

On Real Space Scalings for the Transverse Ising Model

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Abstract We discuss the use of self-dual clusters to investigate the critical properties of the quantum transverse Ising model. It is shown how calculations can be simplified by means of a partial decimation. The results using self-dual clusters are generally more accurate than those obtained by a simple decimation scheme.

1. INTRODUCTION

The Renormalization Group (RG) formalism¹ has contributed to a broader view of critical phenomena. In particular, its real-space (or block-spin) versions^{2,3} have been extensively used in the study of classical (i.e. Ising-like) systems. The most widely used approximation consists in treating a cluster as representative of the whole lattice, so that RG recursion relations¹ are obtained by summing out some of the degrees of freedom within the cluster. When dealing with quantum systems (e.g. Heisenberg-like), however, the cluster approximation involves neglecting commutation aspects between cluster and lattice Hamiltonians. Provided we keep track of the commutation relations at the cluster level, this approximation has proved quite useful, and not too drastic.

While the success of block-spin scalings^{2,3} stems from their simplicity, their accuracy is not usually as impressive as that of the so-called phenomenological scaling^{4,5}. Nevertheless, the simple features of block-scaling methods make them a powerful tool when dealing with problems such as randomness and other crossover phenomena.

Recently, a simple block-spin method (decimation) has been applied⁶ to the Transverse Ising Model (TIM). The model is described by the Hamiltonian

$$H = - \Gamma \sum_i \sigma_i^x - \sum_{\langle i,j \rangle} J_{ij} \sigma_i^z \sigma_j^z \quad (1.1)$$

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where the σ 's are Pauli matrices, Γ is the transverse field and J_{ij} is the exchange interaction between nearest neighbour sites i and j of a two-dimensional lattice. The Hamiltonian (1.1) was first introduced as a model for hydrogen-bonded ferroelectrics such as KH_2PO_4 . Since then it has been used to describe a variety of other systems (for a partial list of references, see ref.6). It is instructive to summarize some features of the TIM in d -dimensions⁹⁻¹¹. Firstly, the critical behaviour at finite temperatures is the same as that of the d -dimensional Ising Model (i.e. $\Gamma=0$), the effect of the transverse field being simply to shift the critical temperature to $T_c(\Gamma)$. Secondly, at zero temperature there is a competition between the field and exchange interactions, so that a phase transition takes place at some critical value of $j \approx J/\Gamma$, with the same critical exponents as those of the $(d+1)$ -dimensional Ising model.

Although the results obtained⁶ from the simple decimation approach were not very accurate (where comparison with series results⁸ were available), it was possible to pin-point several qualitative aspects of dilution related to the role of quantum fluctuations.

The purpose of this work is to investigate the properties of another block-spin method¹² when applied to the TIM at zero temperature. This method, though close in spirit to decimation, is usually more accurate and can be easily extended to treat antiferromagnetism and lattice anisotropy, in both pure and random cases.

The plan of the paper is as follows. In Section 2 we present the clusters used in our calculations and discuss the approximations involved; the results are presented and discussed in Section 3, and Section 4 summarizes our findings.

2 CLUSTER APPROXIMATIONS

The clusters in Figs. 1 and 2 have been used with considerable success in the study of classical systems¹²⁻¹⁵, where self-duality plays a crucial role¹⁶ in the location of the critical point. The RG prescription for the cluster in Fig. 2 preserves sub-lattice symmetry¹⁵ as well as the symmetry under the interchange of lattice cartesian directions. For classical systems, the summation of degrees of freedom is equivalent to performing a sequence of series and parallel combination of bonds with the aid of the break-collapse method¹².

