Low Energy Behaviour of XXZ Antiferromagnetic Spin Chain

B. Roostaei*

Department of Physics, Sharif University of Technology, P.O. Box 19395-5534, Tehran-Iran
and Institute for Studies in Theoretical Physics and Mathematics (IPM), P.O. Box 11365-9161, Tehran-Iran

Abstract

The zero temperature phase diagram of XXZ spin chain in external magnetic field is investigated at low energies using path integral approach. It has been shown by spin wave analysis and then by nonlinear sigma model transformation that below some critical field the system undergoes quantum Kosterlitz-Thouless phase transition. Above that critical field for low anisotropies the system is saturated while at strong anisotropy the system has Ising antiferromagnetic order.

1 Introduction

Considerable effort has been made to understand the long range (low energy) behaviour of quantum spin systems specially in low dimensions. The importance of these studies is in their applicability in various physical phenomena in for example quantum Hall ferromagnets[1], high $T_c$ superconductors[2] and many other magnetic systems. On the other hand we know very few models to be exactly solvable, nevertheless development of field theoretical approaches has greatly changed the language in this part of strongly correlated systems and has provided us with effective methods to be applied to our problems of spin systems. One of the great observations by means of field theoretical approach has been the problem of ground state of 1D Heisenberg antiferromagnet: after separating out the rapidly varying fluctuations we obtain a nonlinear sigma model (NLσM) with a topological term which is responsible for destroying the long range order of ground state for integer spin chains according to Haldane’s conjecture[3] while we know that this problem is exactly solvable by Bethe’s ansatz only for spin half problem[4]. The Haldane’s conjecture has been now confirmed by strong experimental and numerical evidence[4,5,6].

*Email: Bahmanr@mehr.sharif.ac.ir
The method of separating out short wavelength fluctuations which resulted in NLσM+topological term for antiferromagnetic spin chains is now widely used for various spin systems including Ferrimagnets[7] and spin ladders[8]. In this paper I am going to apply this method of obtaining low energy behaviour to anisotropic spin chains.

2 Spin Wave Analysis

For the anisotropic Heisenberg model in magnetic field:

\[ \hat{H} = J \sum_{<ij>} \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+) + \lambda S_i^z S_j^z + \sum_{j=1}^N \mathbf{B} \cdot \mathbf{S} \]  

(1)

where \(0 \leq \lambda \leq 1\) there are numerical evidence[9] that under some critical value for the magnetic field \(B_c\) the \(S_z\) fluctuations become negligible and the system behaves as XY model in long range. On the other hand we know that the isotropic Heisenberg antiferromagnet becomes massive by turning on magnetic field[8]. These two considerations suggest that \(B_c \propto (1 - \lambda)^{-\nu}\) for XXZ model. This may be examined by some crude spin wave analysis: I apply the Holstein-Primakov transformation which is some kind of perturbation around saturation point: \(S_i^z = s - a_i^+ a_i^0\) and \(S_i^- = (2s) \frac{a_i^+}{a_i^0}(1 - \frac{a_i^+ a_i^0}{a_i^0})^2\). Here \(a_i^+\) creates a boson to lower the \(S_z\) by one. We are in a situation where the number of bosons are low enough to approximate the square root and obtain: \(S_i^- \approx (2s)^\frac{1}{2} a_i^+\). Applying this transformation to the Hamiltonian (1) for \(B = B \hat{z}\) and Fourier expanding we find:

\[ \hat{H} \approx \sum_k [2(\gamma_k - z \lambda) J s - B] a_k^+ a_k \]  

(2)

in which \(\gamma_k = \sum_a e^{ik \cdot a} = \gamma_{-k}\). \(a\) represents the translation vectors to the neighboring sites and \(z\) is the number of nearest neighbors.

In one dimension the spin wave spectrum becomes gappful: \(E_k = 4J s (\cos ak - \lambda) - B\) with the gap \(\Delta = 4Js(1 - \lambda) - B\). This estimation confirms my suggestion and sets \(\nu = 1\). Under \(B_c\) the saturation point becomes unstable. This elementary analysis will be invalid as \(B\) approaches zero and is valid just near \(B_c\). This result shows that near \(B_c\) the correlation length of \(S_z\) fluctuations \(\xi \propto |B - B_c|^{-1}\).

