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CRITICALITY OF THE ANISOTROPIC QUANTUM HEISENBERG MODEL ON A SIMPLE CUBIC LATTICE

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ABSTRACT

Within a Real Space renormalization group framework, we study the criticality (phase diagram, and critical thermal and crossover exponents) of the spin 1/2 - anisotropic quantum Heisenberg ferromagnet on a simple cubic lattice is studied. The results obtained are in satisfactory agreement with known results whenever available. (Author)

Key-words: Heisenberg model; Cubic lattice; Anisotropy; Criticality

Over the last years, many attempts have been made to generalize the Real-Space Renormalization Group approach [1] to quantum spin systems such as Heisenberg, XY and Transverse Ising models (for a partial list of references, see Pfeuty et al [2]). In particular, one is interested in the effects generated by the non-commutation aspects of the Hamiltonian. Along these lines, several results have been obtained [3-9] for quantum Heisenberg and XY models within a Migdal-Kadanoff approximation [10].

The purpose of this letter is to present the results obtained for the criticality of the spin 1/2 - anisotropic quantum Heisenberg model on a simple cubic lattice within a new Real-Space Renormalization Group framework [11,12].

We consider the following ferromagnetic (dimensionless) Hamiltonian:

$$\mathcal{H} = \sum_{<ij>} K\left[(1+\Delta)\sigma_i^z\sigma_j^z + (1-\Delta)(\sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y)\right] \qquad (1)$$

where $K=J/k_BT$ (J is the exchange coupling) is the same for all bonds, the σ's are Pauli spin operators, $<ij>$ denotes first - neighbouring sites on a simple cubic lattice, and the anisotropy parameter Δ is restricted to the interval $[-1,1]$. We note that for some special values of Δ we recover well-known models, namely the Ising ($\Delta=1$), the isotropic

Heisenberg ($\Delta=0$) and the XY ($\Delta=-1$) ones.

Within the block-spin approximation for the simple cubic lattice, we use the hierarchical lattice generated by the two-terminal graphs [13] in Fig.1. The b=2 cluster in Fig.1a is renormalized into the b=1 cluster in Fig. 1b (the linear scaling factor is s=2) by performing a partial trace on the internal sites, in such a way that the partition function is preserved, i.e.,

$$e^{\mathcal{H}'_{12}} = \mathrm{Tr}_{3,4,5,6}\, e^{\mathcal{H}_{123456}} \tag{2}$$

where

$$\mathcal{H}'_{12} = K'_0 + K'\left[(1+\Delta')\sigma_1^z\sigma_2^z + (1-\Delta')(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y)\right] \tag{3}$$

where K'_0 is a normalization constant and

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

where the sum runs over the twelve bonds of the graph in Fig. 1.a.

The evaluation of the trace in Eq. (2) is carried out through a procedure previously developed [11,12].

We start off expanding the density matrices as follows:

$$e^{\mathcal{H}'_{12}} = \varepsilon' + b'_{12}(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y) + c'_{12}\sigma_1^z\sigma_2^z \tag{5}$$

and

$$e^{\mathcal{H}_{12?456}} = a + \sum_{i<j} \left[b_{ij} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) + c_{ij} \sigma_i^z \sigma_j^z \right] +$$

$$+ \sum_{(i<j),(k<\ell)} \left[d_{(ij)(k\ell)} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) \sigma_k^z \sigma_\ell^z + e_{(ij)(k\ell)} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) \right.$$

$$\left. (\sigma_k^x \sigma_\ell^x + \sigma_k^y \sigma_\ell^y) + f_{(ij)(k\ell)} \sigma_i^z \sigma_j^z \sigma_k^z \sigma_\ell^z \right] +$$

$$+ \sum_{(i<j)(k<\ell)(m<n)} \left[g_{(ij)(k\ell)(mn)} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y)(\sigma_k^x \sigma_\ell^x + \sigma_k^y \sigma_\ell^y) \sigma_m^z \sigma_n^z + \right.$$

$$+ h_{(ij)(k\ell)(mn)} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) \sigma_k^z \sigma_\ell^z \sigma_m^z \sigma_n^z + q_{(ij)(k\ell)(mn)} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y)$$

$$\left. (\sigma_k^x \sigma_\ell^x + \sigma_k^y \sigma_\ell^y)(\sigma_m^x \sigma_n^x + \sigma_m^y \sigma_n^y) + r_{(ij)(k\ell)(mn)} \sigma_i^z \sigma_j^z \sigma_k^z \sigma_\ell^z \sigma_m^z \sigma_n^z \right] \quad (6)$$

where the sum runs over all sites of the graph in Fig.1.a, and $(i,j) \neq (k,\ell) \neq (m,n)$.

