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1984 J. Phys. A: Math. Gen. 17 L697

(http://iopscience.iop.org/0305-4470/17/13/004)

J. Phys. A: Math. Gen. 17 (1984) L697–L702. Printed in Great Britain

LETTER TO THE EDITOR

Quantum spin systems: dynamical mean field renormalisation group approach

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Received 19 June 1984

Abstract. The mean field renormalisation group approach is applied to the study of the static and dynamical critical properties of the spin-$\frac{1}{2}$ anisotropic Heisenberg model in a transverse field. The critical surface and estimates of static and dynamical critical exponents are obtained for the one-, two-, and three-dimensional models.

In this letter we treat the spin-$\frac{1}{2}$ anisotropic Heisenberg model in a transverse field. The Hamiltonian can be defined as

$$H=-J\sum_{(i,j)}[\sigma_i^z\sigma_j^z+\eta(\sigma_i^x\sigma_j^x+\sigma_i^y\sigma_j^y)]-\Omega\sum_i\sigma_i^x, \tag{1}$$

where η ranges from 0 (Ising limit) to 1 (isotropic Heisenberg limit), J is the nearest-neighbour exchange interaction, Ω is the transverse field, and σ's are Pauli spin matrices. The sums run over spins on a d-dimensional lattice.

In the Ising limit the Hamiltonian (1) reduces to that of the transverse Ising model. In one-dimension Pfeuty (1970) has exactly shown that this model exhibits a long-range order at zero temperature for Ω less than a critical value Ω_c. Series expansions results in higher dimensions (Elliott and Wood 1971, Pfeuty and Elliott 1971, Yanase 1977) have shown that the effect of the transverse field is simply to shift the critical temperature without altering the critical exponents (provided the critical temperature remains non-zero). For transitions at zero temperature it has been proved that the critical behaviour of the d-dimensional transverse Ising model corresponds to that of the $(d+1)$-dimensional Ising model with $\Omega=0$ (Young 1975, Hertz 1976, Suzuki 1976). It is also known that the dynamical exponent z for the critical slowing down of the transverse Ising model at zero temperature is equal to 1 (Young 1975, Hertz 1976).

At zero transverse field the model (1) reduces to the anisotropic Heisenberg model. This system has been recently treated by using a real space renormalisation group transformation (Suzuki and Takano 1979, Stinchcombe 1981, Caride *et al* 1983). It has been shown that the critical temperature T_c of the ferromagnetic transition decreases as a function of the anisotropy. In particular, in the isotropic Heisenberg limit T_c vanishes for the two-dimensional model, while for the three-dimensional model T_c remains finite. It has also been proved that the vanishing of T_c for the two-dimensional isotropic Heisenberg model is an exact result (Mermin and Wagner 1966).

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In order to study the dynamical critical properties of the model (1) we employ the mean field renormalisation group (MFRG) method. This method has been proposed by Indekeu *et al* (1982) for computing critical properties of lattice spin systems. It is based upon a comparison of the behaviour of clusters of different sizes in the presence of symmetry breaking boundary conditions (mean field) which simulate the effect of the surrounding spins in the infinite system. The MFRG has been successfully applied to the study of the static critical properties of ordered (Indekeu *et al* 1982, Slotte 1984) and disordered (Droz *et al* 1982, Plascak 1984a) spin models and geometric phase transitions (De'Bell 1983). More recently, the MFRG has been applied to the study of the dynamical critical properties of classical kinetic Ising models (Indekeu *et al* 1984). In the present letter we extend the MFRG to the study of the dynamical critical properties of quantum spin systems.

We consider herein one- and two-spin clusters respectively, and we follow closely the procedure suggested by Indekeu *et al* (1982, 1984). In the one-spin cluster the single spin $\boldsymbol{\sigma}_1$ interacts with its c nearest neighbours, where c is the coordination number of the lattice. The z-component of these boundary spins is fixed to a time-dependent 'effective magnetisation' $b_1(t)$. While mean field theory identifies $b_1(t)$ with the z-component of the average magnetisation $m_1(t)=\langle\sigma^\alpha\rangle(t)$, the MFRG assumes that the effective magnetisation 'scales' in the same way. Since in the scaling regime the magnetisation is infinitesimal, $b_1(t)$ is assumed to be very small. The Hamiltonian of the one-spin cluster then reads

$$H_1=-\Omega\sigma_1^x-cJb_1(t)\sigma_1^z. \tag{2}$$

In the linear response theory (see, for example, Kubo 1957) the Fourier transform of the average magnetisation in the z direction, $m_1(t)$, is given by

$$m_1(K,\alpha,\omega)=\chi_1^{zz}(K,\alpha,\omega)b_1(\omega), \tag{3}$$

where χ_1^{zz} is the dynamical longitudinal susceptibility of the single spin in a transverse field and the variables are defined by $\alpha=\Omega/J$ and $K=J/k_BT$. For this one-spin cluster χ_1^{zz} is easily evaluated, giving

$$\chi_1^{zz}(K,\alpha,\omega)=\frac{c\tanh K\alpha}{\alpha}\left(1+\frac{\omega^2}{4\Omega^2-\omega^2}\right). \tag{4}$$

