ISSN 0029-3865

CNPq

CBPF - CENTRO BRASILEIRO DE PESQUISAS FÍSICAS

Notas de Física

CBPF-NF-036/93

Phase Diagram of the Quantum Anisotropic Heisenberg Model on a Self-Dual Hierarchical Lattice

by

André M.C. de Souza

Rio de Janeiro
1993

Abstract

A good approximation for the phase diagram of the quantum anisotropic spin $\frac{1}{2}$ Heisenberg ferromagnet on a self-dual hierarchical latice is calculated within a real-space renormalization group framework . We extend the results to the antiferromagnetic case and show that T_c vanishes for values of the anisotropy parameter $\Delta \leq 0.399$, i.e, for small anisotropy the order is destroyed by quantum fluctuations at any <u>finite</u> temperature.

Key-words: Heisenberg model; Hierarchical lattice; Renormalization group; Criticality.

PACS numbers: 64.60.-i, 75.10.Jm, 75.30.Gw, 75.40.-s

In 1987 Anderson[1] proposed that the behavior of the high-temperature superconductivity might be described by the two-dimensional spin $\frac{1}{2}$ Heisenberg antiferromagnetic model (see ref. [2]). This suggestion increased the interest on this model which has been representing a challenge for more than 60 years. There is still a great controversy on the existence of Néel order and considerable effort has been done in order to solve this problem, unfortunatly without success. Rigorous results at temperature $T=0$ were summarized by Kubo and Kishi[3] for two- (three-) dimensions on the square (simple cubic) lattice, most of them based on a previous paper by Dyson, Lieb and Simon[4]. For the anisotropic spin $\frac{1}{2}$ Heisenberg on the square lattice, they proved that, for certain values of the anisotropy parameter(Δ), long-range order exists at temperature $T=0$.

Caride, Tsallis and Zanette[5] applied with success the real-space renormalization group(RG) approach to the study of the anisotropic spin $\frac{1}{2}$ Heisenberg ferromagnet model on a self-dual Wheatstone bridge hierarchical lattice[5,6]. Their results are either exact or very good approximations for the square lattice.

For classical and for some quantum systems(e.g, XY model), there is a unitary operator that automatically brings the ferromagnetic case into the antiferromagnetic one, but for the general quantum Heisenberg model no such symmetry exists.

In this paper we generalize the analysis of ref.[5,6] for the antiferromagnetic case. We have chosen the simplest hierarchical lattice that preserves (a) the symmetry of the ground state under the renormalization group operation, (b) the self-duality of square lattice and (c) the Hamiltonian form (i.e., there is no parameter proliferation). It is defined through the aggregation process (see ref. [7]) of clusters that can be seen in fig. 1a and has led good results for several models[7].

The dimensionless Hamiltonian is defined by

$$\mathcal{H} = -\beta H = \frac{4J}{k_B T} \sum_{<ij>} [(1-\Delta)(S_i^x S_j^x + S_i^y S_j^y) + S_i^z S_j^z], \tag{1}$$

where $\beta \equiv 1/k_B T$, $< ij >$ denotes first-neighboring lattice sites, Δ is the anisotropic parameter and the S_i^α $\{\alpha = x, y, z\}$ is the spin $\frac{1}{2}$ on the site i.

To obtain the RG recurrence equations we preserve the two-body correlation function[5, 6], by imposing

$$exp(\mathcal{H}_{12}' + C) = \mathop{\mathrm{Tr}}_{sites\ 3,4,5,6} exp(\mathcal{H}_{123456}) \tag{2}$$

where

$$\mathcal{H}_{123456} = 4K \sum_{<ij>} [(1-\Delta)(S_i^x S_j^x + S_i^y S_j^y) + S_i^z S_j^z] \tag{3}$$

is the Hamiltonian of the cluster under consideration (Fig. 1a); the sum runs over the nine bonds of the graph; $K \equiv J/k_B T$;

$$\mathcal{H}_{12}' = 4K'[(1-\Delta')(S_1^x S_2^x + S_1^y S_2^y) + S_1^z S_2^z] \tag{4}$$

denotes the Hamiltonian of the renormalized two-site cluster (Fig.1b) and C is an additive constant included to make equation (2) possible. The eq.

