi/l, ... 2i\pi$, where l is some number of $O(L)$. First, we have to show that $|\psi_1\rangle$ is degenerate with $|\psi_0\rangle$ in the $L \rightarrow \infty$ limit. To do that, we compute

$$\langle \psi_1 | H - E_0 | \psi_1 \rangle = \langle \psi_0 | U^\dagger (H - E_0) U | \psi_0 \rangle, \tag{17}$$

where $H|\psi_0\rangle = E_0|\psi_0\rangle$. Now using the commutation relations of the spins, we can show that

$$\langle \psi_1 | H - E_0 | \psi_1 \rangle = \frac{2J\pi^2}{3l^2} e_0(2l + 2), \tag{18}$$

where J is the coupling constant of the spins and $e_0 = E_0/L$. The point to note here is that the R.H.S. is of $O(l)$ and goes to zero as $l \to \infty$. This shows that for an infinite chain, $|\psi_0\rangle$ and $|\psi_1\rangle$ are degenerate. There is still a possibility that asymptotically $|\psi_0\rangle \to |\psi_1\rangle$, so that we have only one state. But to disprove that, let us look at the behaviour of $|\psi_1\rangle$ under parity. Under parity, $S_i^z \to S_{-i}^z$ and under rotation about the y-axis through π, $S_i^z \to -S_i^z$. Note that both parity and rotation about the y-axis through π, are symmetries of the Hamiltonian. Hence, under a combined action of both these symmetries, $S_i^z \to -S_{-i}^z$. So

$$U = e^{(i\pi/L)\Sigma'_{j=-l}(j+1)S_j^z} \to U = e^{(-2\pi i)\Sigma'_{j=-l}S_j^z}. \tag{19}$$

Hence, the state $|\psi_1\rangle = U|\psi_0\rangle$, under a combined symmetry operation of parity and rotation, goes to $Ue^{(-2\pi i)\Sigma'_{j=-l}S_j^z}|\psi_0\rangle$ $= e^{(-2\pi i)\Sigma'_{j=-l}S_j^z}|\psi_1\rangle$. But since $\Sigma'_{j=-l}S_j^z = (2l+1)S$, we see that $e^{(i\pi/L)\Sigma'_{j=-l}(j+1)S_j^z} = -1$ if the spin S is odd and is equal to $+1$ if the spin S is even. Hence, for 1/2 integer spins, the state $|\psi_1\rangle$ has odd parity and is distinct from $|\psi_0\rangle$. In fact, $\langle\psi_0|\psi_1\rangle = 0$. Hence, for 1/2 odd integer spins, we have proven that as $L \to \infty$, there exists a state $|\psi_1\rangle$ distinct from $|\psi_0\rangle$, but degenerate with $|\psi_0\rangle$. Hence, either there exists a massless excitation with odd parity, or if there is a gap, then there is a degeneracy in the spectrum. This result is the LSM theorem. The Bethe ansatz solution for the Heisenberg AFM with massless excitations falls in the first class and the Majumdar-Ghosh model with two degenerate ground states and massive excitations falls in the second class.

II. Field theory treatment of fluctuations

The idea here is to derive a low energy continuum limit of spin models, keeping only the lowest derivative terms [1,6]. We shall first derive the field theory is detail for the Heisenberg AFM, and then briefly discuss how it is done for other general models, including the Majumdar-Ghosh model [13].

For the Heisenberg AFM, we start by defining two fields

$$\phi_{2i+1/2} \equiv \phi x_{2i+1/2} = \frac{S_{2i} - S_{2i+1}}{2S}$$

$$l_{2i+1/2} \equiv l x_{2i+1/2} = \frac{S_{2i} + S_{2i+1}}{2a} \tag{20}$$

Here, a is the lattice spacing and the fields are defined at a point $x_{2i+1/2}$ between the sites $2i$ and $2i + 1$ where the spins are defined. So that pair of spin variables are now replaced by the pair of fields ϕ and l. The commutation relations for the spins imply that $\phi(x)$ and $l(x)$ behave like a scalar field and angular

momentum field respectively. We can also check that $\phi^2 = 1 + 1/S - a^2l^2/S^2 = 1$ in the large S limit. Hence, ϕ is a constrained field.

