## **ISTANBUL TECHNICAL UNIVERSITY ★ INSTITUTE OF SCIENCE AND TECHNOLOGY**

#### QUANTUM PHENOMENON IN ANISOTROPIC XXZ HEISENBERG SPIN CHAINS WITH FERROMAGNETIC AND ANTIFERROMAGNETIC INTERACTIONS: RENORMALIZATION-GROUP CALCULATION

M.Sc. Thesis by Ozan Sabahattin SARIYER, B.Sc.

**Department : Physics Engineering** 

**Programme:** Physics Engineering

**JUNE 2007** 

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## <u>İSTANBUL TEKNİK ÜNİVERSİTESİ ★ FEN BİLİMLERİ ENSTİTÜSÜ</u>

# FERROMANYETİK VE ANTİFERROMANYETİK ETKİLEŞMELİ ANİZOTROPİK XXZ HEISENBERG SPİN ZİNCİRLERİNDE KUANTUM OLGULARI: RENORMALİZASYON GRUBU ÇÖZÜMÜ

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## ABBREVIATIONS

XXX model	: Isotropic quantum Heisenberg model $(J_x = J_y = J_z)$
XXZ model	: Anisotropic quantum Heisenberg model $(J_x = J_y)$
XYZ model	: Fully anisotropic quantum Heisenberg model
RGT	: Renormalization-group theory

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## LIST OF SYMBOLS

d	: Lattice dimensionality
i, j, k,	: Lattice sites
s <sup>m</sup>	: Pauli spin operator at site i $(m = x, y, z)$
–βΗ, Η	: Hamiltonian, dimensionless and in enegy dimensions
β	: Inverse temperature $(1/k_BT)$
k <sub>B</sub>	: Boltzman's constant
Т	: Temperature
$\mathbf{J}, \mathbf{J}_{xy}, \mathbf{J}_{z}$	: Nearest-neighbor spin-spin interaction constants
Si	: Classical Ising spin variable
G	: Additive constant
-βH(i,j)	: Dimensionles Hamiltonian of one bond between sites i and j
Z	: Partition function
$\mathbf{J'}, \mathbf{J'}_{xy}, \mathbf{J'}_{z}, \mathbf{G'}$	: Renormalized interaction constants
<b>-β'H'</b> , <b>-β'H'</b> (i,j)	: Renormalized dimensionless Hamiltonians
b	: Rescaling factor
R	: Anisotropy parameter $(J_z/J_{xy})$
$\mathbf{u}_{i},\overline{\mathbf{u}}_{i}^{},\mathbf{v}_{k}^{},\overline{\mathbf{v}}_{k}^{},\mathbf{w}_{j}^{}$	: Quantum single-site spin-1/2 state variables
$\left  \mathbf{\phi}_{\mathbf{p}}  ight angle, \left  \mathbf{\psi}_{\mathbf{q}}  ight angle$	: Two- and three-site basis eigenstates
$\Lambda_p, \lambda_q$	: Two- and three-site Hamiltonian eigenvalues
σ, τ, μ, ν	: Three-site eigenstate coefficients and normalization factors
γ <sub>p</sub>	: Two-site exponentiated Hamiltonian eigenstates
$\hat{\mathbf{T}}$ , $\mathbf{T}_{\boldsymbol{\beta}\boldsymbol{\alpha}}$	: Recursion-matrix and its $\beta \alpha$ element
$\overline{\mathbf{M}}$ , $\overline{\mathbf{K}}$ , $\mathbf{M}_{a}$ , $\mathbf{K}_{a}$	: Density, interaction constant vectors, and their $\alpha^{th}$ components
$\left\langle s_{i}^{m}s_{j}^{m}\right\rangle$	: Nearest-neighbor spin-spin correlations $(m = x, y, xy, z)$
$\vec{\mathbf{M}}^{(n)}, \vec{\mathbf{M}}^{*}$	: Density vector at the n <sup>th</sup> step and at a fixed point
$N_{\alpha}$	: Number of α-type interactions
$\mathbf{J}_{xy}, \mathbf{J}_{z}, \mathbf{J}^{C}$	: Interaction constants at fixed points and critical point
U	: Internal energy
C	: Specific heat
ħ	: Planck's constant / $2\pi$
Ø	: Magnon angular frequency
c	: Spin-wave stiffness constant
k	: Spin-wave number
n	: Spin-wave exponent
A <sub>i</sub>	: High-temperature series coefficients for specific heat
T <sub>0</sub>	: Sign-reversal temperature
γ	: arccos(-R)
$\Delta, \Delta_{\text{spinon}}, \Delta_{\text{spinwave}}$	: Excitation spectrum gaps
d"	: Lower critical dimension

## QUANTUM PHENOMENON IN ANISOTROPIC XXZ HEISENBERG SPIN CHAINS WITH FERROMAGNETIC AND ANTIFERROMAGNETIC INTERACTIONS: RENORMALIZATION-GROUP CALCULATION

#### SUMMARY

The statistical mechanics of anisotropic XXZ Heisenberg spin chains is solved for both ferromagnetic and antiferromagnetic interactions, thoughout the entire temperature and anisotropy ranges, via the renormalization-group method developed for electronic system calculations. Spin-spin correlations and specific heats are calculated in detail. The spin-wave stiffness constant, excitation spectrum gap, and spin-wave to spinon crossever are obtained. From these solutions, completely quantum mechanical phenomenon are obtained: The XY interaction induces antiferromagnetic  $s_z$  spin correlations, while on the other hand, antiferromagnetic  $s_z$  interaction induces XY spin correlations. The specific heat maxima values and temperatures respond to anisotropy in a completely different way for ferromagnetic and antiferromagnetic systems. One can see this fact as a harbinger of the quantum phenomenon of different ferromagnetic and antiferromagnetic phase transition temperatures for higher dimensions. The 3dimensional global phase diagram is calculated, showing that ferromagnetic and antiferromagnetic regions indeed do not map onto each other. In addition, in this global phase diagram, one can see the expected order of the critical temperatures, namely the Ising model critical temperature being the highest, and the Heisenberg model critical temperature being the lowest, and the XY model critical temperature being in between. This effect is due to order of degree of freedom of each spin in the models, i.e. 1 for Ising model, 2 for XY model, and 3 for Heisenberg model.

## FERROMANYETİK VE ANTİFERROMANYETİK ETKİLEŞMELİ ANİZOTROPİK XXZ HEISENBERG SPİN ZİNCİRLERİNDE KUANTUM OLGULARI: RENORMALİZASYON GRUBU ÇÖZÜMÜ

### ÖZET

Anizotropik XXZ Heisenberg spin zincirlerinin istatistik mekaniği, elektronik sistem çözümleri için geliştirilen kuantum renormalizasyon grubu yöntemi kullanılarak, hem ferromanyetik hem antiferromanyetik etkilesmeler icin, bütün sıcaklıklar ve bütün spin anizotropi değerleri için çözülmüştür. Spin-spin bağlantıları ve özgül ısılar ayrıntılarıyla hesaplanmıştır. Spin dalgası katılıkları, uyarılma spektrum ayrılıkları ve spin dalgasından spinona öte geçiş elde edilmiştir. Bu çözümlerden, tümüyle kuantum mekaniksel olan olgular bulunmuştur: XY spin etkileşmeleri, antiferromanyetik sz spin bağlantıları oluşturmaktadır. Buna karşılık da, antiferromanyetik sz etkileşmeleri, XY spin bağlantıları oluşturmaktadır. Özgül ısının pik değerlerinin ve sıcaklıklarının anizotropiye bağlantısı, ferromanyetik ve antiferromanyetik sistemlerde tamamen değişiktir. Bu, üst boyutlarda, antiferromanyetik ve ferromanyetik faz geçiş sıcaklıklarının değişik olması kuantum olgusunun habercisi olarak görülebilir. 3-boyutta global faz diyagramı elde edilmis ve gerçekten de ferromanyetik ve antiferromanyetik bölgelerin üstüste çakışmadıkları bulunmuştur. Buna ek olarak, global faz diyagramında, Ising modeli kritik sıcaklığının en yüksek, Heisenberg modeli kritik sıcaklığının en düşük, XY modeli kritik sıcaklığının da ikisinin arasında olduğu haliyle, beklenen kritik sıcaklık sıralaması görülebilir. Bu etkinin sebebi, modellerdeki her spinin serbestlik derecesinin sıralanışıdır. Serbestlik dereceleri Ising modeli için 1, XY modeli için 2, Heisenberg modeli için ise 3 şeklindedir.