In the two-spin cluster, $\boldsymbol{\sigma}_1$ interacts directly with $\boldsymbol{\sigma}_2$ and both $\boldsymbol{\sigma}_1$ and $\boldsymbol{\sigma}_2$ interact with their $(c-1)$ nearest neighbours fixed to a time-dependent effective magnetisation $b_2(t)$. The Hamiltonian then reads

$$H_2=-J[\sigma_1^z\sigma_2^z+\eta(\sigma_1^x\sigma_2^x+\sigma_1^y\sigma_2^y)]-\Omega(\sigma_1^x+\sigma_2^x)-(c-1)Jb_2(t)(\sigma_1^z+\sigma_2^z). \tag{5}$$

Similarly, in the linear response theory the Fourier transform of the average magnetisation in the z direction, $m_2(t)=\frac{1}{2}\langle\sigma_1^z+\sigma_2^z\rangle(t)$, is given by

$$m_2(K,\alpha,\eta,\omega)=\chi_2^{zz}(K,\alpha,\eta,\omega)b_2(\omega). \tag{6}$$

Diagonalisation of the time-independent part of the Hamiltonian (5) is simple. Without entering into the details of the calculation we give below just the final expression for the dynamical susceptibility of H_2:

$$\chi_2^{zz}(K, \alpha, \eta, \omega) = 2(c-1) \times\left[A\left(1+\frac{\omega^2}{[J(\lambda_1-\lambda_4)]^2-\omega^2}\right)+B\left(1+\frac{\omega^2}{[J(\lambda_2-\lambda_4)]^2-\omega^2}\right)\right], \tag{7}$$

where

$$\begin{aligned} &A = 4a^2(e^{-K\lambda_4}-e^{-K\lambda_1})/(\lambda_1-\lambda_4)\Delta, \\ &B = 4b^2(e^{-K\lambda_2}-e^{-K\lambda_4})/(\lambda_4-\lambda_2)\Delta, \\ &\begin{Bmatrix} a \\ b \end{Bmatrix} = \left\{\frac{\alpha^2}{R[R\pm(1-\eta)]}\right\}^{1/2}, \\ &R = [4\alpha^2+(1-\eta)^2]^{1/2}, \\ &\lambda_1 = -\eta+R, \qquad \lambda_2 = -\eta-R, \qquad \lambda_3 = 1+2\eta, \qquad \lambda_4 = -1, \\ &\Delta = \sum_{i=1}^{4} e^{-K\lambda_i}. \end{aligned} \tag{8}$$

We impose now a scaling relation of the form

$$m_2(K, \alpha, \eta, \omega) = L^{-d+y_H+z} m_1(K', \omega', L^z\omega) \tag{9}$$

between such approximate magnetisations, where $L = 2^{1/d}$ is the rescaling factor, y_H is the static magnetic exponent, z is the dynamical exponent, and $\omega \to 0$ (long-time regime). Assuming now that the effective magnetisations scale in the same way, i.e.

$$b_2(\omega) = L^{-d+y_H+z} b_1(L^z\omega), \tag{10}$$

one obtains

$$\chi_2^{zz}(K, \alpha, \eta, \omega) = \chi_1^{zz}(K', \alpha', L^z\omega), \tag{11}$$

which is independent of the rescaling factor L^{-d+y_H+z}. From equations (4), (7), (10), and (11) one has, in the limit $\omega \to 0$,

$$c(\tanh K'\alpha')/\alpha' = 2(c-1)(A+B), \tag{12}$$

which gives the static critical properties, and

$$L^{2z} = \frac{4\alpha^2}{A+B}\left(\frac{A}{(\lambda_1-\lambda_4)^2}+\frac{B}{(\lambda_4-\lambda_2)^2}\right)\Bigg|_{FP}. \tag{13}$$