To derive an effective field theory, we write the Hamiltonian as

$$H = J\sum \sum S_{2i} \cdot S_{2i+1} + S_{2i-1} \cdot S_{2i} \tag{21}$$

then write the spins in terms of the fields and then Taylor expand the fields. After doing a lot of algebra, we find that [2, 16]

$$H = 2Ja\int dx \left[\left(l + \frac{S}{2}\phi' \right)^2 + \frac{S^2\phi'}{4} \right] \tag{22}$$

where $\phi' = \frac{\sigma\psi}{dx}$ and $\Sigma_{2i}(2a) = \int dx$. We now introduce the spin-wave volocity $v_s = 2JaS$ and also the coupling constants $g^2 = 2/S$ and $\theta = 2\pi S$. This allows is to rewrite the Hamiltonian density as

$$H = \frac{v}{\text{--}} g^2 \left| l + \frac{\theta}{4\pi}\phi' \right| + \frac{v}{\text{--}} \tag{23}$$

which, with some more algebra can be shown to be derived from the Lagrangian density given by

$$L = \frac{1}{2g^2}\partial_\mu\phi\partial^\mu\phi + \frac{\theta}{8\pi}\varepsilon^{\mu\nu}\phi \cdot \partial_\mu\phi \times \partial_\nu\phi \tag{24}$$

with $\phi^2 = 1$. Note that we have already taken the large S limit. This is necessary not only to have $\phi^2 = 1$, but also to justify the Taylor expansion. By keeping terms only upto second order in derivatives, we are assuming that the deviations from the equilibrium positions of the spins are small, which is justified only in the large S limit. With these assumptions, we find that the spinwave modes or fluctuations in the HAFM are described by an $O(3)$ non-linear sigma model ($NLSM$) with a Hopf term (the term proportional to θ).

The Hopf term is a total derivative, but its integral is an integer. Hence, the action

$$S = \int dtdxL = \frac{1}{2g^2}\int d^2x\partial_\mu\phi\partial^\mu\phi + i\theta Q \tag{25}$$

where

$$Q = \frac{1}{8\pi}\int d^x\varepsilon^{\mu\nu}\phi \cdot \partial_\mu\phi \times \partial_\nu\phi \tag{26}$$

is an integer (in Euclidean space). Hence, in the partition function,

$Z = \int \mathcal{D}\phi e^{-S} \; e^{i\theta Q} = e^{2\pi S Q}$ is periodic in $S.S = 0$ is equivalent to all $S =$ integers and $S = 1/2$ is equivalent to all $S = 1/2$ integers. Also, we note that for integer spins, the topological term can be dropped because $e^{2\pi i S Q} = 1$ for all configurations, but for half integer spins, it is either $+1$ or -1 depending on value of Q. Thus, the Hopf term plays an important role for half-integer spins. This was what in fact, led to the famous Haldane conjecture that the *HAFM* for integer spins has a gapped spectrum and is massless for half-integer spins.

From the field theory mapping, in fact, it is easy to see that integer spins models have a gap, but it is more non-trivial to show that half-integer spin models are gapless. Let us start with a semi-classical analysis of the integer spin models. Semiclassically, we assume that the $SO(3)$ symmetry of the Lagrangian is spontaneously broken to $U(1) \simeq SO(2)$ by the Neel state or vacuum state given by $\phi = (0, 0, 1)$. Fluctuations about this state are described by

$$\tilde{\phi}_1, \tilde{\phi}_2, \left(1 - \tilde{\phi}_1^2 - \tilde{\phi}_2^2\right)^{1/2} \simeq \left(\tilde{\phi}_1, \tilde{\phi}_2, 1\right) \tag{27}$$

to linear order in fluctuations. Hence, the Lagrangian

$$L = \frac{1}{2g^2}\partial_\mu\phi\partial^\mu\phi = \frac{1}{2g^2}\partial_\mu\tilde{\phi}_1\partial^\mu\tilde{\phi}_1 + \frac{1}{2g^2}\partial_\mu\tilde{\phi}_2\partial^\mu\tilde{\phi}_2 \tag{28}$$

is just the Lagrangian of two free bosons. This is the same as the result that was obtained using spin-wave theory.

