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The 2D transverse Ising model at T = 0: a finite-size rescaling transformation approach

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Abstract. The critical behaviour of the spin- $\frac{1}{2}$ Ising model with a transverse field at zero temperature in triangular and square lattices is investigated through a finite-size rescaling transformation. This technique enables the critical properties of infinite systems to be calculated from the scaling properties of systems of finite size, in a generalisation of the so-called phenomenological renormalisation group. The critical field and correlation length exponent calculated using systems of fairly small sizes have reasonable accuracy, but calculations on larger clusters are limited by computer time and storage.

1. Introduction

The renormalisation group (RG) ideas (Wilson and Kogut 1974) have contributed a great deal to our understanding of critical phenomena. In particular, they have provided us with a formal interpretation of universality and also with a means of calculating critical exponents.

The great flexibility in defining an RG transformation in real space (Niemeijer and van Leeuwen 1976, Wallace and Zia 1978) allows several approximation schemes to be set up. For classical (i.e. Ising-like) spins even the simplest approximations are able to elucidate several aspects of pure (Niemeijer and van Leeuwen 1973, Kadanoff and Houghton 1975, Barber 1975) as well as of diluted systems (Young and Stinchcombe 1976, Yeomans and Stinchcombe 1978, 1979). As these simple approximations are improved, one usually faces the uncontrolled appearance of coupling constants of longer range than the ones one started with. These difficulties are worse when dealing with quantum spins, i.e. systems described by Hamiltonians containing non-commuting terms, where couplings involving other spin components are also generated under an RG transformation (dos Santos 1980). These are usually dealt with by referring the transformation to a certain basis (Friedman 1976, 1978, Subbarao 1976, Um 1977, 1978, dos Santos 1980).

A completely different approach for classical spins was proposed by Nightingale (1976, 1977), in which the RG transformation is defined at a macroscopic level, through the scaling of the correlation length. As there is no explicit relationship between site and cell spins, this scheme is free from the proliferation of coupling constants found in standard RG approaches. Another feature of this scheme is the high accuracy of the results obtained for classical spins (Nightingale 1976, 1977, Sneddon 1978, 1979,

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Nightingale and Blöte 1980, Blöte *et al* 1981). This method was also successfully applied to a quantum model through its classical equivalent (Sneddon and Stinchcombe 1979) and also to the percolation (Derrida and Vannimenus 1980) and self-avoiding walk (Derrida 1981) problems.

The above method relies on the possibility of computing the correlation length as a function of the coupling constants for semi-infinite systems (i.e. infinite strips of finite width) through transfer matrix (Domb 1960) techniques. Although transfer matrices can be defined for some quantum systems (Denbigh 1978), the calculation of the correlation length is not as straightforward as for classical spins (Domb 1960).

This phenomenological approach (Nightingale 1976, 1977) has been reinterpreted at a more formal level by dos Santos and Sneddon (1981), enabling a transformation to be derived from the scaling properties of not just the correlation length but of any thermodynamic quantity such as susceptibility, specific heat, etc, calculated for systems of finite size. This approach is equally applicable to classical and quantum spins. It is worth pointing out that due to the absence both of multi-dimensional flows in the parameter space and of a definite relationship between cell and site spins, this transformation is quite different from the usual RG transformations, as well as being a finite-size transformation. To make these distinctions it will here be referred to as a finite-size rescaling transformation (FSRT). These ideas were tested in the calculation of the critical properties of the one-dimensional transverse Ising model at zero temperature, for which exact results are known (Pfeuty 1970, Young 1975, Hertz 1976), and yielded excellent estimates for the critical field and exponents (dos Santos and Sneddon 1981).

In the present work we apply the FSRT approach to the two-dimensional transverse Ising model (TIM[d], d = 2) (de Gennes 1963, Stinchcombe 1973) at zero temperature, described by the Hamiltonian (in units of the exchange coupling)

$$\mathscr{H} = -g \sum_{i} \sigma_{i}^{x} - \sum_{\langle i,j \rangle} \sigma_{i}^{z} \sigma_{j}^{z} - h \sum_{i} \sigma_{i}^{z}$$
(1.1)

where g and h are the transverse and longitudinal fields respectively, σ^x and σ^z are Pauli matrices and the second sum runs over nearest-neighbour sites on a triangular or square lattice. As was first suggested (Elliott *et al* 1970) and then proved (Pfeuty 1970, Young 1975, Hertz 1976, Suzuki 1976), the critical behaviour of the TIM[d] (with h = 0) at finite temperatures is the same as that of the d-dimensional Ising model, but at zero temperature there is a phase transition at a critical field g_c , with the same critical exponents (defined in terms of $|g - g_c|$) as the (d + 1)-dimensional Ising model.