Equation (12) can be viewed as a renormalisation recursion relation among the parameters of the Hamiltonian (1). It is clear that one cannot determine the full renormalisation flow diagram in the K, α, η space from this equation alone. Interestingly, however, the fixed point solution of (12) gives exactly the same critical surface as that obtained by using a variational approach for the free energy (Plascak 1984b). Such equivalence between MFRG using one- and two-spin clusters and the variational approach for the free energy in the pair approximation has already been reported for the diluted transverse Ising model (Plascak 1984a). Equation (12) can also be used to estimate static critical exponents associated with some invariant sets in the K, α, η space. This is done by computing

$$[\partial\mu'/\partial\mu]_{FP} = L^{y_\mu}, \tag{14}$$

where μ can be K or α (note that η does not appear in the one-spin cluster calculations) and the derivative is taken at the fixed point of the invariant set considered. Similarly, the dynamical exponent z, at criticality, is obtained from equation (13). It is interesting to note that, in the zero temperature limit, (13) reduces to

$$L^z = 2\alpha/(\lambda_1 - \lambda_4)|_{\mathrm{FP}} = G_1/G_2|_{\mathrm{FP}}, \tag{15}$$

where G_i is the energy gap of the cluster i. This is a well known result (Hertz 1976). It is also worthwhile to mention that the z exponent obtained from (15) is independent of the anisotropy. We summarise below the results for the one-, two-, and three-dimensional models.

For the one-dimensional model ($c = 2$) equation (12) presents only zero temperature fixed points solutions, as expected. In the Ising limit ($\eta = 0$) one has

$$\alpha' = R(R-1)/(R+1), \qquad R = (1+4\alpha^2)^{1/2}, \tag{16}$$

which is the same renormalisation recursion relation as that given by the SLAC method (Jullien *et al* 1978, Jullien 1981). The present MFRG approach is then, in the Ising limit, identical to the SLAC method for $d = 1$, when in the latter one considers two-spin cell.

For finite values of η, it is noted that α_c decreases to zero as $\eta \to 1$ while the critical exponents y_α ($=0.68$) and z ($=0.55$) are independent of the anisotropy.

For the two-dimensional model we consider the square lattice, i.e. $c = 4$. For completeness, we reproduce in figure 1 the critical temperature as a function of α for various values of η, as obtained from equation (12), for the two-dimensional model. The critical temperature decreases as a function of α. At $\eta = 0$ one has $\mathrm{d}T_c/\mathrm{d}\alpha \to \infty$ as $\alpha \to \alpha_c$, in agreement with series expansions results. For intermediate values of η the system remains long-range ordered at $T = 0$ for $\alpha < \alpha_c$ but, $\mathrm{d}T_c/\mathrm{d}\alpha$ is finite as $\alpha \to \alpha_c$. Close to the isotropic Heisenberg limit the long-range order can be broken at finite low temperatures producing a kind of re-entrant phenomena. For further details on the critical surface see Plascak (1984b).

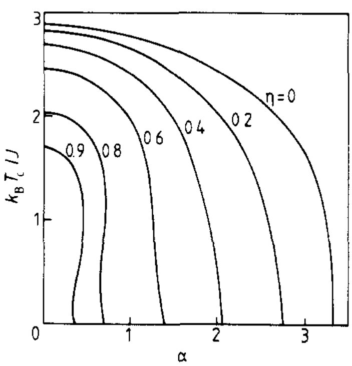

Figure 1. Critical temperature $k_B T_c/J$ as a function of $\alpha = \Omega/J$ for various values of the anisotropy η for the two-dimensional model.

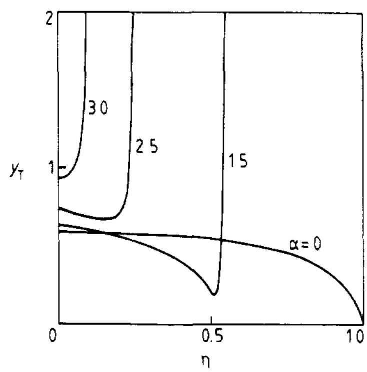

Figure 2. Critical exponent y_T as a function of the anisotropy for various values of α for the two-dimensional model.

At zero transverse field this model has been recently studied by using the MFRG approach (Plascak 1984c). It is noted that the critical temperature T_c and the critical exponent y_T decrease as a function of the anisotropy. In the isotropic Heisenberg limit, the exact results $T_c = 0$ (Mermin and Wagner 1966) and $y_T = 0$ (Polyakov 1975) are reproduced even by considering the present simple choice for the clusters. The crossover from Ising to isotropic Heisenberg behaviour is given through a continuous variation of y_T as a function of η, while the crossover should actually occur all at the isotropic Heisenberg point. This continuous variation of y_T with η is due to having only one recursion relation for the parameters of the system. Figure 2 shows the critical exponent y_T as a function of the anisotropy for various values of α.