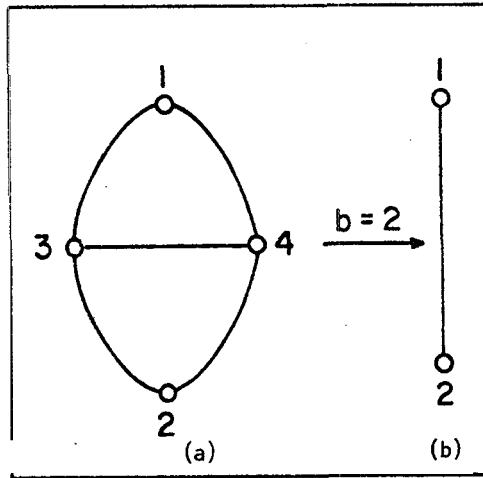


Fig.1 - A four-site cluster (a) is renormalized into a two-site cluster (b) by summing out spins 3 and 4.

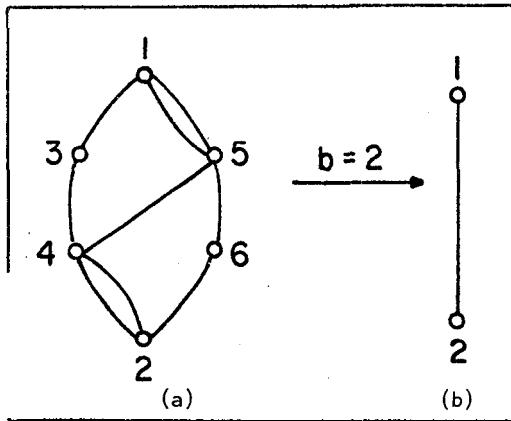


Fig.2 - A six-site cluster (a) is renormalized into a two-site cluster (b) by summing out spins 3, 4, 5 and 6.

For quantum systems at zero temperature, the **self-duality** nature of these clusters **is** not important, since the Hamiltonian does not share this property. Nevertheless, the other **symmetries** present in the cluster of Fig. 2a are still very important in the study of lattice anisotropy and of spin-glass behaviours.

In order to define the RG transformation, we first note that the Hamiltonian for **both** renormalized cells (Figs. 1b and 2b) **is** (in units of Γ')

$$H' = -(\sigma_1^x + \sigma_2^x) - j' \sigma_1^z \sigma_2^z \quad (2.1)$$

where $j' = J'/\Gamma'$. For the original cells of Figs. 1a and 2a, the Hamiltonians can be written (in units of Γ) as

$$H = -(\sigma_1^x + \sigma_2^x + \sigma_3^x + \sigma_4^x) - j(\sigma_1^z \sigma_3^z + \sigma_1^z \sigma_4^z + \sigma_3^z \sigma_4^z + \sigma_2^z \sigma_3^z + \sigma_2^z \sigma_4^z) \quad (2.2)$$

and

$$H = - \sum_{i=1}^6 \sigma_i^x - j \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z \quad (2.3)$$

respectively. Note that, according to Fig. 2a each of the terms $\sigma_1^z \sigma_5^z$ and $a_i^z a_j^z$ appears twice in eq.(2.3). At zero temperature, the ground state projector plays the role of the density matrix, so that the RG recursion relations $j'(j)$ and $c'(j)$ (where c' is a normalization constant) can be obtained **implicitly** from⁶

$$\langle m_1 m_2 | P'_0(j', c') | m_1 m_2 \rangle = \sum_{m_3, m_4} \langle m_1 m_2 m_3 m_4 | P_0(j) | m_1 m_2 m_3 m_4 \rangle \quad (2.4)$$

where $P'_0(j', c')$ and $P_0(j)$ are the ground-state projectors for eq. (2.1) and for eq. (2.2) (for eq.(2.3) one must also include m_5 and m_6), respectively. The $|m_i\rangle$'s are eigenstates of σ_i^z and the sum runs over all states of **non-terminal** spins.