#### **1. INTRODUCTION**

The quantum Heisenberg chain, including the possibility of spin-space anisotropy, is the simplest nontrivial quantum spin system and has thus been widely studied since the very beginning of the spin concept in quantum mechanics [1-3]. Interest in this model continued [4-10] and redoubled with the exposition of its richly varied lowtemperature behavior [11-13] and of its relevance to high-temperature superconductivity [14-18]. It has become clear that antiferromagnetism and superconductivity are firmly related to, adjoining and overlapping each other.

A large variety of theoretical tools have been employed in the study of the various isotropic and anisotropic regimes of the quantum Heisenberg chain, including finite-systems extrapolation [6, 19], linked-cluster [7] and dimer-cluster [20] expansions, quantum decimation [21], decoupled Green's functions [22], quantum transfer matrix [23, 24], high-temperature series expansion [25], and numerical evaluation of multiple integrals [26].

In the present study, a position-space renormalization-group method introduced by Suzuki and Takano [27, 28] for d = 2 dimensions and already applied to a number of d > 1 systems [27-33] is used to compute the spin-spin correlations and the specific heat of the anisotropic quantum Heisenberg chain, resulting in a global description and detailed information for the entire temperature and anisotropy ranges. By comparing with other works done in the various regimes of the model, we see that the method is overall quantitatively successful. A number of characteristics of the quantum nature of the system are seen: The interaction  $s_i^x s_j^x + s_i^y s_j^y$  induces an antiferromagnetic correlation in the  $s_i^z$  component, not only in the XY subcase, but for a range of anisotropies and temperatures, competing with the  $s_i^z s_j^z$  interaction when the latter is ferromagnetic. We find that the converse effect also occurs: an antiferromagnetic  $s_i^z s_j^z$  interaction induces a correlation in the  $s_i^{xy}$  component. The specific heat maxima and their response to anisotropy are distinctly opposite in the antiferromagnetic and ferromagnetic cases, again a purely quantum effect and precursor to different phase transition temperatures in three dimensions [29,33-35].

# 2. RENORMALIZATION-GROUP TRANSFORMATION FOR ONE-DIMENSIONAL CLASSICAL SYSTEMS

Ising model, a well-known classical model, is defined by the dimensionless Hamiltonian

$$-\beta \mathbf{H} = \sum_{\langle ij \rangle} \left[ \mathbf{J} \ \mathbf{s}_i \ \mathbf{s}_j + \mathbf{G} \right] \equiv \sum_{\langle ij \rangle} -\beta \mathbf{H} \left( i, j \right), \tag{2.1}$$

where  $\beta = 1/k_BT$ ,  $\langle ij \rangle$  denotes summation over nearest-neighbor pairs of sites and  $s_i$ , for every site i, can take values  $\pm 1/2$ . The additive constant G is generated by the renormalization-group transformation and is used in the calculation of thermodynamic functions.  $-\beta H(i,j) \equiv J s_i s_j + G$  is the Hamiltonian involving the bond between sites i and j. The partition function for the system is

$$Z = \sum_{\{s\}} e^{-\beta H(\{s\})} = \sum_{s_1} \sum_{s_2} \sum_{s_3} \cdots \sum_{s_i} \sum_{s_j} \sum_{s_k} \cdots \sum_{s_N} e^{-\beta H(1,2) - \beta H(2,3) \cdots - \beta H(i,j) - \beta H(j,k) \cdots - \beta H(N,1)}, \quad (2.2)$$

where i, j, k are three successive lattice sites. Performing this infinite series of sums and obtaining Z (and thus obtaining the thermodynamics) may be seen as impossible, however renormalization-group transformation opens up the possibility.

First of all, we will perform the summation over one variable, i.e.,  $s_j$ . The only part of the exponentiated Hamiltonian including  $s_j$  is  $exp[-\beta H(i,j) -\beta H(j,k)]$ , and the rest is constant with respect to  $s_j$ . Therefore, performing the sum over  $s_j$  yields

$$\begin{split} \sum_{s_{j}=\pm\frac{1}{2}} e^{-\beta H(i,j)-\beta H(j,k)} &= \sum_{s_{j}=\pm\frac{1}{2}} e^{J s_{i} s_{j} + G + J s_{j} s_{k} + G} \\ &= \sum_{s_{j}=\pm\frac{1}{2}} e^{J s_{j}(s_{i} + s_{k}) + 2G} \\ &= e^{2G} \left( e^{\frac{1}{2} J(s_{i} + s_{k})} + e^{-\frac{1}{2} J(s_{i} + s_{k})} \right) \\ &= e^{J' s_{i} s_{j} + G'} = e^{-\beta' H'(j,k)} , \end{split}$$
(2.3)

where we have redefined the result of the sum as a transformed dimensionless Hamiltonian. Here and throughout this paper, the primes are used for the renormalized system. From Eq.(2.3), one can derive the renormalized interaction constants with respect to unrenormalized ones as

$$\mathbf{J}' = 2\ln\left[\cosh\left(\frac{\mathbf{J}}{2}\right)\right] , \ \mathbf{G}' = 2\mathbf{G} + \frac{1}{2}\ln\left[4\cosh\left(\frac{\mathbf{J}}{2}\right)\right].$$
(2.4)

Two of the properties of the above recursion relations are general for renormalization-group transformation: Firstly, the derivative  $\partial_G G' = 2 = b^d$ , where b = 2 is the rescaling factor and d = 1 is the dimensionality of the lattice. Secondly J' is independent of the additive constant G.

After applying the same procedure for every even lattice site, the partition function from Eq.(2.2) takes the renormalized form

$$Z = \sum_{s_1} \sum_{s_3} \cdots \sum_{s_k} \sum_{s_k} \cdots \sum_{s_{N-1}} e^{-\beta' H'(1,3) \cdots -\beta' H'(N-1,1)} \equiv Z'.$$
(3.4)

This form of the partition function is identical with the unrenormalized one, although we have eliminated half of the degrees of freedom. One can exploit this identity in order to derive the thermodynamics as will be seen in the Sec.3.3.

# 3. THE ANISOTROPIC QUANTUM HEISENBERG MODEL AND THE RENORMALIZATION-GROUP METHOD

#### 3.1. The Anisotropic Quantum Heisenberg Model

The spin-<sup>1</sup>/<sub>2</sub> anisotropic Heisenberg model (XXZ model) is defined by the dimensionless Hamiltonian

$$-\beta H = \sum_{\langle ij \rangle} \left\{ \left[ J_{xy} \left( s_i^x s_j^x + s_i^y s_j^y \right) + J_z s_i^z s_j^z \right] + G \right\}.$$
(3.1)

Here the  $s_i^m$  are the quantum mechanical Pauli spin operators at site i, unlike the scalar  $\pm \frac{1}{2}$  values for the classical Ising model. The anisotropy coefficient is defined as  $R = J_z / J_{xy}$ . The model reduces to the isotropic Heisenberg model (XXX model) for |R| = 1, to the XY model for R = 0, and to the Ising model for  $|R| \rightarrow \infty$ .