Figure 3 shows the critical exponent y_α as a function of α for various values of η. As can be seen from this figure, the crossover from finite temperature to zero temperature behaviour still remains and it is more pronounced as $\eta \to 1$. At $T=0$, the critical exponent y_α ($=0.70$) is independent of the anisotropy. The inset shows y_α as a function of η at zero transverse field. Another crossover driven by the anisotropy is also apparent in this case. In the isotropic Heisenberg limit one has $y_\alpha = 2$ at $\alpha = 0$.

The results of the dynamical exponent z for the critical slowing down are shown in figure 4. Again, at $T=0$, z ($=0.43$) is independent of the anisotropy. It is interesting

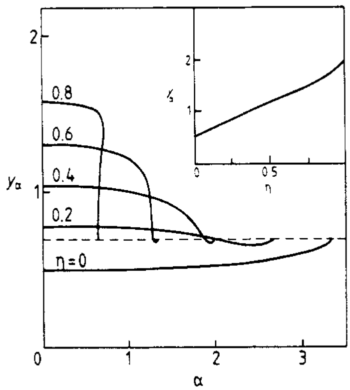

Figure 3. Critical exponent y_α as a function of α for various values of the anisotropy for the two-dimensional model. The broken line represents the results at $T=0$. The inset shows the critical exponent y_α as a function of the anisotropy at $\alpha = 0$.

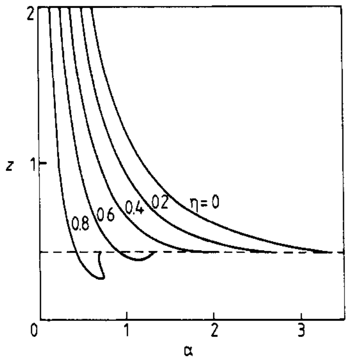

Figure 4. Dynamical exponent z as a function of α for various values of the anisotropy for the two-dimensional model. The broken line represents the results at $T=0$.

to note the crossover from zero temperature to finite temperature behaviour. In this case $z \to \infty$ as $\alpha \to 0$ for any value of η.

The critical points and estimates of critical exponents obtained from the present calculations at $T=0$ are shown in table 1 in comparison with exact (if available) or other approximated results. For the two-dimensional model, the critical transverse field and the exponent s are in good agreement with series expansions results. On the other hand, the values of the exponents y_α and z are poorer, even when compared with the SLAC approximation. It is, however, worthwhile to mention that the SLAC method for $d=2$ considers cell of four spins, while in the present MFRG we consider a two-spin cluster.

Finally, the present approach is easily extended to the three-dimensional model ($c=6$). Similar results as shown in figures 1–4 are obtained in this case. Numerical values for the critical transverse field and estimates of critical exponents at $T=0$ are presented in table 1 in comparison with series expansions results.

As a final remark, we mention that the unexpected behaviour of the critical exponents as shown in figures 2–4 (mainly for $\eta \leqslant 1$ and $\alpha \leqslant \alpha_c$) is related to the particular re-entrant phenomena observed at low temperatures. Although quite good results are obtained in the zero transverse field limit or in the Ising limit (even in the

Table 1. Critical points and critical exponents obtained from the present method at $T=0$ in comparison with exact (if available) and other approximated results.

	d = 1		d = 2			d = 3	
	present, SLAC[a]	exact[e]	present	SLAC[b]	series[c]	present	series[c]
α_c	1.27	1	3.33	2.63	3.08	5.35	5.1
y_α	0.68	1	0.70	0.91	1.59	0.707	1.72
z	0.55	1	0.43	0.546	1[d]	0.404	1[d]
s	0.805	1	0.62	0.60	0.63	0.57	0.58

[a] Jullien *et al* (1978), [b] Penson *et al* (1979), [c] Pfeuty and Elliott (1971), [d] exact (Young 1975, Hertz 1976), [e] Pfeuty (1970).

neighbourhood of $T=0$) this rather pathological behaviour for $\eta \neq 0$ and $\alpha \neq 0$ could be associated to the fact that the MFRG is deficient at low temperatures (Slotte 1984). Such peculiar results have been previously obtained by applying the present approach to the random field Ising model (Droz *et al* 1982) and to the triangular Ising antiferromagnet (Slotte 1984).

The author is indebted to Dr R B Stinchcombe and Dr A L Stella for helpful discussions and comments. Particular thanks are due to Dr R B Stinchcombe for a critical reading of the manuscript. Financial support from Conselho Nacional de Desenvolvimento Cientifico e Tecnologico (CNPq, Brazil) and Universidade Federal de Minas Gerais (Brazil) is also gratefully acknowledged.

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