(2) establishes the relation between the set of parameters (K, Δ) and the set of renormalized parameters (K', Δ', C).

The Hamiltonian $\mathcal{H}_{123456}$ is not the total Hamiltonian, since the hierarchical lattice contains an infinite number of clusters. The eq. (2) neglects the noncommutativity between the Hamiltonians associated with neighboring clusters and therefore is an approximation for all temperatures, being asymptotically exact at high temperatures(see [6] and references therein).

To calculate the partial trace (2) we will diagonalize the 64x64 matrix associated with $\mathcal{H}_{123456}$. As we can see, the z-component of the total angular momentum always commutes with the Hamiltonian. Using the basis vectors eigenvectors of S^z(corresponding to the eigenvalues M) the matrix associated with $\mathcal{H}_{123456}$ can be presented in a block-diagonal structure where the largest block is a 20x20 (M=0) matrix.

Following the treatment of [5] we expand $exp(\mathcal{H}'_{12})$ as

$$exp(\mathcal{H}'_{12}) = a' + 4b'_{12}(S_1^x S_2^x + S_1^y S_2^y) + 4c'_{12} S_1^z S_2^z \qquad (5)$$

and, straightforwardly from eqs.(3) and (5), we obtain that

$$exp(4K') = \frac{(a' + c'_{12})^2}{(a' - c'_{12})^2 - 4(b'_{12})^2}$$

$$
\begin{aligned}
exp(4K'\Delta') &= \frac{a' - c_{12}' + 2b_{12}'}{a' - c_{12}' - 2b_{12}'} \\
exp(C) &= \frac{a' + c_{12}'}{exp(K')}.
\end{aligned}
\tag{6}
$$

Analogously,

$$
\begin{aligned}
exp(\mathcal{H}_{123456}) &= a + 4\sum_{(i<j)}[b_{ij}(S_i^xS_j^x + S_i^yS_j^y) + c_{ij}S_i^zS_j^z] \\
&+ 16 \sum_{(i<j)\neq(k<l)} [d_{ij,kl}(S_i^xS_j^x + S_i^yS_j^y)S_k^zS_l^z \\
&+ e_{ij,kl} (S_i^xS_j^x + S_i^yS_j^y)(S_k^xS_l^x + S_k^yS_l^y) + f_{ij,kl}S_i^zS_j^zS_k^zS_l^z] \\
&+ 64 \sum_{(i<j)\neq(k<l)\neq(m<n)} [g_{ij,kl,mn}(S_i^xS_j^x + S_i^yS_j^y)S_k^zS_l^zS_m^zS_n^z \\
&+ q_{ij,kl,mn} (S_i^xS_j^x + S_i^yS_j^y)(S_k^xS_l^x + S_k^yS_l^y)(S_m^xS_n^x + S_m^yS_n^y)] \\
&+ 64\, r\, S_1^zS_2^zS_3^zS_4^zS_5^zS_6^z
\end{aligned}
\tag{7}
$$

where $a, b_{ij}, c_{ij}, d_{ij,kl}, \ldots$ are functions of K and Δ, which can be determined diagonalizing $\mathcal{H}_{123456}$ which was done numerically. From equation (2),(5) and (7), it follows that

$$
\begin{aligned}
a' &= 16\, a \\
b_{12}' &= 16\, b_{12} \\
c_{12}' &= 16\, c_{12}
\end{aligned}
\tag{8}
$$

which determine the set of parameters (K', Δ', C) as functions of (K, Δ)

and consequently the phase diagram.

In Fig. 2a we present the phase diagram in the $(k_BT/J, \Delta)$ space for $k_BT/J > 0$, i.e., the ferromagnetic case. We verify the existence of two phases, namely, a paramagnetic(P) and a ferromagnetic(F) one, respectively, characterized, by fully stable fixed points $(k_BT/J, \Delta)$ at: $(\infty,1)$ -(P) and (0,1) -(F). This case was treated by [5,6] on the Wheatstone bridge hierarchical lattice, and those results agree very well with ours.