#### **3.2 Renormalization-Group Recursion Relations**

The Hamiltonian in Eq.(3.1) can be rewritten as

$$-\beta H = \sum_{i} \{-\beta H(i, i+1)\},$$
(3.2)

where  $\beta H(i,i+1)$  is a Hamiltonian involving sites i and i+1 only. The renormalizationgroup procedure, which eliminates half of the degrees of freedom and keeps the partition function unchanged, is done approximately [27, 28]:

$$\begin{aligned} & \operatorname{Tr}_{odd} e^{-\beta H} = \operatorname{Tr}_{odd} e^{\sum_{i}^{\{-\beta H(i,i+1)\}}} \\ &= \operatorname{Tr}_{odd} e^{\sum_{i}^{odd} \{-\beta H(i-1,i)-\beta H(i,i+1)\}}} \\ &\simeq \prod_{i}^{odd} \operatorname{Tr}_{i} e^{\{-\beta H(i-1,i)-\beta H(i,i+1)\}}} \\ &= \prod_{i}^{odd} e^{-\beta' H'(i-1,i+1)} \\ &\simeq e^{\sum_{i}^{odd} \{-\beta' H'(i-1,i+1)\}} \\ &= e^{-\beta' H'}. \end{aligned}$$
(3.3)

Thus, at each successive length scale, we ignore the non-commutativity of the operators beyond three consecutive sites, in the two steps indicated by  $\approx$  in the above equation. Since the approximations are applied in opposite directions, one can expect some mutual compensation. Earlier studies [27, 28, 30-32] have been successful in obtaining finite-temperature behavior on a variety of quantum systems.

The transformation above is summarized by

$$e^{-\beta'H'(i,k)} = Tr_{j}e^{\{-\beta H(i,j) - \beta H(j,k)\}},$$
(3.4)

where i, j, k are three successive sites. The operator  $-\beta H(i,k)$  acts on two-site states, while the operator  $-\beta H(i, j) -\beta H(j, k)$  acts on three-site states, so that we can rewrite Eq.(3.4) in the matrix form,

$$\left\langle u_{i}v_{k}\left|e^{-\beta'H'(i,k)}\left|\overline{u}_{i}\overline{v}_{k}\right\rangle = \sum_{w_{j}}\left\langle u_{i}w_{j}v_{k}\right|e^{-\beta H(i,j)-\beta H(j,k)}\left|\overline{u}_{i}w_{j}\overline{v}_{k}\right\rangle,\tag{3.5}$$

where state variables can take spin-up or spin-down values at each site. The unrenormalized 8×8 matrix on the right-hand side is contracted into the renormalized 4×4 matrix on the left-hand side of Eq.(3.5). We use two-site basis states vectors  $\{|\phi_p\rangle\}$  and three-site basis states vectors  $\{|\psi_q\rangle\}$  to diagonalize the matrices in Eq.(3.5). The states  $\{|\phi_p\rangle\}$ , given in Table 3.1, are eigenstates of parity, total spin

magnitude, and total spin z-component. These  $\{|\phi_p\rangle\}$  diagonalize the renormalized matrix, with eigenvalues

$$\Lambda_1 = \frac{1}{4}J'_z + G', \quad \Lambda_2 = \Lambda_3 = -\frac{1}{4}J'_z + \frac{1}{2}J'_{xy} + G', \quad \Lambda_4 = -\frac{1}{4}J'_z - \frac{1}{2}J'_{xy} + G'.$$
(3.6)

The states  $\{|\psi_q\rangle\}$ , given in Table 3.2, are eigenstates of parity and total spin zcomponent. The  $\{|\psi_q\rangle\}$  diagonalize the unrenormalized matrix, with eigenvalues

$$\lambda_{1} = \frac{1}{2} \mathbf{J}_{z} + 2\mathbf{G} , \qquad \lambda_{2} = -\frac{1}{4} \Big( \mathbf{J}_{z} + \sqrt{8 \mathbf{J}_{xy}^{2} + \mathbf{J}_{z}^{2}} \Big) + 2\mathbf{G} ,$$

$$\lambda_{3} = -\frac{1}{4} \Big( \mathbf{J}_{z} - \sqrt{8 \mathbf{J}_{xy}^{2} + \mathbf{J}_{z}^{2}} \Big) + 2\mathbf{G} , \qquad \lambda_{4} = 2\mathbf{G} .$$
(3.7)

With these eigenstates, Eq.(3.5) is rewritten as

$$\begin{split} \gamma_{p} &\equiv \left\langle \phi_{p} \left| e^{-\beta' H'(i,k)} \left| \phi_{p} \right\rangle = \sum_{\substack{u,v,\overline{u},\\\overline{v},w,q}} \left\langle \phi_{p} \left| u_{i}v_{k} \right\rangle \left\langle u_{i}w_{j}v_{k} \left| \psi_{q} \right\rangle \left\langle \psi_{q} \left| e^{-\beta H(i,j) - \beta H(j,k)} \left| \psi_{q} \right\rangle \right. \right. \right. \right. \\ &\left. \left\langle \psi_{q} \left| \overline{u}_{i}w_{j}\overline{v}_{k} \right\rangle \left\langle \overline{u}_{i}\overline{v}_{k} \left| \phi_{p} \right\rangle \right. \end{split}$$
(3.8)

Thus, there are three independent  $\gamma_p$  that determine the renormalized Hamiltonian and, therefore, three renormalized interactions in the Hamiltonian closed under renormalization-group transformation, Eq.(3.1). These  $\gamma_p$  are

$$\begin{split} \gamma_{1} &= e^{\frac{1}{4}J'_{z}+G'} = e^{2G-\frac{1}{4}J_{z}} \left[ e^{\frac{3}{4}J_{z}} + \cosh\left(\frac{1}{4}\sqrt{8J_{xy}^{2}+J_{z}^{2}}\right) - \frac{J_{z}\sinh\left(\frac{1}{4}\sqrt{8J_{xy}^{2}+J_{z}^{2}}\right)}{\sqrt{8J_{xy}^{2}+J_{z}^{2}}} \right], \\ \gamma_{2} &= e^{\frac{1}{2}J'_{xy}-\frac{1}{4}J'_{z}+G'} = 2e^{2G-\frac{1}{4}J_{z}} \left[ \cosh\left(\frac{1}{4}\sqrt{8J_{xy}^{2}+J_{z}^{2}}\right) + \frac{J_{z}\sinh\left(\frac{1}{4}\sqrt{8J_{xy}^{2}+J_{z}^{2}}\right)}{\sqrt{8J_{xy}^{2}+J_{z}^{2}}} \right], \end{split}$$
(3.9)  
$$\gamma_{4} &= e^{-\frac{1}{2}J'_{xy}-\frac{1}{4}J'_{z}+G'} = 2e^{2G}, \end{split}$$

which yield the recursion relations

$$\mathbf{J}'_{xy} = \ln\left(\frac{\gamma_2}{\gamma_4}\right) , \quad \mathbf{J}'_z = \ln\left(\frac{\gamma_1^2}{\gamma_2 \gamma_4}\right) , \quad \mathbf{G}' = \frac{1}{4}\ln\left(\gamma_1^2 \gamma_2 \gamma_4\right) . \tag{3.10}$$