But using the field theory, we can do a lot better. Firstly, we can use renormalisation group (RG) to go beyond naive perturbation theory, *i.e.*, we can compute the β-function. Since the manifold here (of values taken by the fields (ϕ_1, ϕ_2, ϕ_3)) is a sphere, we can use geometric methods to compute the RG equation and we find that

$$\beta(g^2) = \frac{dg^2}{d\ln L/a} = \frac{g^2}{2\pi}$$

$$\Rightarrow g_{eff}^2(L) = \frac{g_0^2}{\left(1 - \left(g_0^2 \ln L/a\right)/2\pi\right)}, \tag{29}$$

where g^2 is the microscopic coupling that was derived at length scale $L = a$ to be $2/S$. From this, it is clear that the coupling constant blows up when $\left(g_0^2 \ln L/a\right)/2\pi = 1$ which implies $L/a = e^{2\pi/g^2} = e^{\pi S}$. Thus, as a function of g^2, we expect a phase transition to the strong coupling regime, where the earlier perturbative result of two massless bosons is no longer valid. Since the length scale is of $O(e^{\pi S})$, masses of order $O(e^{-\pi S})$ are expected *i.e.*, one expects to flow to a strong coupling regime,

where there is a gap of $O(e^{-\pi S})$ to excitations.

One can also substantiate this by solving the field theory in the large N limit, *i.e.*, by extending the $O(3)$ *NLSM* to $O(N)$ [1,2], with a Lagrangian

$$L = \frac{N}{2g^2}\partial_\mu\phi\partial^\mu\phi \tag{30}$$

with $\phi^2 = \phi_1^2 + \phi_2^2 + \phi_3^2 + ... + \phi_N^2 = 1$. In other words, instead of having just the usual spin variables with three components, we have extended it to N components. This can also be thought of as taking the number of dimensions in which the spin moves to be N. In the limit of large N, it is actually possible to compute the path integral explicitly and obtain the mass generated and we find that

$$m = Ae^{-\pi S} \tag{31}$$

for each of the N bosons, where A is an ultra-violet cutoff. As $N \to \infty, S \to \infty$ but $A \to \infty$ as well, so as to keep m fixed. Higher order corrections will go as $O(1/N)$. Having obtained this result for large N, we now bravely set $N = 3$ (assuming corrections will be small) and conclude that the integer spin HAFM has an excitation spectrum consisting of a triplet of massive bosons with masses of the order of $e^{-\pi S}$

All of this was for integer spins. Now what about 1/2 integer spins ? Here, the field theory incldues the non-trivial Hopf term and is quite difficult to solve. However, Affleck [2] has mapped the model to a $k = 1$ Wess-Zumino-Witten (*WZW*) model and by studying its symmetries, he has argued that the $\theta = \pi$ case is massless. This difference between the integer and half-integer spins was the big contribution of field theories in spin models.

Similar mappings have also been used to write down field theories of other models, such as the Majumdar-Ghosh model and its generalisations [16, 17]. For instance, for the *MG* model for arbitary spins, we can write down as $SO(3)_L \times SO(2)_R$ field theory [16] by introducing an $SO(3)$ group valued R field as follows –

$$R = \begin{pmatrix} \phi_{11} & \phi_{21} & \phi_{31} \\ \phi_{12} & \phi_{22} & \phi_{32} \\ \phi_{13} & \phi_{23} & \phi_{33} \end{pmatrix} \tag{32}$$