In section 3 after separating out short range Neel field we can see that the correlation length of \(S_z\) fluctuations is actually \(\xi \propto (1 - \lambda)^{-\frac{1}{2}}\) for \(\lambda \leq 1\). For the case of \(\lambda \geq 1\) the analysis is a bit complicated. In this regime to find the fluctuations around Ising antiferromagnetic order (IAF) we can again apply the Holstein-Primakov transformation for two sublattices: \(S_i^z = s - a_i^+ a_i^0\) and \(S_i^- = \sqrt{2s} a_i^+ (1 - \frac{a_i^+ a_i^0}{a_i^0})^2\) for \(i\) in sublattice A and for sublattice B: \(S_i^z = -s + b_i^+ b_i^0\) and \(S_i^- = \sqrt{2s}(1 - \frac{b_i^+ b_i^0}{b_i^0})^2 b_i\). Here we have two kind of Bosons one \(a^+ (b^+)\) lowers(adds)
the $S_z$ by one in sublattice $A(B)$. By applying the first order approximation: $S_i^- \approx \sqrt{2s_a}a_i^\dagger$ for $A$ and $S_i^- \approx \sqrt{2s_b}b_i$ for $B$, and inserting in the Hamiltonian (1) we find:

$$\hat{H} \approx Js \sum_{i \in A} \sum_{j \in B} [a_i b_j + a_i^\dagger b_j^\dagger + \lambda(a_i^\dagger a_i + b_j^\dagger b_j)] + B \sum_{i \in B} b_i^\dagger b_i - B \sum_{i \in A} a_i^\dagger a_i$$

(3)

$$= Js \sum_k \gamma_k (a_k b_{-k} + a_k^\dagger b_{-k}^\dagger) + \alpha \sum_k b_k^\dagger b_k + \beta \sum_k a_k^\dagger a_k.$$  

Where $\alpha \equiv Js \lambda z + B$ and $\beta \equiv Js \lambda z - B$ and we have Fourier expanded the operators in the last equality. Now to diagonalize (3) I apply the (canonical) Bogoliubov transformation:

$$c_k = u_k a_k - v_k b_{-k}^\dagger$$
$$d_k = u_k b_k - v_k a_{-k}^\dagger$$

For the transformation to be canonical we must have: $u^2 - v^2 = 1$ and for (3) to be diagonal we must have: $Js \gamma(u^2 + v^2) + (\alpha + \beta) uv = 0$. No problem arises if we assume $u$ and $v$ are real. Finally we obtain:

$$\hat{H} \approx \sum_k \mathcal{E}^{(1)}_k c_k^\dagger c_k + \sum_k \mathcal{E}^{(2)}_k d_k^\dagger d_k$$

(5)

$$\mathcal{E}^{(1,2)}_k = 2Js(\lambda^2 - \cos^2 ak)\frac{1}{2} \pm B.$$  

One of the branches is always gapfull which has to be the spectrum of fluctuations trying to align spins against the magnetic field direction and the other one is also gapfull which tries to saturate the system, but in this branch the gap vanishes at: $B_c = 2Js(\lambda^2 - 1)\frac{1}{4}$. This result shows that for $\lambda \geq 1$ the correlation length $\xi \propto (\lambda - 1)^{-\frac{1}{2}}$ that is $\nu = \frac{1}{2}$ above the critical point $\lambda = 1$. This result is more reliable for the following reason:

we can compute the site magnetization reduction due to quantum fluctuations in our spin wave approximation:

$$| \Delta < S_z > | = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} v_k^2 dk = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \left( \frac{\lambda z}{2\sqrt{\lambda^2 z^2 - \gamma_k^2}} - \frac{1}{2} \right) dk$$

(6)

$$= -\frac{2\pi}{a} + \frac{4\sqrt{2\lambda} F(\frac{1}{\sqrt{\lambda^2 - 1}})}{a \sqrt{\lambda^2 - 1}}.$$  

Where $F$ is the complete elliptic integral of first kind. We can see in Fig.I that this reduction is finite at $\lambda > 1$ and vanishes very fast as $\lambda$ grows.

Now we can sketch the line of transition from saturation to IAF and other phases as follows (fig.II):

$$B_c(\lambda) = 2Js\sqrt{\lambda^2 - 1} \quad \lambda \geq 1$$
$$B_c(\lambda) = 4Js(1 - \lambda) \quad \lambda \leq 1.$$  

(7)
3 Field Theoretic Discussion

In this section I am going to analyze the anisotropic spin chain by means of nonlinear sigma model transformation. The Minkowskian action for anisotropic Heisenberg chain \( \mathcal{H} = \sum_{j=1}^{N} \alpha_{\mu\nu} S_{j}^{\mu} S_{j+1}^{\nu} - \sum_{j=1}^{N} B \cdot S \) with the symmetric rank two tensor \( \alpha \) is:

\[
S_{\text{eff}} = S_{\text{WZ}[\mathbf{n}_{j}]} - \int_{0}^{\beta \hbar} dx_{0} \sum_{j=1}^{N} \alpha_{\mu\nu} n_{j}^{\mu} n_{j+1}^{\nu} - \int_{0}^{\beta \hbar} dx_{0} \sum_{j=1}^{N} B \cdot n . \tag{8}
\]