**Table 3.1:** The two-site basis eigenstates that appear in Eq.(3.8). These are the well-known singlet and triplet states. The state  $|\phi_3\rangle$  is obtained by spin reversal from  $|\phi_1\rangle$ , with the same eigenvalue.

p	S	m <sub>s</sub>	Two-site basis eigenstates
	1	1	$ \phi_1\rangle =  \uparrow\uparrow\rangle$
+	1	0	$\left \phi_{2}\right\rangle = \frac{1}{\sqrt{2}}\left\{\left \uparrow\downarrow\right\rangle + \left \downarrow\uparrow\right\rangle\right\}$
-	0	0	$ \phi_{4}\rangle = \frac{1}{\sqrt{2}} \left\{  \uparrow\downarrow\rangle -  \downarrow\uparrow\rangle \right\}$

**Table 3.2:** The three-site basis eigenstates that appear in Eq.(3.8) with coefficients  $\sigma = \left(-J_z + \sqrt{8J_{xy}^2 + J_z^2}\right)/2J_{xy}$ ,  $\tau = \left(-J_z - \sqrt{8J_{xy}^2 + J_z^2}\right)/2J_{xy}$  and normalization factors  $\mu$ , v. The states  $|\psi_{5-8}\rangle$  are obtained by spin reversal from  $|\psi_{1-4}\rangle$ , with the same respective eigenvalues.

р	m <sub>s</sub>	Three-site basis eigenstates				
	3/2	$\left  \psi_{1} \right\rangle = \left  \uparrow \uparrow \uparrow \right\rangle$				
+	1/2	$ \psi_{2}\rangle = \mu \left\{  \uparrow\uparrow\downarrow\rangle + \sigma  \uparrow\downarrow\uparrow\rangle +  \downarrow\uparrow\uparrow\rangle \right\}$				
	1/2	$\left \psi_{3}\right\rangle = \nu\left\{\left \uparrow\uparrow\downarrow\right\rangle + \tau\left \uparrow\downarrow\uparrow\right\rangle + \left \downarrow\uparrow\uparrow\right\rangle\right\}$				
_	1/2 $ \psi_4\rangle = \frac{1}{\sqrt{2}} \{ \uparrow\uparrow\downarrow\rangle -  \downarrow\uparrow\uparrow\rangle\}$					

As expected,  $J'_{xy}$  and  $J'_z$  are independent of the additive constant G and the derivative  $\partial_G G' = b^d = 2$ .

For  $J_{xy} = J_z$ , the recursion relations reduce to the spin-½ isotropic Heisenberg (XXX) model recursion relations, while for  $J_{xy} = 0$  they reduce to spin-½ Ising model recursion relations. The  $J_z = 0$  subspace (XY model) is not (and need not be) closed

under these recursion relations [27, 28]: The renormalization-group transformation induces a positive  $J_z$  value, but the spin-space easy-plane aspect is maintained.

In addition, there exists a mirror symmetry along the  $J_z$ -axis, so that  $J'_{xy}(-J_{xy}, J_z) = J'_{xy}(J_{xy}, J_z)$  and  $J'_z(-J_{xy}, J_z) = J'_z(J_{xy}, J_z)$ . The thermodynamics of the system remains unchanged under flipping the interactions of the x and y spin components, since the renormalization-group trajectories do not change. In fact, this is part of a more general symmetry of the XYZ model, where flipping the signs of any two interactions leaves the spectrum unchanged [8]. Therefore, with no loss of generality, we take  $J_{xy} > 0$ . Independent of the sign of  $J_{xy}$ ,  $J_z > 0$  gives the ferromagnetic model and  $J_z < 0$  gives the antiferromagnetic model.

# **3.3.** Calculation of Densities and Response Functions by the Recursion-Matrix Method

Just as the interaction constants of two consecutive points along the renormalizationgroup trajectory are related by the recursion relations, the densities are connected by a recursion matrix  $\hat{T}$ , which is composed of derivatives of the recursion relations. For our Hamiltonian, the recursion matrix and density vector  $\vec{M}$  are

$$\hat{\mathbf{T}} = \begin{pmatrix} \frac{\partial \mathbf{G}'}{\partial \mathbf{G}} = 2 & \frac{\partial \mathbf{G}'}{\partial \mathbf{J}_{xy}} & \frac{\partial \mathbf{G}'}{\partial \mathbf{J}_{z}} \\ \frac{\partial \mathbf{J}'_{xy}}{\partial \mathbf{G}} = 0 & \frac{\partial \mathbf{J}'_{xy}}{\partial \mathbf{J}_{xy}} & \frac{\partial \mathbf{J}'_{xy}}{\partial \mathbf{J}_{z}} \\ \frac{\partial \mathbf{J}'_{z}}{\partial \mathbf{G}} = 0 & \frac{\partial \mathbf{J}'_{z}}{\partial \mathbf{J}_{xy}} & \frac{\partial \mathbf{J}'_{z}}{\partial \mathbf{J}_{z}} \end{pmatrix} , \qquad \mathbf{\overline{M}} = \begin{pmatrix} 1 & 2 \left\langle \mathbf{s}_{i}^{xy} \, \mathbf{s}_{j}^{xy} \right\rangle & \left\langle \mathbf{s}_{i}^{z} \, \mathbf{s}_{j}^{z} \right\rangle \end{pmatrix} .$$
(3.11)

These are densities  $M_{\alpha}$  associated with each interaction  $K_{\alpha}$ ,

$$M_{\alpha} = \frac{1}{N_{\alpha}} \frac{\partial \ln Z}{\partial K_{\alpha}} , \qquad (3.12)$$

where  $N_{\alpha}$  is the number of  $\alpha$ -type interactions and Z is the partition function for the system, which can be expressed both via the unrenormalized interaction constants as  $Z(\vec{K})$  or via the renormalized interaction constants as  $Z(\vec{K})$ . By using these two equivalent forms, one can formulate the density recursion relation [36]

$$M_{\alpha} = b^{-d} \sum_{\beta} M_{\beta}' T_{\beta\alpha} \quad , \quad T_{\beta\alpha} \equiv \frac{N_{\beta}}{N_{\alpha}} \frac{\partial K_{\beta}'}{\partial K_{\alpha}} \quad .$$
(3.13)

Since the interaction constants, under renormalization-group transformation, stay the same at fixed points such as critical fixed points or sinks, the above Eq.(3.13) takes the form of a solvable eigenvalue equation,

$$\mathbf{b}^{\mathrm{d}} \mathbf{\widetilde{M}}^* = \mathbf{\widetilde{M}}^* \cdot \mathbf{\widehat{T}}, \qquad (3.14)$$

at fixed points, where  $\vec{M} = \vec{M'} = \vec{M}^*$ . The fixed point densities are the components of the left eigenvector of the recursion matrix with left eigenvalue b<sup>d</sup> [36]. At ordinary points, Eq.(3.13) is iterated until a sink point is reached under successive renormalization-group transformations. In algebraic form, this means,

$$\vec{M}^{(0)} = b^{-nd} \vec{M}^{(n)} \hat{T}^{(n)} \hat{T}^{(n-1)} \cdots \hat{T}^{(1)}, \qquad (3.15)$$

where the upper indices indicate the number of iteration (transformation), with  $\overrightarrow{M}^{(n)} \simeq \overrightarrow{M}^*$ .

This method is applied on our model Hamiltonian. The sink of the system is at infinite temperature  $J_{xy}^* = J_z^* = 0$  for all initial conditions  $(J_{xy}, J_z)$ . One can see that, since reaching this sink needs less renormalization-group steps for high-temperature (low-J) than for low-temperature (high-J), our approximate renormalization-group method works better in high-temperature than in low-temperature. We already know that the method is exact in  $|R| \rightarrow \infty$  (Ising) limit, since the model is classical in this limit. With the additional information of the sink of the model (i.e. sink at infinite temperature), we also know that the method is exact in  $T \rightarrow \infty$  limit too. At the  $T \approx 0$  regime, the method works at its worst, since in order to reach the sink from initial conditions in this regime, we need the most renormalization-group steps, which are approximate and summarized by Eq.(3.4).