In terms of the R field, the Lagrangian is given by

$$L = \frac{1}{4cg^2}tr\left(\dot{R}^T\dot{R}\right) - \frac{c}{2g^2}tr\left(R'^T R' I_2\right) \tag{33}$$

with $g^2 = \sqrt{6}/S$ and $c = JSa\sqrt{27/8}$ and I_2 being a diagonal 3 × 3 matrix with diagonal entries (1, 1, 0) and all other entries zero. Here, $\dot{R}$ denotes the time derviative of the matrix-valed field R

and R', its space derivative. The fields ϕ_i are related to the spins as

$$(\phi_1)_{3i} = \frac{S_{3i-1} - S_{3i+1}}{\sqrt{3}S},$$

$$(\phi_2)_{3i} = \frac{S_{3i-1} + S_{3i+1} - 2S_{3i}}{\sqrt{3}S}$$

$$(\phi_3)_{3i} = (\phi_1)_{3i} \times (\phi_2)_{3i}. \tag{34}$$

Note that the field theory has no topological term. This is not unexpected, because here the manifold of the fields is $SO(3)$ and $\Pi_2(SO(3)) = 0$, whereas for the *HAFM*, the manifold was S^2 and $\Pi_2(S^2) = Z$. So at least naively, no difference is expected for integer and half-integer spin models. Also, note that the global symmetry of the action is $SO(3)_L \times SO(2)_R$, which means that the effective action at any length scale can be written as

$$L = \left(\frac{1}{2g_1^2} - \frac{1}{4g_2^2}\right)tr\left(\dot{R}^T\dot{R}\right) + \left(\frac{1}{2g_2^2} - \frac{1}{2g_1^2}\right)tr\left(\dot{R}^T R I_2\right)$$

$$+ \left(\frac{1}{2g_3^2} - \frac{1}{4g_4^2}\right)tr\left(R'^T R'\right) + \left(\frac{1}{2g_4^2} - \frac{1}{2g_3^2}\right)tr\left(R'^T R'I_2\right)$$

with the microscopically derived Lagrangian having $g_1^2 = g_2^2 = g_3^2 = 2g_4^2 = g^2 = \sqrt{6}/S$. But these values change as we go to larger length scales in accordance with the *RG* equations or β-functions given by

$$g_1^2 = \frac{g_1^-}{2\pi}\left[\frac{g_1^- g_3 g_4}{g_2^2} \frac{2}{(g_1 g_4 + g_2 g_3)} + g_1 g_3\left(\frac{1}{g_1^2} - \frac{1}{g_2^2}\right)\right]$$

$$g_2^2 = \frac{g_2^4}{2\pi}\left[g_1^3 g_3\left(\frac{2}{g_1^2} - \frac{1}{g_2^2}\right)^2 + 2g_1 g_3\left(\frac{2}{g_2^2} - \frac{1}{g_1^2}\right)\right]$$

$$g_3^2 = \frac{g_3^4}{2\pi}\left[\frac{g_3^2 g_1 g_2}{g_4^2} \frac{2}{(g_1 g_4 + g_2 g_3)} + g_1 g_3\left(\frac{1}{g_3^2} - \frac{1}{g_4^2}\right)\right]$$

$$g_4^2 = \frac{g_4^4}{2\pi}\left[g_3^3 g_1\left(\frac{1}{g_3^2} - \frac{1}{g_4^2}\right)^2 + 2g_1 g_3\left(\frac{1}{g_4^2} - \frac{1}{g_3^2}\right)\right] \cdot \tag{35}$$

We integrated these equations numerically [16] and found that the length scale where strong coupling takes over is $\zeta = L/a = e^{5.76S}$, which is of the same order as $e^{\pi S}$ that we had found for the *HAFM*. Moreover, we found that the flow is such

that g_1/g_2 and g_3/g_4 flow to unity, so that the symmetry gets enhanced to $SO(3)_L \times SO(3)_R$, and Lorentz invariance is restored. Thus, the Majumdar-Ghosh model for arbitrary values of the spin flows to a disordered phase. We shall come back to this analysis in the last section where we study a general dimerised and frustrated model.