Where \( x_{0} \) is the real time and \( \beta = 1/k_B T \) that in this paper we discuss the zero temperature situation \( \beta \hbar \to \infty \). The first term known as Wess-Zumino term is a Berry phase for each spin and represents the area of a cap of the unit sphere formed by the closed path passed by the unit vector \( \mathbf{n} \) from \( x_{0} = 0 \) to \( x_{0} = \beta \hbar[10] \). Under the critical magnetic field \( B_c \) we can separate out rapidly varying fluctuations as follows:

First of all we stagger the field: \( \mathbf{n}_{j} \to (-1)^{j} \mathbf{n}_{j} \) then we write \( \mathbf{n}_{j} \) as a short range Ne\( \ddot{e} \)l field \( \mathbf{l} \) plus fluctuations around it \( \mathbf{m}_{j} : \mathbf{n}_{j} = \mathbf{m}_{j} + a_{0}(-1)^{j} \mathbf{l} \) where \( \mathbf{m}^2 = 1, \mathbf{m} \cdot \mathbf{l} = 0 \) and \( a_0 \) is the lattice constant. This method works only for two sublattice systems close to Ne\( \ddot{e} \)l state which is not the eigenstate of \( \mathcal{H} \) of course!

Expanding the action up to second order in \( \mathbf{l} \) and integrating it out we obtain

\[
Z = \int \mathcal{D}\mathbf{m} \delta(\mathbf{m}^2 - 1) e^{i S_{\text{eff}}} \text{ where :}
\]

\[
S_{\text{eff}} = \int d^{2}x \left[ \frac{1}{a_0} \alpha_{\mu\nu} m^{\mu} m^{\nu} + \frac{a_0}{2} \alpha_{\mu\nu} m^{\mu} \partial_{i} m^{\nu} \right] + \frac{s}{2} \int d^{2}x \mathbf{m} \cdot (\partial_{0} \mathbf{m} \times \partial_{1} \mathbf{m}) + \frac{s^2}{4a_0} \int \alpha_{\mu\nu} \left( (\mathbf{m} \times \partial_{0} \mathbf{m})_{\mu} (\mathbf{m} \times \partial_{0} \mathbf{m})_{\nu} \right) d^{2}x - \frac{1}{J_{s} \lambda a_0} \mathbf{B} \cdot \left( \mathbf{m} \times \partial_{0} \mathbf{m} \right) .
\]

For the XXZ model \( \alpha_{\mu\nu} = J s^2 \text{ diag}(1,1,1) \) by which we find:

\[
\mathcal{L}_{\text{eff}} = \frac{s}{4a_0 J} (\partial_{0} m_{z})^2 - \frac{a_{0} J}{2} (\partial_{1} m_{z})^2 - \frac{J}{a_0} (1 - \lambda) m_{z}^2 - \frac{a_0 J}{2} (\partial_{1} m_{x})^2 + \frac{1}{4a_0 J} \left( (\partial_{0} m_{y})^2 (m_{z}^2 + \lambda^{-1} m_{x}^2) + (\partial_{0} m_{x})^2 (m_{z}^2 + \lambda^{-1} m_{y}^2) + \right.
\]

\[
-2(m_{y} m_{z} \partial_{0} m_{y} + m_{x} m_{z} \partial_{0} m_{x} + \lambda^{-1} m_{y} m_{z} \partial_{0} m_{y} \partial_{0} m_{x}) \right) + \frac{B}{J_{s} \lambda a_0} (\mathbf{m} \times \partial_{0} \mathbf{m}) \cdot \hat{z} + \frac{\theta}{8\pi} \epsilon_{\mu\nu\rho} \mathbf{m} \cdot (\partial_{\rho} \mathbf{m} \times \partial_{\mu} \mathbf{m}) .
\]

where for the last term \( \mu, \nu = 0, 1 \). The last term is the Pontryagin index (or winding number) of field \( \mathbf{m} \) as a map from \( S^{2} \) (real space-time) to \( S^{2} \) (configuration space) and is a topological term and \( \theta = 2\pi s[10] \). This is the well known \( \theta \)-term that for isotropic Heisenberg chain resulted in Haldane’s conjecture, however in XXZ chain as we can see in (10) due to massive fluctuations
of \( m_z (\Delta \propto 1 - \lambda) \) the \( z \) component will be negligible in ground state, in other words this component is short range and so at long wavelengths (low energies) is irrelevant. To find the low energy behavior we can use the mean-field approximation \( m_z \approx 0 \). In this approximation the winding number will be ineffective.