Response functions are calculated by differentiation of densities. For example, the internal energy is  $U = -2 \langle s_i^{xy} s_j^{xy} \rangle - R \langle s_i^z s_j^z \rangle$ , employing  $T = 1/J_{xy}$ , and  $U = -2 \langle s_i^{xy} s_j^{xy} \rangle / R - \langle s_i^z s_j^z \rangle$ , employing  $T = 1/|J_z|$ . The specific heat  $C = \partial_T U$  follows from the chain rule.

#### 4. CORRELATIONS SCANNED WITH RESPECT TO ANISOTROPY

The ground-state and excitation properties of the XXZ model offer a variety of behaviors [11, 12, 37, 38]: The antiferromagnetic model with R < -1 is Isinglike and the ground state has Néel long-range order along the z spin component with a gap in the excitation spectrum. For  $-1 \le R \le 1$ , the system is a "spin liquid", with a gapless spectrum and power-law decay of correlations at zero temperature. The ferromagnetic model with R > 1 is also Isinglike, the ground state is ferromagnetic along the z spin component, with an excitation gap.

Our calculated  $\langle s_i^z s_j^z \rangle$  and  $\langle s_i^{xy} s_j^{xy} \rangle \equiv \langle s_i^x s_j^x \rangle = \langle s_i^y s_j^y \rangle$  nearest-neighbor spin-spin correlations for the whole range of the anisotropy coefficient R are shown in Fig.4.1, for various temperatures.

The xy correlation is always non-negative. Recall that we use  $J_{xy} > 0$  with no loss of generality. In the Isinglike antiferromagnetic (R < -1) region, the z correlation is expectedly antiferromagnetic. As the  $\langle s_i^z s_j^z \rangle$  correlation saturates for large |R|, the transverse  $\langle s_i^{xy} s_j^{xy} \rangle$  correlation is somewhat depleted. In the Isinglike ferromagnetic (R > 1) region, the  $\langle s_i^z s_j^z \rangle$  correlation is ferromagnetic, saturates quickly as the  $\langle s_i^{xy} s_j^{xy} \rangle$  correlation quickly goes to zero. In the spin-liquid (IRI < 1) region, the  $\langle s_i^z s_j^z \rangle$  correlation is maximal. The remarkable quantum behavior of  $\langle s_i^z s_j^z \rangle$  around R = 0 is discussed in Sec.6 below. It is seen in the figure that these changeovers are increasingly sharp as temperature is decreased and, at zero temperature, become discontinuous at R = 1. As seen in Fig.4.1(b), at zero temperature, our calculated  $\langle s_i^z s_j^z \rangle$  and  $\langle s_i^{xy} s_j^{xy} \rangle$  correlations show very good agreement with the known exact points [4, 39-41]. Also, our results for R > 1 fully

overlap the exact results of  $\langle s_i^z s_j^z \rangle = 0.25$  and  $\langle s_i^{xy} s_j^{xy} \rangle = 0$  [37]. We also note that zero-temperature is the limit in which our approximation is at its worst.



**Figure 4.1:** (a) Calculated nearest-neighbor spin-spin correlations  $\langle s_i^z s_j^z \rangle$ , (thick curves from lower left) and  $\langle s_i^{xy} s_j^{xy} \rangle$ , (thin curves from upper left) as a function of anisotropy coefficient R for temperatures  $1/J_{xy} = 0, 0.1, 0.2, 0.4, 0.8$ . (b) Calculated zero-temperature nearest-neighbor spin-spin correlations (thin and thick curves, as in the upper panel) compared with the exact points of Ref.[4, 37, 39-41] shown with filled and open symbols for  $\langle s_i^z s_j^z \rangle$ , and  $\langle s_i^{xy} s_j^{xy} \rangle$ , respectively. At R = 1,  $\langle s_i^z s_j^z \rangle$ , discontinuously goes from antiferromagnetic to the exact result of 0.25 [37] of saturated ferromagnetism and  $\langle s_i^{xy} s_j^{xy} \rangle$ , discontinuously goes from ferromagnetic to the exact result of constant zero [37].

#### 5. ANTIFERROMAGNETIC XXZ CHAIN



**Figure 5.1:** Calculated nearest-neighbor spin-spin correlations  $\langle s_i^z s_j^z \rangle$  (lower thick curves in each panel) and  $\langle s_i^{xy} s_j^{xy} \rangle$  (upper thin curves in each panel) for the antiferromagnetic XXZ chain, as a function of temperature for anisotropy coefficients R = 0, -0.25, -0.50, -0.75, -1, -2, -4, -8, - $\infty$  spanning the spin-liquid (upper panel) and Isinglike (lower panel) regions.

For the antiferromagnetic XXZ chain, our calculated  $\langle s_i^z s_j^z \rangle$  and  $\langle s_i^{xy} s_j^{xy} \rangle$  nearestneighbor spin-spin correlations as a function of temperature are shown in Fig.5.1 for various anisotropy coefficients R. We find that when  $J_{xy}$  is the dominant interaction (spin liquid), the  $\langle s_i^{xy} s_j^{xy} \rangle$  correlation is weakly dependent on anisotropy R. Conversely, when  $J_z$  is the dominant interaction (Isinglike), the  $\langle s_i^z s_j^z \rangle$  correlation is weakly dependent on anisotropy R, but only at the higher temperatures. Our results are compared with multiple-integral results [26] in Fig.5.2.



**Figure 5.2:** Comparison of our results (thick lines) for the correlation functions of the antiferromagnetic XXZ chain, with the multiple-integral results of Ref.[26] (thin lines), for various anisotropy coefficients R spanning the spin-liquid and Isinglike regions.

The calculated antiferromagnetic specific heats are shown in Fig.5.3 for various anisotropy coefficients and compared, in Fig.5.4 and Fig.5.5, with finite-lattice expansion [6, 19], quantum decimation [21], transfer matrix [24], high-temperature series expansion [25] results and, for the R = 0 case, namely the XY model, with the exact result  $\frac{1}{4\pi\Gamma}\int_0^{\pi} \left[\cos\omega/\cosh\left(\frac{\cos\omega}{2\Gamma}\right)\right]^2 d\omega$  [5]. The maximum C(T) temperature is highest for the isotropic case (Heisenberg) and decreases with anisotropy increasing in either direction (towards Ising or XY). The maximum value of C(T) is only weakly dependent on anisotropy, especially for the Isinglike systems.



**Figure 5.3:** Calculated specific heats C of the antiferromagnetic XXZ chain, as functions of temperature for anisotropy coefficients  $R = 0, -0.25, -0.50, -0.75, -1, -2, -4, -8, -\infty$  spanning the spin-liquid (upper panel) and Isinglike (lower panel) regions.



**Figure 5.4:** Comparison of our antiferromagnetic specific heat results (thick lines) with the results of Refs.[5] (open circles), [6] (dotted), [19] (thin lines), [21] (dash-dotted), and [23, 24] (dashed), for anisotropy coefficients R = 0, -0.5, -1, -2 spanning the spin-liquid and Isinglike regions.



**Figure 5.5:** Comparison of our antiferromagnetic specific heat results (thick lines) with the high-temperature  $J \rightarrow 0$  behaviors (thin lines) obtained from series expansion in Ref.[25], for anisotropy coefficients  $R = 0, -0.50, -0.75, -1, -2, -\infty$  spanning the spin-liquid and Isinglike regions.