III. Numerical methods

The third method that has been used to study spin chains is through numerical computation. Here, I shall only quote various results.

Exact diagonalisation of small systems

The frustrated Heisenberg antiferromagnet modeled by

$$H = J\sum S_i S_{i+1} + \alpha\sum S_i S_{i+2} \tag{36}$$

has been studied for $S = 1/2$ to upto 20 sites and it was found that the critical value of α for which a gap opens up in the spectrum is give by $\alpha_c = 0.2411 \pm 0.0001$ [18]. This is the point at which the fluid-dimer transition takes place.

Density-matrix renormalisation group (DMRG) [19]

This is recent method which has gained ground and is remarkably accurate. The idea is to combine exact diagonalisation methods with the idea of renormalisation group. So a small system is first diagonalised exactly and then the system size is increased by adding two spins at a time on either side. This is done repeatedly using *RG* ideas. For the same model as above, DMRG also finds $\alpha_c = 0.241$. DMRG was also used to study a more general model involving bond alternation [20].

3. Frustrated and dimerised AFM spin chain

The idea is to study the $J_1 - J_2 - \delta$ model given by

$$H = J_1\left[\sum_i [1 + (-1)^i\delta]S_i S_{i+1} + J_2\sum_i S_i S_{i+2}\right] \tag{37}$$

in detail [17]. Classically, the ground state is a coplanar configuration of the spins with energy per spin.

$$E_0 = S^2\left[\frac{J_2}{2}(1 + \delta)\cos\theta_1 + \frac{J_1}{2}(1 - \delta)\cos\theta_2 + J_2\cos(\theta_1 + \theta_2)\right]. \tag{38}$$

Minimising this energy with respect to θ_i gives three phases

Neel phase

$$\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow. \tag{39}$$

This is stable for $(1-\delta^2) > 4J_2/J_1$.

Spiral phase

Here, the angles between neighbouring spins alternate

$$\uparrow \nearrow \rightarrow \searchrow \swarrow \nearrow \nwarrow \uparrow \uparrow$$

between θ_1 and θ_2 where

$$\cos\theta_1 = -\frac{1}{1+\delta}\frac{1-\delta^2}{4J_2/J_1} + \frac{\delta}{1+\delta^2}\frac{4J_2}{J_1}$$

and
$$\cos\theta_1 = -\frac{1}{1+\delta}\frac{1-\delta^2}{4J_2/J_1}\frac{\delta}{1-\delta^2}\frac{4J_2}{J_1} \qquad (40)$$

This phase is stable for $1-\delta^2 < 4J_2/J_1 < (1-\delta^2)/\delta$.

Collinear phase

This phase can be thought of as a special case of the spiral phase where $\theta_1 = \pi$ and $\theta_1 = 0$. It can be denoted as

$$\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow...... \qquad (41)$$

This phase needs both frustration and dimerisation and is stable for $(1-\delta^2)/\delta < 4J_2/J_1$.

These three phases in the classical phase diagram are depicted in Figure 1.
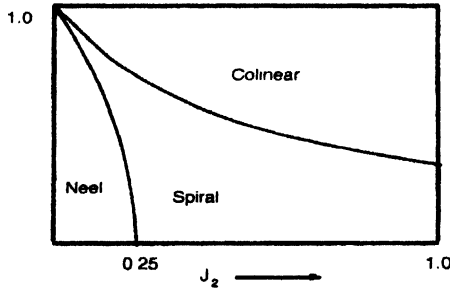

Figure 1. Semi-classical phase diagram of the $J_1 - J_2 - \delta$ model.

We can study fluctuations about the classical ground state as described earlier. In the *Neel* phase, there are two modes with equal velocity and the Fourier transform of the spin-spin correlation function $S(q)$ is peaked at $q = \pi$. In the spiral phase, we have three modes, two of them with equal velocity describe out-of-plane fluctuations and the third one with a higher velocity describes in-plane fluctuations. $S(q)$ is peaked at $\pi/2 < q < \pi$. In the collinear phase, once again, there are two modes with equal velocity, but here $S(q)$ is peaked at $q = \pi/2$. But as we have already seen earlier, we do not expect spinwave theory to be accurate in one dimension because, there is no long-range

order, no spontaneous symmetry breakdown and no Goldstone modes in one dimension.