The plan of this paper is as follows: in § 2 we briefly review the method (dos Santos and Sneddon 1981) and discuss the quantities used to define the FSRT. The results for the triangular and square lattices are presented in §§ 3 and 4. In § 5 we present our conclusions.

2. The finite-size rescaling transformation approach

2.1. The transformation

The FSRT approach is closely related to the RG, in the sense that we define a recursion relation for the (n, n/b) scaling

$$g' = R_b(n;g) \tag{2.1}$$

$$X_{n/b}(g') = b^{-p} X_n(g)$$
(2.2)

where X_m is an intensive quantity (such as the susceptibility, specific heat, correlation length, etc) calculated for the system of finite size m, and p is a constant to be determined.

As in standard RG schemes (Wilson and Kogut 1974, Wallace and Zia 1978), we search for a fixed point $g_n^*(p)$ satisfying

$$g_n^*(p) = R_b(n; g_n^*(p))$$
(2.3)

around which the linearised recursion relation yields an eigenvalue

$$\lambda_b(n;p) = \frac{\mathrm{d}R_b}{\mathrm{d}g}\Big|_{g=g^*_n(p)}.$$
(2.4)

The connection with the actual critical behaviour of the infinite system is established from the assumption that the limit

$$\lim_{n \to \infty} g_n^*(p) = g^* \tag{2.5}$$

exists and is independent of p. It then follows that (dos Santos and Sneddon 1981)

$$\lim_{n \to \infty} \lambda_b(m; p) = \lambda_b = b^{\nu} \tag{2.6}$$

for some y independent of b, and that

$$X(g) = \lim_{n \to \infty} X_n(g) \tag{2.7}$$

has a power-law singularity

$$X(g) \sim |g - g_c|^{-x}$$
 (2.8)

defining the critical exponent x, with $g_c = g^*$. Finally, the parameter p is found to be (dos Santos and Sneddon 1981)

$$p = yx = x/\nu \tag{2.9}$$

where ν is the correlation length exponent.

As the thermodynamic limit $(n \rightarrow \infty)$ is usually computationally inaccessible, fixed points and eigenvalues obtained for systems of finite sizes will depend on p, but as the sizes of the systems considered are increased the results should improve. In practical applications we must calculate p, which can be done in several ways as discussed below.

2.2. Adjusting the parameter p

The simplest situation is when p is known. When the correlation length for semi-infinite systems is used as the quantity X, we have x = v, so that p = 1. Also, for quantum models at zero temperature in which the longest time scale is given by the inverse of the energy gap between the two lowest states, we have p = -z, where z is the dynamic critical exponent (Hohenberg and Halperin 1977). In particular, for the TIM[d] at zero

temperature we have the exact result z = 1 (Young 1975, Hertz 1976, Sneddon and Stinchcombe 1979). Another special situation is when x/ν is known either from series expansions or exactly.

The more common situation is when no information about p is available. If computations with three systems of finite size $(n_1 > n_2 > n_3)$ can be performed, we can determine two curves $g_{n_1}^*(p)$ and $g_{n_2}^*(p)$ from equation (2.3) with $b_1 = n_1/n_2$ and $b_2 = n_2/n_3$, respectively. The parameter p is then chosen from the intersection of these two curves, artificially reproducing the very large n limit in which the estimates should be independent of p. The corresponding exponents ν_{n_1} and ν_{n_2} will, in general, be different, with ν_{n_1} closer to the limiting value than ν_{n_2} . This approach was applied to the TIM[1] at zero temperature and yielded estimates for the critical field and correlation length exponents less than 1% of the exact values (dos Santos and Sneddon 1981).

When computer time or storage prevents calculations being performed on more than two systems with different sizes we can use two different quantities X and V. (As an exponent $v \neq x$ is associated with V, we must determine a second parameter q = v/v, in addition to p = x/v). The recursion relation (2.2) can then be solved separately for X and V, giving the 'fixed curves' $g_{X,n}^*(p)$ and $g_{V,n}^*(q)$, respectively. Also, with these we can calculate the 'eigenvalue curves' $\lambda_{b,X}(n, p)$ and $\lambda_{b,V}(n, q)$. The constants q and p are then determined by demanding

$$g_{X,n}^{*}(p) = g_{V,n}^{*}(q), \qquad \lambda_{b,X}(n,p) = \lambda_{b,V}(n,p).$$
 (2.10)

This procedure was tested for the TIM[1] at T = 0 (dos Santos 1980) and in spite of a rather poor accuracy for g^* , p and q, it yielded extremely accurate results for ν (less than 0.1% of the exact value).