The parameters K_0', K' and A' can be determined analytically [11,12] as functions of a', b_{12}' and c_{12}'. The trace of Eq.(6) yields $a'=16a$, $b_{12}'=16b_{12}$ and $c_{12}'=16c_{12}$; the remaining terms vanish since they always involve a term in σ_i^α, $i \neq 1,2$. Finally, the coefficients a, b_{12} and c_{12} are determined numerically as functions of K and A. In this way we obtain the recursion relations $K_0'(K,A)$, $K'(K,A)$ and $A'(K,A)$.

The following remarks about these recursion relations are in order. First, they are independent of the basis used to manipulate Eq. (6). Secondly, they are exact at the cluster level, although the cluster approximation involves neglecting non-commutation aspects between clusters. This approximation, however, is not too drastic, as pointed out by Takano and Suzuki [7].

Solving the recursion relations for fixed points (Δ^*, K^*) and eigenvalues (λ_i) we get the results displayed in Table 1, where

$$\nu_i = \frac{\ln s}{\ln \lambda_i} \quad (i=T,\Delta)$$

where λ_i are relevant eigenvalues ($\lambda_i>1$); T and Δ respectively correspond to the thermal and anisotropy correlation length critical exponents. For the sake of comparison, we also quote the results obtained from the Migdal-Kadanoff (MK) approximation [7] and from series expansions [14-17].

From Table 1 we see that the present approach somewhat overestimates the critical temperatures which are underestimated in the MK approximation [7]. The fact that the XY model ($\Delta=-1$) does not renormalize into itself (as a consequence of $\sigma^z\sigma^z$ terms being generated by products of $(\sigma^x\sigma^x + \sigma^y\sigma^y)$ in Eq. (6)) is reflected in a residual Ising interaction ($\Delta^*\neq-1$) in the XY fixed point; this feature is also present in the MK

approximation [7]. The XY critical coupling (quoted in brackets in Table 1) is obtained as the intersection of the critical curve with the line $\Delta=-1$.

The estimates we get for the correlation length exponent ν_T represent a systematic improvement over those obtained through the MK approximation [7]. In particular, arbitrarily close to the Heisenberg fixed point the critical curve is given by

$$T_c(\Delta) = T_c(0) + A_\pm |\Delta|^{1/\phi} \quad ; \quad |\Delta| \ll 1$$

where $A_\pm$ are constants respectively corresponding to $\Delta \to \pm 0$, and $\phi = \nu_T/\nu_\Delta = 1.27$ is the crossover exponent.

In Fig.2 we show the critical line, obtained as the (unique) RG trajectory linking the three non-trivial fixed points. The Heisenberg fixed point is unstable for both thermal and anisotropy perturbations whereas the Ising and XY fixed points are unstable only for thermal perturbations, as one would expect from symmetry arguments (which lead to universality). The fact that the low temperature XY region ($\Delta<0$) is driven towards the zero temperature Heisenberg fixed point under iteration of the RG is spurious and can be attributed to the different ground state properties of the clusters in Fig.1 when the interaction is predominantly XY in character. As pointed out by Castellani et al [8] (in the context of the MK approximation),

for $\Delta<0$ the zero temperature limit of the right hand-side of an equation similar to Eq.(2) yields a 3-fold degenerate ground state whereas the two-site cluster has a single ground state.

In summary the finite-temperature critical behaviour of the quantum anisotropic Heisenberg model is well described by the present approach: the critical exponents improve on those obtained within the MK approximation, and the entire para-ferro critical line can be given with reasonable quantitative confidence (the error being of roughly 20%).

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TABLE CAPTION

Table 1 - Results for fixed points $(\frac{k_B T^*}{J}, \Delta^*)$, critical expoents ν_T (correlation length exponent) and ϕ (crossover exponent) from the present calculations; for comparison we also quote Migdal-Kadanoff [7] and series results [14,17]. The XY critical coupling (quoted in square brackets) is obtained as the intersection of the critical curve with the line $\Delta=-1$.