4 Topological Phase Transition at \( T=0 \)

In our mean-field approximation removing the \( z \) component in the Lagrangian density results in:

\[
\mathcal{L}_{eff} = -\frac{a_0 J}{2} [ (\partial_1 m_x)^2 + (\partial_1 m_y)^2 ] + \frac{1}{4\alpha_0 J \lambda} [ (\partial_0 m_y)^2 m_x^2 + (\partial_0 m_x)^2 m_y^2 - 2 m_x m_y \partial_0 m_x \partial_0 m_y ] - \frac{B}{J \lambda \alpha_0} (m_x \partial_0 m_y - m_y \partial_0 m_x) \to \frac{1}{2g} [ (\partial_0 \varphi)^2 - (\partial_1 \varphi)^2 ] - \frac{2B}{gs} (\partial_0 \varphi) .
\]

Where in the last line we have parametrized \( m \) as \((\cos \varphi, \sin \varphi, 0)\) and scaled the space-time so that the spin wave velocity is one and \( g = (2\lambda)^{1/2} \) is the coupling constant. This is the Lagrangian for massless fluctuations of XXZ model in 1+1 dimensions. (The term coupled to magnetic field is a total derivative, i.e. the magnetic field has no effect on in plane excitations in mean-field approximation.) The Lagrangian in (11) has topological defects for the field \( \varphi(x_0, x) \) is an angle. These defects drastically alter the behavior of system when they are present. In this scenario (Kosterlitz-Thouless), at weak couplings \((g < g_c)\) the ground state has bound vortices (defects in space-time) and is partially ordered with algebraically falling correlations. At strong couplings the vortices become unbound and the partial order completely vanishes and the correlations fall off exponentially with correlation length \( \xi \propto 1/\ln(2g) \). This drastic change is a second order quantum phase transition at zero temperature without symmetry breaking.

5 Summary

The low energy phase diagram of antiferromagnetic XXZ chain in magnetic field is shown in fig. II. At \( 0 \leq \lambda < 1 \) and under \( B_c \approx 4Js(1 - \lambda) \) we have two kind of ground states: at \( \lambda < \lambda_{KT} \) the ground state is partially ordered while at \( \lambda > \lambda_{KT} \) the ground state has free vortices and is disordered. Above the critical magnetic field the \( z \) component is no longer ignored and we have saturated ferromagnetic (SF) order. At \( \lambda > 1 \) and \( B < B_c \) obviously the system has antiferromagnetic Ising (IAF) behaviour at low energies while in this regime and above \( B_c \) we have again saturated phase. For \( B = 0 \) it is inferred that we have a quantum phase transition at \( \lambda = 1 \) from disordered phase to ordered
IAF phase which has already been shown in continuum limit for spin half case by Bosonization method[10].

6 Acknowledgement

The author is grateful to IPM for funding this research as a student research work.

7 References

[1] S.M. Girvin, cond-mat/9711233 and references therein.
[2] P.W. Anderson, Science235,1196(1987), S.Chakravarty, B.I. Halperin, D.R. Nelson, Phys. Rev. B,39,2344(1989) and references therein.
[3] F.D.M. Haldane, Phys. Rev. Lett.,50,1153(1983).
[4] E. Fradkin, Field theories of Condensed Matter Systems(Addison-Wesely,1991),Chp.4
[5] I. Affleck, J. Phys. :Cond. Matt. 1,3047(1989).
[6] A. Auerbach, Interacting Electrons and Quantum Magnetism(Springer-Verlag,New York,1995).
[7] R. Abolfath, H. Hamidian, A. Langari, Cond-Matt/9901063.
[8] B. Normand, J. Kyriakidis, D. Loss, Cond-Matt/9902104.
[9] A. Langari, Phys. Rev.B,58,14467(1998).
[10] Ref.4 charter 5.
[11] A. Lopez, A. G. Rojo, E. Fradkin, Phys. Rev. B,49,15139(1994).

Figure caption

Fig. I) Site magnetization reduction due to quantum fluctuations at ground state in the regime of higher anisotropy \( \lambda > 1 \).

Fig. II) The low energy phase diagram of the XXZ antiferromagnetic chain. The straight line shows the threshold of saturation. The curve \( \sqrt{B^2 + 1} \) is the threshold of Ising Antiferromagnetism (IAF).
This figure "fig.jpg" is available in "jpg" format from:

http://arxiv.org/ps/cond-mat/0108086v1
This figure "fig1.jpg" is available in "jpg" format from:

http://arxiv.org/ps/cond-mat/0108086v1