The linearity, at low temperatures, of the spin liquid ( $|\mathbf{R}| \leq 1$ ) specific heat with respect to temperature is expected on the basis of spin-wave calculations for the antiferromagnetic XXZ model [42, 43]. This linear form of C(T) reflects the linear energy-momentum dispersion of the low-lying excitations, the magnons. The lowtemperature magnon dispersion relation is  $\hbar \omega = ck^n$ , where c is the spin-wave stiffness and n = 1 for the antiferromagnetic XXZ model in d = 1 [37]. The internal energy, given by  $U = \frac{1}{2\pi} \int_0^{\infty} \left[ \hbar \omega(k) / (e^{\beta \hbar \omega(k)} - 1) \right] dk$ , is dominated by the magnons at low temperatures, yielding  $U \sim T^2$  and  $C \sim T$  for n = 1 in the dispersion relation. From this relation, our calculated spin-wave stiffness c as a function of anisotropy R is given in Fig.5.6. The exactly known value of  $c = 2\pi$  at R = -1 [42, 43] is also shown in Fig.5.6. Our calculated value of c = 6.78620 is only in 8% error with respect to this exact value of  $c = 2\pi = 6.28319$ . Our simultaneous fit to the dispersion relation exponent n, expected to be 1, yields  $1\pm 0.02$ . However, for the Isinglike |R| > 1, the unexpected linearity instead of an exponential form caused by a gap in the excitation spectrum, points to the approximate nature of our renormalization-group calculation. The correct exponential form is obtained in the large R limit, where the renormalization-group calculation becomes exact.



**Figure 5.6:** Our calculated antiferromagnetic spin-wave stiffness c versus the anisotropy coefficient R. The single point shows the exact result of  $c = 2\pi$  at R = -1 [42, 43]. The lower line is the fit to the dispersion relation exponent n, expected to be 1 [37].

Rojas et al. [25] have obtained the high-temperature expansion of the free energy of the XXZ chain to order  $\beta^3$ , where  $\beta$  is the inverse temperature. The specific heat from this expansion is

$$C = \frac{2 + R^2}{16}\beta^2 - \frac{3R}{32}\beta^3 + \frac{6 - 8R^2 - R^4}{256}\beta^4.$$
 (5.1)

This high-temperature specific heat result is also compared with our results, in Fig.5.5, and very good agreement is seen. In fact, when in the high-temperature region of  $0 < \beta < 0.1$ , we fit our numerical results for C( $\beta$ ) to the fourth degree polynomial C =  $\sum_{i=1}^{4} A_i \beta^i$ , and we do find (1) the vanishing A<sub>0</sub> < 10<sup>-5</sup> and A<sub>1</sub> < 10<sup>-7</sup> for all R and (2) the comparison in Fig.5.7 between our results for A<sub>2</sub> and A<sub>3</sub> and those of Eq.(5.1) from Ref.[25], thus obtaining excellent agreement for all regions of the model.



**Figure 5.7:** Comparison of our results with the high-temperature expansion of Ref.[25] for all regions: antiferromagnetic (outer panels) and ferromagnetic (inner panels), spin-liquid (left panels) and Isinglike (right panels). Triangles and circles denote our results, while solid and dashed lines denote the results of Ref.[25] for A<sub>2</sub> and A<sub>3</sub>, respectively. The error bars, due to the statistical fitting procedure of the coefficients A<sub>2</sub> and A<sub>3</sub>, have half-heights of  $1.7 \times 10^{-4}$  and  $2.6 \times 10^{-3}$  respectively.

#### 6. FERROMAGNETIC XXZ CHAIN

For the ferromagnetic (i.e., R > 0) systems in Fig.4.1, the  $\left\langle s_{i}^{z} s_{j}^{z} \right\rangle$  expectation value becomes rapidly negative at lower temperatures for R < 1, even though for  $R \ge 0$  all couplings in the Hamiltonian are ferromagnetic. This is actually a real physical effect, not a numerical anomaly. In fact, we know the spin-spin correlations for the ground state of the one-dimensional XY model (the R = 0 case of our Hamiltonian), and we can compare our low-temperature results with these exact values. The ground-state properties of the spin-1/2 XY model are studied by making a Jordan-Wigner transformation, yielding a theory of non-interacting spinless fermions. Analysis of this theory yields the exact zero-temperature nearest-neighbor spin-spin correlations [4] shown in Table 6.1. Our renormalization-group results in the zerotemperature limit, also shown in this table, compare quite well with the exact results, as with the other exact points in Fig.4.1(b), although in the worst region for our approximation. Finally, by continuity, it is reasonable that for a range of R positive but less than one, the z component correlation function is as we find, intriguingly but correctly negative at low temperatures. Thus, the interaction  $s_i^x s_j^x + s_i^y s_j^y$  (irrespective of its sign, due to the symmetry mentioned at the end of Sec.3.2) induces an antiferromagnetic correlation in the  $s^{z}_{i}$  component, competing with the  $s^{z}_{i}\,s^{z}_{j}$ interaction when the latter is ferromagnetic.

Zero-temperature correlations of the spin-½ XY chain	Exact values from Ref.[4]	Our RGT results
$\left\langle s_{i}^{xy}s_{j}^{xy} ight angle$	0.15915	0.17678
$\left< {{s_i^z}{s_j^z}} \right>$	-0.10132	-0.12500

Table 6.1: Zero-temperature nearest-neighbor correlations of the spin-½ XY chain.

For finite temperatures, our calculated nearest-neighbor spin-spin correlations are shown in Fig.6.1, for different values of R. These results are compared with Green's function calculations [22] in Fig.6.2. As expected from the discussion at the beginning of this section, in the spin-liquid region, the correlation  $\langle s_i^z s_j^z \rangle$  is negative at low temperatures. Thus, a competition occurs in the correlation  $\langle s_i^z s_j^z \rangle$  between the XY-induced antiferromagnetism and the ferromagnetism due to the direct coupling between the  $s^z$  spin components. In fact, this effect is also seen in the antiferromagnetic model discussed in the previous section, as detected in the lower panel of Fig.5.1: For  $|J_z| \leq 2.7$ , the antiferromagnetic correlations of  $\langle s_i^z s_j^z \rangle$  are increased by increasing  $J_{xy}$ . Moreover, we find that the converse effect also occurs, as seen in the upper panel of Fig.5.1: For  $|J_z|$  increases the correlations of  $\langle s_i^z s_j^z \rangle$ .



**Figure 6.1:** Calculated nearest-neighbor spin-spin correlations  $\langle s_i^z s_j^z \rangle$  and  $\langle s_i^{xy} s_j^{xy} \rangle$ , (thick and thin curves in each panel respectively) for the ferromagnetic XXZ chain, as functions of temperature, for anisotropy coefficients R = 0, 0.25, 0.50, 0.75, 1, 2, 4, 8,  $\infty$  spanning the spin-liquid (upper panel) and Isinglike (lower panel) regions.



Figure 6.2: Comparison of our ferromagnetic R = 1, 5/3 results with Green's function calculations [22].

As a consequence of the competition mentioned above, a sign reversal in  $\langle s_i^z s_j^z \rangle$  occurs from negative to positive correlation, at temperatures  $T_0(R)$ . At this temperature, by cancelation of the competing effects, the nearest-neighbor correlation  $\langle s_i^z s_j^z \rangle$  is zero. Our calculated  $T_0(R)$  curve is shown in Fig.6.3, and has very good agreement with the exact result  $T_0 = (\sqrt{3} \sin \gamma/2\gamma) \tan[\pi(\pi - \gamma)/2\gamma]$ , where  $\gamma \equiv \cos^{-1}(-R)$  [23].