One should make the following remarks about the above prescription: (i) for zero longitudinal field, which is our case, eq. (2.4) only yields two independent equations (for the unknowns j' and c') namely, when $m_1=m_2$ and when $m_1=-m_2$; (ii) only the diagonal elements are considered, which is an approximation that can be **justified**, to some extent, by the fact that the full trace is **preserved**² under this transformation; (iii)

the RG transformation thus defined is critically dependent on the basis used, but it can be shown¹⁷ that for the Hamiltonian (1.1) the states of a^z form an appropriate basis (essentially it is because the order parameter is $\langle \sigma^z \rangle$). Actually, these restrictions are related, but can be lifted in some cases^{18,19}.

In actual calculations, we diagonalize a $2^N \times 2^N$ matrix (N is the number of spins in the original cluster) to obtain the ground-state projector. This task is considerably harder when we allow for randomness, since configurational averages have to be performed. Nevertheless, one can simplify the calculations for the cluster in Fig. 2a if, before using eq. (2.4), we make a "series" combination (partial decimation) of the bonds linking 1 to 3 and 3 to 4 (the same for 2, 6 and 5) based on an exact result for the Transverse Ising chain at zero temperature²⁰: under scaling, a "series" combination of b bonds yields

$$j' = j^b \quad (2.5)$$

Note that the fixed point of eq. (2.5) is $j^* = 1$ and the correlation length exponent $\nu = \text{Re} \ln b / \ln \left(\frac{dj'}{dj} \right)_{j^* = 1}$, which are the exact results in one dimension²¹.

The net effect of this partial decimation, together with adding up the two bonds between 2 and 4 (and 1 and 5) is to reduce the original cluster in Fig. 2a to that in Fig. 1a, but with different couplings. Clearly one may question whether this partial decimation could involve neglecting commutation aspects at a cluster level; we will return to this point in the following section.

3. RESULTS AND DISCUSSION

The fixed point j^* of the recursion relation $j'(j)$ is the critical value for the reduced coupling $j \equiv J/\Gamma$, above (below) which the ground state is ordered (disordered). As usual¹, linearization of the recursion relation around the fixed point yields the eigenvalue $\lambda = \left(\frac{dj'}{dj} \right)_{j^*}$, from which the correlation length exponent is related through

$$\nu = \frac{\ln b}{\ln \lambda} \quad (3.1)$$

where $b=2$ for the clusters used in this work, although in the context of hierarchical lattices $b=3$ seems to be a more appropriate choice²².

The results of our calculations are summarized in Table 1, where comparison is made with decimation⁶ and with series⁸. There is an overall improvement over the decimation approach, and the good results for the cluster in Fig. 2 is attributed to its larger connectivity, being more similar to the real lattice. Clearly, the accurate result for ν we get using Fig.2 without partial decimation should be regarded as fortuitous, although the choice of $b=3$ would imply in $\nu=1.00$.

Table 1 - Results for fixed point (j^*) and correlation length exponent (ν) from our RG calculations; for comparison we also quote other results.

Cluster	j^*	ν
Figure 1	0.49	0.91
Figure 2 with partial decimation	0.43	0.66
Figure 2 without partial decimation	0.44	0.63
Decimation ⁶	0.64	0.50
Series ⁸	0.33	0.63

It is interesting to note the closeness of both results for the cluster in Fig.2; this means that, in this case, the partial decimation is a good approximation. The results are not so close when we allow for lattice anisotropy^{2,3} and take the limit of linear chain: partial decimation implies in worse results because the remaining chain is smaller.

As a final remark, we should point out that these clusters can be thought of as a cell that generates the whole lattice upon translations, in which the boundary sites are collapsed. One would then be tempted to assign 2Γ to each of the terminal spins in the clusters, as is usually done for classical spins in a longitudinal field^{2,4}. The crucial difference is that, in our case, the transverse field is not a symmetry-breaking field but, rather, it competes with the exchange in-

teraction. Since there are two "entry" sites in each cell, order sets in through *either* of these sites, and not through *both* simultaneously. Thus, assigning 2Γ instead of Γ to the terminal sites would artificially overestimate the exchange strength necessary to keep the system ordered. In fact, calculations performed for the cluster in Fig. 2, with 2Γ for each terminal site, without partial decimation yield $j^*=0.76$ and $\nu=0.72$, which compare rather poorly with the results quoted in Table 1. Another possibility (C.Tsallis, private communication) is to assign to each site a weight equal to the number of bonds leaving that site. Although this choice is crucial for other systems, it also yields poor results for the TIM.