In the antiferromagnetic case($k_BT/J < 0$), presented in Fig. 2b, we verify the existence of two phases, namely, a paramagnetic(P) and an antiferromagnetic(AF) one, respectively, characterized, by the fully stable fixed points: $(-\infty,1)$ -(P) and (0,1) -(AF). For very low temperatures, extremely accurate results become difficult because of numerical errors, but from Fig. 2b our results strongly support the existence of an ordered phase for $\Delta > \Delta_c \approx 0.399$. Indeed, in [8] it is proved the existence of a long-range order in the ground state for $\Delta > 0.40$ (the equivalence of the anisotropic parameter of ref. [8] ($\Delta^{(8)}$) with the present Δ is given by $\Delta = 1 - \frac{1}{\Delta^{(8)}}$). However, their numerical analysis show the existence of long-range order for $\Delta > 0.09$. In our case, we find the non existence of the ordered phase for $0 \leq \Delta \leq \Delta_c$ at finite T, but in $T = 0$ we cannot conclude anything.

In the region $0.375 < \Delta \leq \Delta_c$, we observe a re-entrance effect, where there is an ordered phase at relatively high temperature but not at very low temperature. This result is not so frequent in the literature and suggests that there might be phase transitions not accompanied by long-range order.

The $\Delta = 0$ and $\Delta = 1$ axes, correspond to isotropic Heisenberg and Ising models, respectively. They are renormalized into themselves, and contains semi-stable critical fixed points, at (0,0) and ($\pm$ 2.269,1). The signal +(-) correspond to the case when J is positive(negative), i.e., for ferromagnetic (antiferromanetic) case. All these fixed points are the exact answers for the square lattice.

The criticality of the ferromagnetic case is Ising like for $0 < \Delta \leq 1$. The same is not true for the antiferromagnetic case; indeed, for small anisotropies ($\Delta \leq \Delta_c$) the ordering is destroyed by quantum fluctuations of the XY part of the Hamiltonian[3,9-11].

As a final comment, it would be important to extend the procedure for spins $S > \frac{1}{2}$ and to compare the behavior for integer and half-integer spins, verifing (or not) the Haldane's conjecture[12] who obtained a qualitative difference between those two types of systems. We will report calculations along these lines elsewhere.

I thank C.Tsallis, F.Tamarit and J.A.Redinz for stimulating discussions, encouragement and critical reading of the manuscript, as well as financial support from CAPES (Brazilian agency).

Caption for figures and tables

Figure 1: Renormalization group transformation associated with the self-dual cell. • and o are internal and terminal sites,respectively. (a) Cluster that generates, through infinite iterations, the self-dual hierarchical lattice under consideration. (b) Two-site cluster.

Figure 2: Phase diagram. Full curves correspond to critical frontiers. ■, • and o respectively, denote, the fully stable, fully unstable and semi-stable fixed points. AF,F and P respectively correspond to antiferromagnetic, ferromagnetic and paramagnetic regions.

(a) Ferromagnetic case ($J > 0$). (b) Antiferromagnetic case ($J < 0$).