**Figure 6.3:** The sign-reversal temperature  $T_0$  of the nearest-neighbor correlation  $\langle s_i^z s_j^z \rangle$ : our results (full curve) and the analytical result from the quantum transfer matrix method (dashed) [23].

The calculated ferromagnetic specific heats are shown in Fig.6.4 for various anisotropy coefficients and compared, in Fig.6.5 and Fig.6.6, with finite-lattice expansion [6], quantum decimation [21], decoupled Green's functions [22], transfer

matrix [23, 24], high-temperature series expansion [25] results and, for the R = 0 case, namely the XY model, with the exact result  $\frac{1}{4\pi T} \int_0^{\pi} \left[ \cos \omega / \cosh \left( \frac{\cos \omega}{2T} \right) \right]^2 d\omega$  [5]. In sharp contrast to the antiferromagnetic case in Sec.5, the maximum C(T) temperature is highest for the most anisotropic cases (XY and Ising) and decreases with anisotropy decreasing from either direction (towards Heisenberg). In the same contrast, the maximum value of C(T) is dependent on anisotropy, decreasing, eventually to a flat curve, as anisotropy is decreased. This contrast between the ferromagnetic and antiferromagnetic systems is a purely quantum phenomenon. Specifically, the marked contrast between the specific heats of the isotropic antiferromagnetic and ferromagnetic systems, seen in the full curves of Fig.5.3 and Fig.6.4 respectively, translates into the different critical temperatures of the respective three-dimensional systems [29, 33-35]. Classical ferromagnetic and antiferromagnetic systems are, on the other hand, identically mapped onto each other. Three-dimensional model will be discussed in Sec.8.

The low-temperature specifics heats are discussed in detail and compared to other results in Sec.7.



**Figure 6.4:** Calculated specific heats C of the ferromagnetic XXZ chain, functions of temperature for anisotropy coefficients  $R = 0, 0.25, 0.50, 0.75, 1, 2, 4, 8, \infty$  spanning the spin-liquid (upper panel) and Isinglike (lower panel) regions.



**Figure 6.5:** Comparison of our ferromagnetic specific heat results (thick lines) with the results of Refs.[5] (dash-double-dotted), [6] (dotted), [21] (dash-dotted), [22] (open circles), and [23, 24] (dashed), for anisotropy coefficients R = 0, 0.5, 1, 5/4, 5/3, 2, 5 spanning the spin-liquid and Isinglike regions.



**Figure 6.6:** Comparison of our ferromagnetic specific heat results (thick lines) with the high-temperature  $J \rightarrow 0$  behaviors (thin lines) obtained from series expansion [25], for anisotropy coefficients R = 0.25, 0.50, 0.75, 1, 2,  $\infty$  spanning the spinliquid and Isinglike regions.

#### 7. LOW-TEMPERATURE SPECIFIC HEATS

Properties of the low-temperature specific heat of the ferromagnetic XXZ chain have been derived from the thermodynamic Bethe-ansatz equations [37]. For anisotropy coefficient  $|\mathbf{R}| \le 1$ , the model is gapless [11, 12] and, except at  $\mathbf{R} = 1$ , the specific heat is linear in  $T = 1/J_{xy}$  in the zero-temperature limit,  $C/T = 2\gamma/(3 \sin \gamma)$ , where again  $\gamma \equiv \cos^{-1}(-\mathbf{R})$ . Note that this result contradicts the spin-wave theory prediction of  $\mathbf{C} \sim T^{\frac{1}{2}}$  for the ferromagnetic chain (n = 2 for the ferromagnetic magnon dispersion relation of the kind given above in Sec.5). The spin-wave result is valid only for  $\mathbf{R} = 1$ , the isotropic Heisenberg case. From the expression given above, we see that C/T diverges as  $\mathbf{R} \to 1^-$ , and at exactly  $\mathbf{R} = 1$  it has been shown that  $\mathbf{C} \sim T^{\frac{1}{2}}$ [37].

In the Isinglike region R > 1, the system exhibits a gap in its excitation spectrum and the specific heat behaves as C ~ T<sup>-3/2</sup> exp( $-\Delta / T$ ), with  $\Delta$  being the excitation spectrum gap [11, 12, 37]. We can fit our calculated C(T) curves, which are shown in the lower panel of Fig.6.4, to this formula in order to obtain the excitation spectrum gap for various anisotropy coefficients (Fig.7.1). There exist two gaps for the energy, called the spinon gap and the spin-wave gap, given by  $\Delta_{spinon} = \frac{1}{2}\sqrt{1-R^{-2}}$  and  $\Delta_{spin-wave} = 1 - R^{-1}$ . These are the minimal energies of elementary excitations [10, 37]. A crossover between them occurs at R = 5/3: below this value, the spinon gap is lower, while above this value the spin-wave gap is lower. As seen in Fig.7.1, as expected, our calculated gap  $\Delta$  behaves linearly in R<sup>-1</sup> for R<sup>-1</sup> close to 1, and crosses over to 1/2 at R<sup>-1</sup> = 0.



**Figure 7.1:** Calculated excitation spectrum gap  $\Delta$  versus inverse anisotropy.

We now turn to the discussion of our specific heat results for the entire ferromagnetic and antiferromagnetic ranges. Our calculated C/T curves are plotted as a function of anisotropy and temperature in Fig.7.2 and Fig.7.3 respectively.



**Figure 7.2:** Calculated specific heat coefficients C/T as functions of anisotropy R, for  $T = 0.10, 0.05, 10^{-10}$ .



**Figure 7.3:** Calculated specific heat coefficients C/T as functions of temperature for anisotropy coefficient R = -2 (thick grey), -1 (dotted), -0.5 (dash-dotted), 0.5 (dashed), and 2 (thin black).

We discuss each region of the anisotropy R separately:

- (i) R > 1: The specific heat coefficient C/T vanishes in the  $T \rightarrow 0$  limit and has the expected exponential form as discussed above in this section. The spin-wave to spinon excitation gap crossover is obtained.
- (ii)  $R \approx 1$ : The double-peak structure of C/T in Fig.7.2 is centered at R = 1. As temperature goes to zero, the peaks narrow and diverge, and the value in-between them sharply dips, but reaches 0.86, not zero. Although we expect  $C \sim T^{\frac{1}{2}}$  at this point, our approximation escapes linearity at  $R = 1^+$  (see end of next paragraph) instead of R = 1.
- (iii)  $-1 \le R < 1$ : The specific heat coefficient is C/T =  $2\gamma/(3 \sin \gamma)$  in this region [11, 37], and our calculated specific heat is indeed linear at low temperatures. The C/T curves for R = -1, -0.5, 0.5 in Fig.7.3 all extrapolate to nonzero limits at T = 0. The spin-wave dispersion relation exponent and stiffness, for the antiferromagnetic system, is correctly obtained for the isotropic case and extended to all anisotropies, as seen in Fig.5.6. Fig.7.4 directly compares C/T =  $2\gamma/(3 \sin \gamma)$  with our results: The curves have the same basic form, gradually rising from R = -1, with a sharp divergence as R nears 1. At R =  $1^+$ , we expect C/T = 0. Our

T =  $10^{-10}$  curve diverges at R = 1 and indeed returns to zero at R = 1.0000001.

(iv) R < -1: We expect a vanishing C/T, which we do find as seen in Fig.7.2 and in the inset of Fig.7.3. The exponential behavior of the specific heat is clearly seen in the Ising limit.