4. CONCLUSION

The use of self-dual clusters in the context of the Renormalization Group represents an improvement over simpler approaches to the Transverse Ising model. The major advantages are that more accurate results are obtained for the critical coupling and correlation length exponent, and that self-dual clusters can be systematically used in other situations of interest. Also, partial decimation was shown to be a good approximation, but should be avoided whenever the problem admits the linear chain as a limit, as is the case of lattice anisotropy or dilution. The choice of weights attributed to the terminal sites was also discussed, with the result that 1 is the appropriate choice. We are currently investigating other aspects of this model such as anisotropic dilution and spin-glass behaviour.

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REFERENCES

1. K.G. Wilson and J. Kogut, Phys. Rep. 22, 75 (1974).
2. Th. Niemeijer and J.M. J. Van Leeuwen, *Phase Transitions and Critical Phenomena*, vol.6, ed. C. Domb and M.S. Green, (London Academic), 1976.

3. A.A. Migdal, Sov. Phys. - JETP **42**, 743 (1976); L.P. Kadanoff, Ann. Phys. (NY) **100**, 559 (1976).
4. M.P. Nightingale, Physica (Utrecht) **83A**, 561 (1976).
5. R.R. dos Santos and L. Sneddon, Phys. Rev. **823**, 3541 (1981).
6. R.R. dos Santos, J. Phys. **C15**, 3141 (1982).
7. P.G. Gennes, Solid St. Comm. **1**, 132 (1963).
8. P. Pfeuty and R.J. Elliott, J. Phys. **C4**, 2370 (1971).
9. J. Mertz, Phys. Rev. **B14**, 1165 (1976).
10. A.P. Young, J. Phys. **C8**, L309 (1975).
11. M. Suzuki, Prog. Theor. Phys. **56**, 1454 (1976).
12. C. Tsallis and S.V.F. Levy, Phys. Rev. Lett. **47**, 950 (1981).
13. (a) A.C.N. Magalhães, C. Tsallis and G. Schwachheim, J. Phys. **C14**, 1393 (1981); (b) P.M.C. de Oliveira, Phys. Rev. Lett. **47**, 1423 (1981).
14. P.M.C. de Oliveira and C. Tsallis, J. Phys. **A15**, 2865 (1982).
15. P.M.C. de Oliveira, Phys. Rev. **825**, 2034 (1982).
16. R. Savit, Rev. Mod. Phys. **52**, 4531 (1980).
17. R.R. dos Santos, D. Phil Thesis, University of Oxford (1980).
18. C. Tsallis, R.B. Stinchcombe and B. Buck, J. Phys. **C17**, 301 (1984).
19. A.O. Caride, C. Tsallis and S. Zanette, Phys. Rev. Lett. **51**, 145 (1984).
20. R.B. Stinchcombe, J. Phys. **C14**, 2193 (1981).
21. P. Pfeuty, Ann. Phys. (NY) **57**, 79 (1970).
22. J.P. Melrose, J. Phys. **A16**, 3077 (1983).
23. Rita M. Zorzenon dos Santos and R.R. dos Santos (in preparation).
24. H.O. Martin and C. Tsallis, J. Phys. **C14**, 5645 (1981).

Resumo

Discutimos o uso de "clusters" auto-duais no estudo das propriedades críticas do modelo quântico de Ising com campo transversal. Mostramos como os cálculos podem ser simplificados por meio de uma dízimação parcial. Os resultados obtidos usando clusters auto-duais são, em geral, mais precisos do que os obtidos usando dízimação simples.