Next, what do we know about the model exactly ? For $J_2 = \delta = 0$, the model is just the *HAFM* and the solution for $S = 1/2$ is a unique ground state with no excitations. For $J_2 = J_1/2$ and $\delta = 0$, which is the *MG* model, the solution for $S = 1/2$ is the doubly degenerate valence bond state, with massive excitations. In fact, this state turns out to be the ground state even with dimerisation along the line $2J_2 + \delta = J_1$.

Now, let us study the field theory model for the fluctuations in the three classical phases.

(i) In the *Neel* phase, even with J_2 and δ, the mapping is to an O(3) *NLSM*, with the Hopf term as given in eq. (24). The only difference is that now $c = 2J_1aS\sqrt{1-\delta^2 - 4J_2/J_1}$, $g^2 = 2/(S(1-\delta^2 - 4J_2/J_1))$ and $\theta = 2\pi S(1-\delta)$. We expect the theory to have a mass gap in general and to be massless only when $\theta = 2\pi S(1-\delta) = \pi$. Note that a topological term is present to distinguish different spins, but spin is not really a continuous variable. So for each spin, integer or half-integer, there are specific values of δ which can be chosen to get massless points.

(ii) For the spiral phase also, the field theory still turn out to be the $SO(3)_L \times SO(2)_R$ invariant, but with a Lagrangian given by

$$L = \frac{1}{4cg^2}tr(\dot{R}^T \dot{R}P_0) - \frac{c}{2g^2}tr(R'^T R'P_1) , \qquad (42)$$

where P_0 and P_1 are diagonal matrices with the diagonal elements given by $P_0 = (1/2g_2^2, 1/2g_2^2, 1/g_1^2 - 1/2g_2^2)$ and $P_1 = (1/2g_4^2, 1/2g_4^2, 1/g_3^2 - 1/2g_4^2)$, respectively. The *RG* equations are the same as the ones given in eq. (35). However, the initial microscopic values of the coupling constants are different now and are given by

$$g_2^2 = g_4^2 = \frac{1}{S}\sqrt{\frac{4J_2 + J_1}{4J_2 - J_1}},$$

$$g_3^2 = 2g_2^2 ,$$

and $g_1^2 = g_2^2 \left[1+(1-J_1/2J_2)^2\right].$ \qquad (43)

As before, the *RG* equations can be integrated numerically with these initial conditions and it can be

shown that the theory flows once again to an $SO(3)_L \times SO(3)_R$ Lorentz invariant field theory.

The interesting point is that this theory turns out to be an exactly solved model [21]. The low energy spectrum consists of a massless spin 1/2 doublet. Hence, in the spiral phase (which requires sufficiently large frustration and dimerisation), we can make the prediction that both integer and half-integer spin models should have massive spin 1/2 excitations. The long wavelength excitations are expected to be 'two-particle' excitations, the spin triplet and the spin singlet excitations.

Although there is no topological term in the Lagrangian, we claim that there does exist a difference between integer and half-integer spins in this phase. Tunneling between soliton sectors can lead to a unique ground state for integer spins, but this is not possible for 1/2 integer spins, which have a doubly degenerate ground state, in accordance with the LSM theorem.

(iii) Finally, we can write down the field theory for the collinear phase as well. Here again, the field thory turns out to be an $O(3)$ $NLSM$, but without the Hopf term. This means that the phase is always gapped both for integer and non-integer spins.

We generally expect these field theories to be valid in the large S limit, but for small values of S such as $S = 1/2$ and $S = 1$, the above analysis is only indicative and numerical studies are needed to get the phase diagram accurately. These have been obtained [18, 20] and we only reproduce the phase diagrams here.