**Figure 7.4:** Calculated specific heat coefficient C/T as a function of anisotropy coefficient R in the spin-liquid region,  $-1 \le R \le 1$ , at constant temperature  $T = 10^{-10}$ . Our renormalization-group result (grey curve) is compared to the zero-temperature Bethe-Ansatz result (black curve). Inset: our calculation (grey curve) at constant  $T = 10^{-2}$  is again compared to the zero-temperature Bethe-Ansatz result (black curve).

# 8. CALCULATION OF RECURSION RELATIONS IN HIGHER DIMENSIONS

Recursion relations for the d = 1 quantum XXZ model obtained in Sec.3.2 are in the form

$$\mathbf{J}_{xy}' = \mathbf{R}_{xy} \left( \mathbf{J}_{xy}, \mathbf{J}_{z} \right) , \quad \mathbf{J}_{z}' = \mathbf{R}_{z} \left( \mathbf{J}_{xy}, \mathbf{J}_{z} \right) , \mathbf{\overline{G}}' = \mathbf{R}_{G} \left( \mathbf{J}_{xy}, \mathbf{J}_{z} \right) , \quad \mathbf{G}' = \mathbf{b}^{d} \mathbf{G} + \mathbf{\overline{G}}' .$$

$$(8.1)$$

The Migdal-Kadanoff approximation for d > 1 is described as [44, 45]

$$\vec{\mathbf{K}}' = \mathbf{R} \left( \mathbf{b}^{d-1} \vec{\mathbf{K}} \right) , \quad \vec{\mathbf{K}} = \left( \vec{\mathbf{G}} , \mathbf{J}_{xy} , \mathbf{J}_{z} \right).$$
(8.2)

Recalling the d = 1 recursion relations from Eq.(3.10) and using these in Eq.(8.2) yield the b = 2 recursion relations for d > 1 quantum XXZ model.

The spin- $\frac{1}{2}$  quantum Heisenberg system ( $J_{xy} = J_z = J$ , R = 1) does not provide any phase transition for  $d \le 2$ . That is to say, the lower critical dimension of the quantum Heisenberg model is  $d_{\text{Heis.}}^{\text{Lc.}} = 2$ , which is an expected result [29, 33]. So, the 3-d Heisenberg model induces a finite temperature second-order phase transition. Another expected result is the ratio of antiferromagnetic transition temperature and the ferromagnetic one, which is found to be approximately 1.22, the same value as computed in [29, 33]. This value can also be compared with the series expansion result of 1.13 [34, 35]. This result of different critical temperatures of ferromagnetic and antiferromagnetic cases was also predicted in Sec.6. The ferromagnetic and antiferromagnetic Ising critical temperatures are found to be 1 and 2 respectively, which are also expected results. In addition, algebraically ordered Kosterlitz-Thouless low-temperature phase is obtained for the two-dimensional quantum XY model [27, 28].

#### 9. PHASE DIAGRAM OF THE THREE-DIMENSIONAL XXZ MODEL

The flow chart of Fig.9.1 presented below is drawn via the recursion relations obtained from Eq.(8.2) for b = 2 recursion relations and with d = 3. The critical points (dots in Fig.9.1) obtained for 3-d ferromagnetic Ising ( $R \rightarrow \infty$ ), isotropic Heisenberg (R = 1), and XY (R = 0) models are  $J_{I-F}^{C} = 0.261065$ ,  $J_{H-F}^{C} = 0.343897$  and  $J_{XY}^{C} = 0.268739$  respectively. These critical points are in an expected order of,  $J_{H-F}^{C} > J_{XY}^{C} > J_{L-F}^{C}$ , due to the decrease in critical temperature (1/J<sup>c</sup>) with the increase in the spin dimension (so in disorder). Three sinks occur in the flow chart of Fig.9.1, namely (0,0), (0,1) and (1,1), which correspond to disordered, s<sup>z</sup>-ordered and s<sup>xy</sup>-ordered phases respectively.



**Figure 9.1:** Flow chart of the 3-d XXZ model plotted as  $tanh(J_z)$  versus  $tanh(J_{xy})$ . Arrows indicate the orientation of flows, while dots indicate the spin- $\frac{1}{2}$  Ising, Heisenberg, and XY model critical points.

One can deduce the phase diagram of the 3-d ferromagnetic anisotropic Heisenberg model from the flow chart of Fig.9.1 as in the Fig.9.2.



**Figure 9.2:** Phase diagram of ferromagnetic XXZ model plotted in the axes  $tanh(J_z)$  versus  $tanh(J_{xy})$ . Full and dashed lines represent second- and first-order phase transitions respectively.

Renormalization-group transformation of a point in the R < 0 antiferromagnetic region maps it on the R > 0 ferromagnetic region, which results in similar phase diagram for antiferromagnetic case, but with numerical values slightly different than the numerical values of the ferromagnetic case. After this very first transformation, the point continues to flow in the R > 0 region. The 3-d antiferromagnetic Ising critical point is found to be  $J_{I-AF}^{C} = -0.261065$ , while the antiferromagnetic isotropic Heisenberg critical point is  $J_{H-AF}^{C} = -0.282388$ . Critical points for antiferromagnetic case are also in the expected order of  $J_{H-AF}^{C} > J_{XY}^{C} > J_{I-AF}^{C}$ .

Below in Fig.9.3 we represent the spin- $\frac{1}{2}$  antiferromagnetic anisotropic Heisenberg model phase diagram joined with the ferromagnetic model. The negative  $J_{xy}$  region is not shown due to above mentioned mirror symmetry along  $J_z$ -axis (see Sec.3.2). Note that the single thin horizontal line of R = 0 is not a phase boundary but just separating the ferromagnetic and the antiferromagnetic regions of the model.



**Figure 9.3:** Phase diagram of antiferromagnetic XXZ model joined with the ferromagnetic one, plotted in the axes  $tanh(J_z)$  versus  $tanh(J_{xy})$ . Full and dashed lines represent second- and first-order phase transitions respectively. The  $J_{xy} < 0$  region is not shown (see text). The thin horizontal line of R = 0, which separates the ferromagnetic (FM) and antiferromagnetic (AFM) regions, is not a phase boundary.

#### **10. CONCLUSION**

A detailed global renormalization-group solution of the XXZ Heisenberg chain, for all temperatures and anisotropies, for both ferromagnetic and antiferromagnetic couplings, has been obtained. In the spin-liquid region, the linear low-temperature specific heat and, for the antiferromagnetic chain, the spin-wave dispersion relation exponent n and stiffness constant c have been obtained. In the Isinglike region, the spin-wave to spinon crossover of the excitation spectrum gap of the ferromagnetic chain has been obtained from the exponential specific heat. Purely quantum mechanical effects have been seen: We find that the xy correlations and the antiferromagnetic z correlations mutually reinforce each other, for a range of temperatures and anisotropies, in both the ferromagnetic and antiferromagnetic systems. The behaviors of the specific heat maximum values and locations with respect to anisotropy are opposite in the ferromagnetic and antiferromagnetic systems. The sharp contrast found in the specific heats of the isotropic ferromagnetic and antiferromagnetic systems is a harbinger of the different critical temperatures in the respective three-dimensional systems. When compared with existing calculations in the various regions of the global model, good quantitative agreement is seen. Even at zero temperature, where our approximation is at its worst, good quantitative agreement is seen with exact data points for the correlation functions (Fig.4.1(b)). The higher-dimensional analysis is also carried out, and the global phase diagram of the three-dimensional anisotropic quantum Heisenberg model is obtained with expeced critical temperature behaviors. Finally, the relative ease with which the Suzuki-Takano decimation procedure is globally and quantitatively implemented should be noted.

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