TABLE 1

		MK[7]	PRESENT	SERIES
Ising	$(\Delta^*, \frac{k_B T_C^*}{J})$	(1,7.66)	(1,10.91)	(1,9.09) (14)
	ν_T	1.06	0.87	0.63 (14)
Isotropic Heisenberg	$(\Delta^*, \frac{k_B T_C^*}{J})$	(0,2.91)	(0,4.18)	(0,3.33) (15)
	ν_T	1.39	1.17	0.72 (15)
	$\phi = \frac{\nu_T}{\nu_z}$	1.56	1.27	1.25 (16)
XY	$(\Delta^*, \frac{k_B T_C^*}{J})$	(-0.88,6.80) [(-1,7.26)]	(-0.65,7.68) [(-1,9.44)]	(-1,8.00) (17)
	ν_T	1.16	1.09	0.67 (17)

FIGURE CAPTIONS

Figure 1 - The two-terminal (indicated by O) graphs. The b=2 cluster (a) is renormalized into a b=1 cluster (b) by summing out internal spins (indicated by ●) 3,4,5 and 6.

Figure 2 - Critical curves (phase diagram) for the anisotropic quantum Heisenberg model on a simple cubic lattice in the $(k_BT/J, \Delta)$ space. The non-trivial Ising (I), isotropic Heisenberg (H) and XY fixed points are shown (● ■ and O respectively denote semi-stable, stable and fully unstable fixed points). P and F respectively denote the para - and ferromagnetic phases.