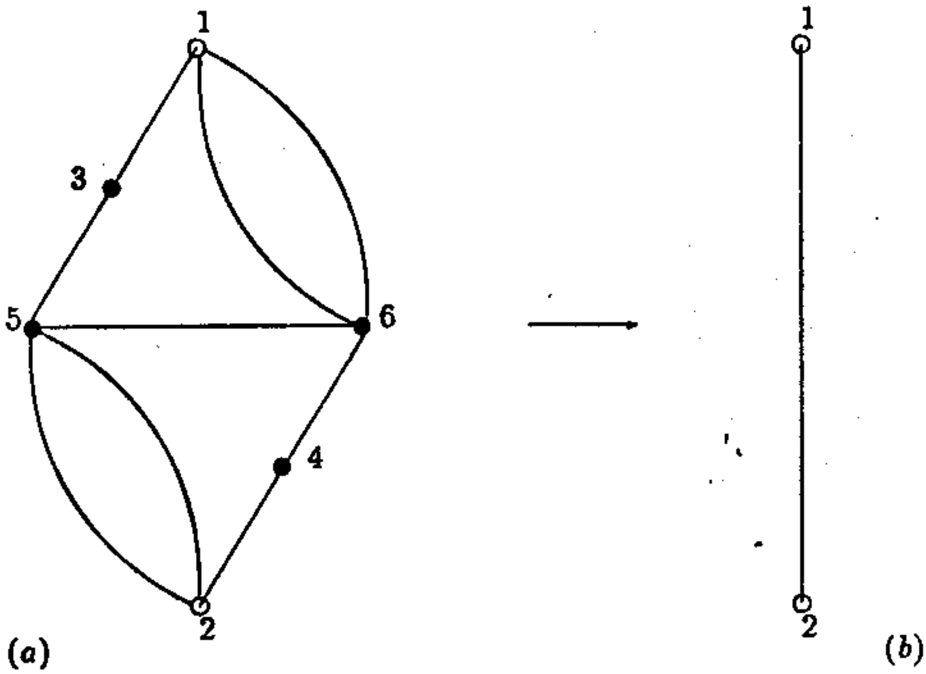

Figure 1

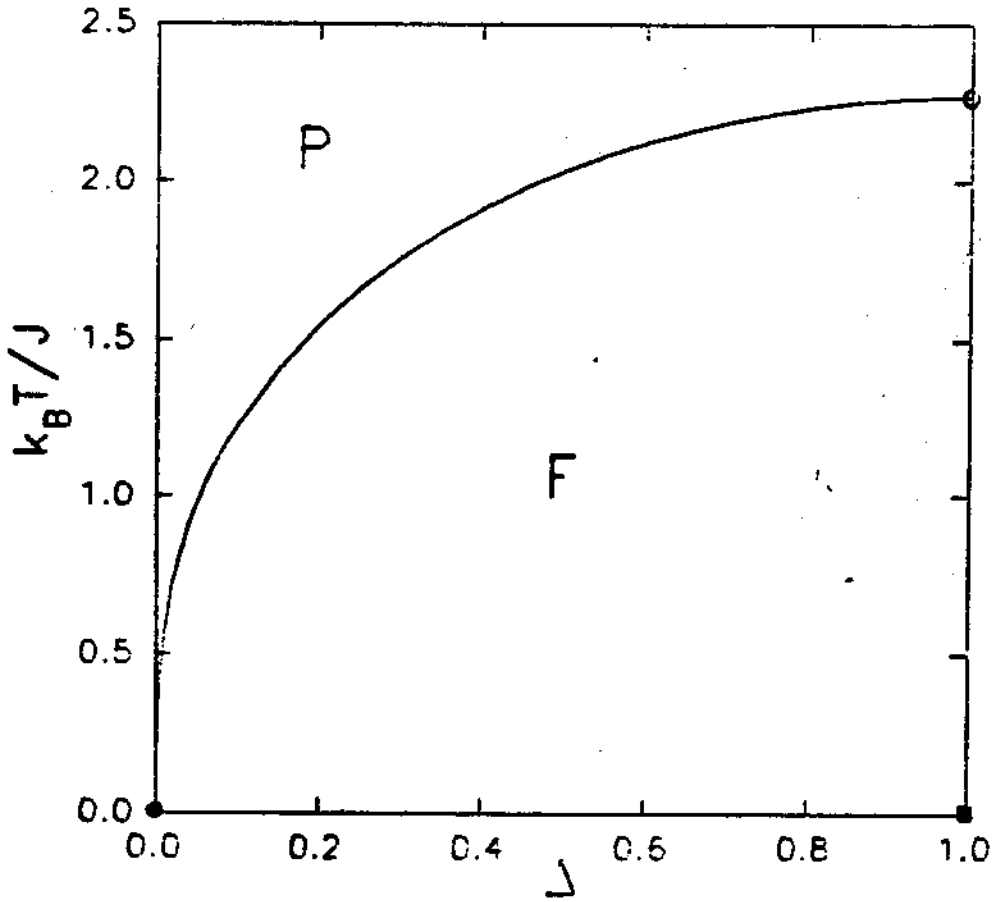

Figure 2(a)