As can be seen by comparing these diagrams, with the classical phase diagram in Figure 1, the qualitative picture is reproduced for spin 1/2, but for spin $S = 1$, there are many new unexpected features in the $S = 1$ phase diagram obtained numerically. For the spin 1/2 chain depicted in Figure 2, in region I $S(q)$ is peaked at $q = \pi$, in region II, $S(q)$ decrease from $q = \pi$ (near region I) to $q = \pi/2$ (near region III) and $S(q)$ is peaked at
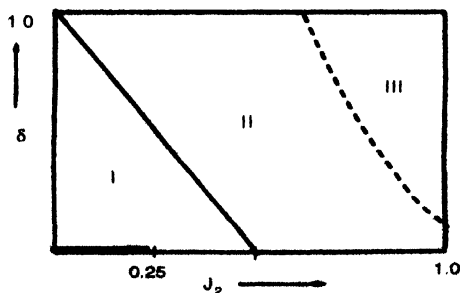

Figure 2. $S = 1/2$ phase diagram of the $J_1 - J_2 - \delta$ model.

$q = \pi/2$ in region III. There exists a gapless line running from J_c $= 0$ to $J_{2c} = 0.241$. It is straight forward to identify region I with the Neel phase, region II with the spiral phase and region III with the collinear phase. However, the phase diagram for spin 1 depicted in Figure 3 is much more complex. There is a gapless solid line and the rest of the phase diagram is gapped. Regions II and III are identified with a Haldane phase, whereas regions I and IV are expected to be non-Haldane singlet phases. For details, see Refs. [18, 20]. It is not clear to us why the semi-classical large S theory, works for spin 1/2 qualitatively, but fails completely for the spin 1 case.
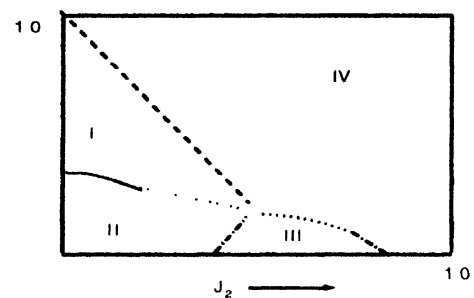

Figure 3. $S = 1$ phase diagram of the $J_1 - J_2 - \delta$ model

4. Conclusion

In this paper, we have given an overview of the field of quantum spin chains, with emphasis on the non-linear sigma model mapping. To recapitulate, quantum spin chains are spin models on a one-dimensional lattice. For parity invariant systems, the Lieb-Schulz-Mattis theorem says that for half-integer spin models, the ground state is either doubly degenerate, or the spectrum contains a massless mode. Using the $NLSM$ mapping, we demonstrated that the difference between 1/2 integer spin chains and integer spin chains was caused by the existence of a topological Hopf term in the Lagrangian. The presence of this term for 1/2 integer chains led to a gapless spectrum, whereas integer spin chains which did not have the Hopf term were gapped. For more general models, such as spin chains with dimerisation and/or frustration, the $NLSM$ approach can only give a qualitative understanding. For instance, the mapping of the Majumdar-Ghosh model (more generally, the spiral phase of a frustrated and dimerised spin chain) to the RG fixed point Lagrangian of an $SO(3)_R \times SO(3)_L$ model leads to the prediction that the low energy spectrum consists of a massive spin 1/2 doublet. But for low values of S, such as 1/2 and 1, often numerical methods are needed to get better results, as seen in the explicit phase diagrams for the spin 1/2 and spin 1 frustrated and dimerised models.

One of the important issues in this field is to get a proper understanding of the Haldane gap. Usually, a gap is formed when some symmetry is broken. So we need a symmetry that

exists for half-integer spins and is broken by all integer spins. Since the distinction between the integer and half-integer spins occurs because of the topological Hopf term, it is expected that the order parameter characterising the massive and massless phases is also topological in nature. A claim is that there exists a hidden $Z_2 \times Z_2$ symmetry in the $S = 1$ model, which when broken leads to the gapped Haldane phase. But this phenomenon is not well-understood.

Acknowledgment

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