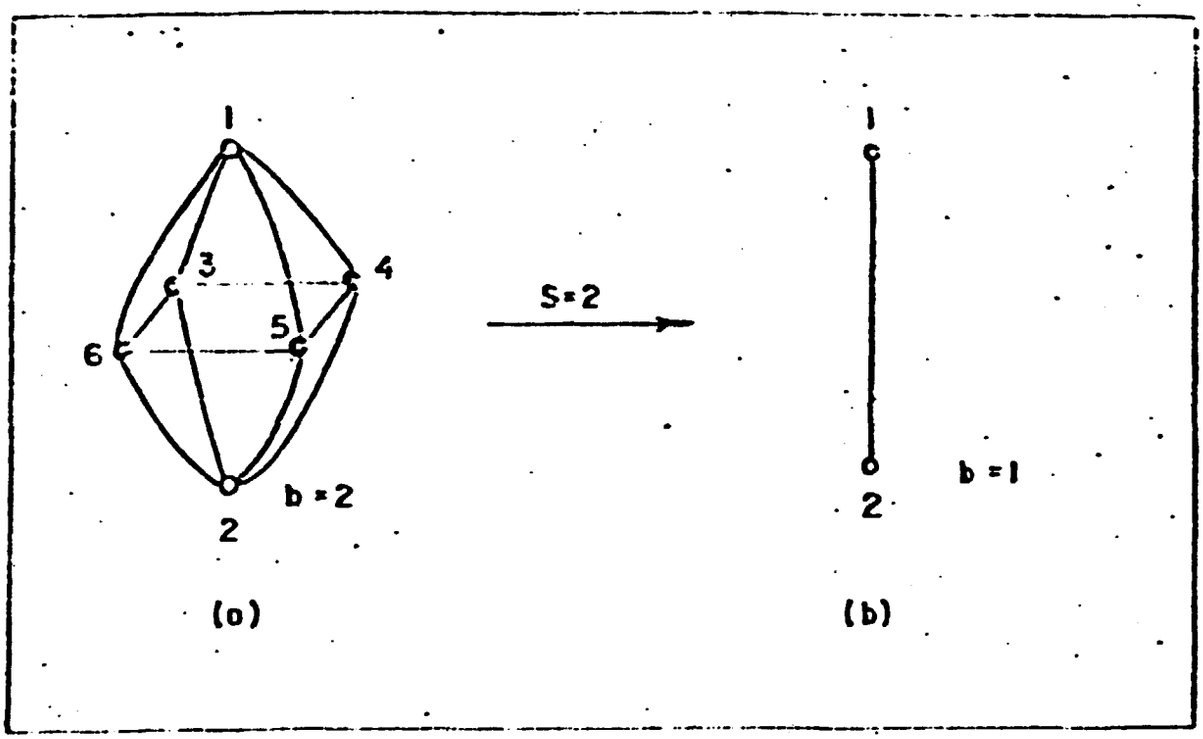

FIGURE 1

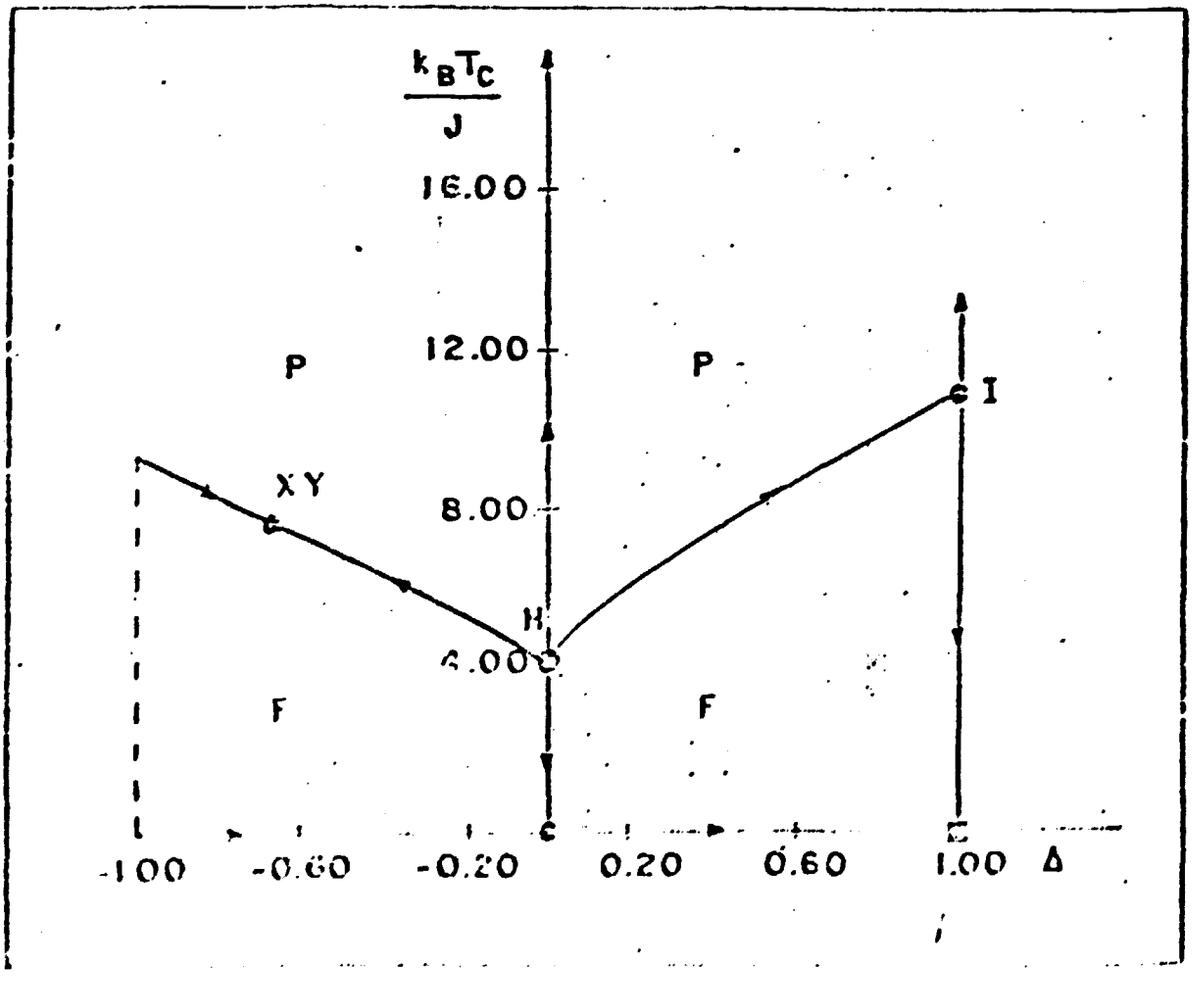

FIGURE 2