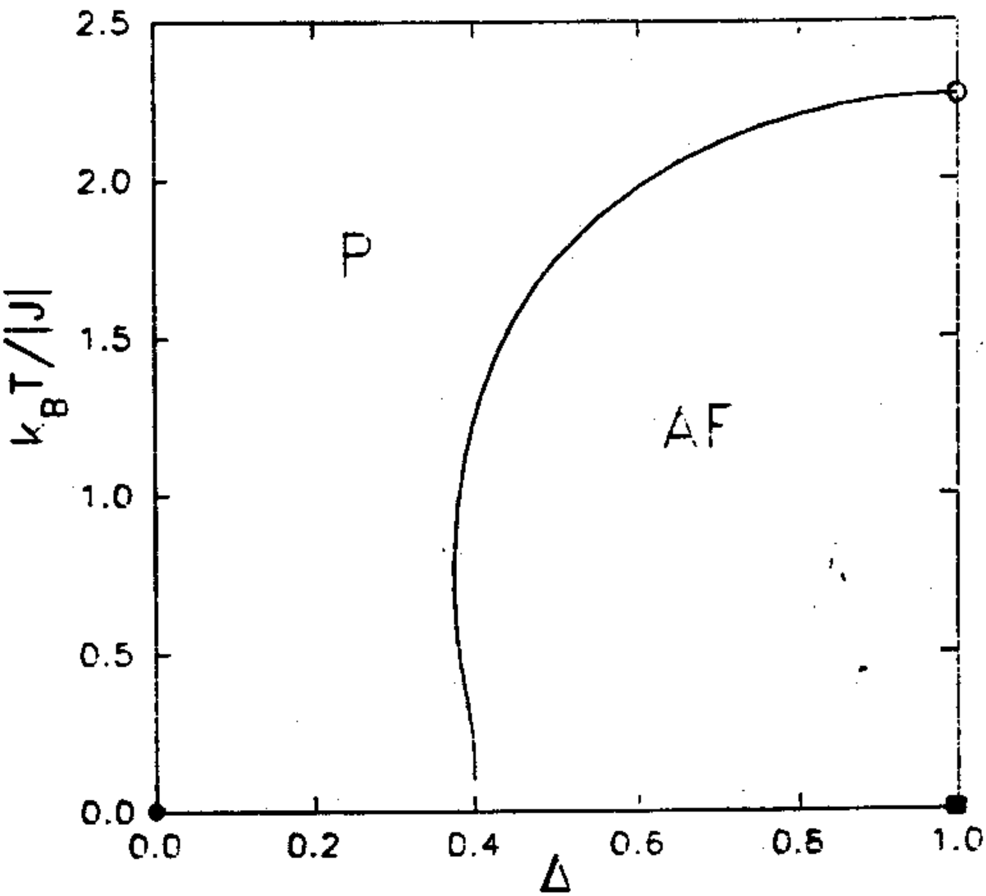

Figure 2(b)

References

[1] P. W. Anderson, Science 235,1196(1987)

[2] E. Manousakis, Rev.Mod.Phys. 63,1(1991)

[3] K. Kubo and T. Kishi,Phys.Rev.Lett. 61,2585(1988)

[4] F. J. Dyson,E. H. Lieb and B. Simon, J.Stat.Phys. 18,335(1978)

[5] A. O. Caride,C. Tsallis and S. I. Zanette, Phys.Rev.Lett. 51,145(1983)

[6] A. M. Mariz,C. Tsallis and A. O. Caride, J.Phys. C 18,4189(1985)

[7] E. P. da Silva,A. M. Mariz and C. Tsallis, J.Phys. A 24,2835(1991);
P. M. C. de Oliveira and C. Tsallis, J.Phys. A 15,2865(1982)

[8] H. Nishimori and Y. Ozeki, J. Phys. Soc. Jpn. 58,1027(1989)

[9] D. W. Robinson, Commun.Math.Phys. 14,195(1969);
J. Ginibre, Commun.Math.Phys. 14,205(1969)

[10] J. Fröhlich and E. H. Lieb, Phys.Rev.Lett. 38,440(1977)

[11] T. Kennedy,E. H. Lieb and B. S. Shastry, J.Stat.Phys. 53,1019(1988)

[12] F. D. M. Haldane, Phys.Rev.Lett. 50,1153(1983)