Other methods of choosing p have been tested (dos Santos 1980), but the ones above turned out to be the most reliable, and will be used in the remainder of this paper.

2.3. Quantities used for the TIM[2] at T = 0

Within the present approach, the limiting (i.e. $n \to \infty$) critical behaviour of the TIM[2] at zero temperature can then be inferred from quantities calculated from the lowest eigenvalues of the Hamiltonian (1.1) for systems with finite size *n*. Indeed, denoting the two lowest eigenvalues of (1.1) by $E_{0,n}(g, h)$ and $E_{1,n}(g, h)$ ($|E_{0,n}| > |E_{1,n}|$) we can calculate the energy gap

$$\Delta_n(g) = E_{1,n}(g,0) - E_{0,n}(g,0), \qquad (2.11)$$

the (longitudinal) zero-field susceptibility

$$\chi_{n}(g) = -\frac{1}{N} \frac{\partial^{2} E_{0,n}(g,h)}{\partial h^{2}} \Big|_{h=0}$$
(2.12)

where N is the *total* number of spins, and the 'specific heat'

$$C_{n}(g) = -\frac{g}{N} \frac{\partial^{2} E_{0,n}(g,0)}{\partial g^{2}}.$$
(2.13)

The existence of a phase transition in the thermodynamic limit is associated with a non-analytic behaviour of these quantities at g_c (Pfeuty 1970, Pfeuty and Elliott 1971, Young 1975, Hertz 1976, Suzuki 1976) described by power laws

$$\Delta(g) \sim |g - g_c|^s, \tag{2.14}$$

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$$\chi(g) \sim |g - g_c|^{-\gamma}, \tag{2.15}$$

$$C(g) \sim \left| g - g_c \right|^{-\alpha},\tag{2.16}$$

where the critical exponents s, γ and α are independent of lattice structures with the same spatial dimensionalities.

The gap exponent s is related to the dynamic critical exponent z (Hohenberg and Halperin 1977) through $z = s/\nu$, where ν is the correlation length exponent defined by

$$\xi(g) \sim |g - g_c|^{-\nu}$$
 (2.17)

so that $s = \nu$ for the TIM[d] at zero temperature, since z = 1 (Young 1975, Hertz 1976, Sneddon and Stinchcombe 1979). From ground-state perturbation expansions (Pfeuty and Elliott 1971, Yanase *et al* 1976) for the TIM[2] at zero temperature we have $\gamma \simeq 1.25$, $\nu \simeq 0.63$ and $\alpha \simeq 0.11$.

As for two-dimensional lattices the total number of spins grows roughly as n^2 , numerical calculations are very lengthy. Even with the aid of group theory (Boardman *et al* 1973), we cannot diagonalise the Hamiltonian (1.1) for $n \ge 5$ and $n \ge 4$ for the triangular and square lattices, respectively, within acceptable computer times. This is particularly unfortunate for the square lattice calculations, because it means we cannot handle three square clusters of different sizes, but only rectangular clusters, as discussed in § 4.

3. Results for the triangular lattice

3.1. Finite-size scaling and the 'specific heat' at zero temperature

Before we proceed to use the quantities above within the FSRT approach, it is instructive to examine the trend of these quantities as the sizes of the systems increase.

If we calculate $\Delta_n(g)$, $\chi_n(g)$ and $C_n(g)$ for the triangular clusters in figure 1, we note that while Δ_n and χ_n are monotonic functions of g, $C_n(g)$ displays maxima (or rounded-off singularities) at $g_c(n)$ as shown in figure 2. In this case some of the critical properties can be estimated from the finite-size scaling theory developed by Fisher and



Figure 1. Triangular clusters of finite size n, where the spins are represented by open circles.



Figure 2. 'Specific heat' at zero temperature as a function of the transverse field g calculated for the triangular clusters of figure 1.

co-workers (Fisher 1971), according to which

$$C_n(g) \approx n^{\alpha/\nu} Q[n^{1/\nu}(g - g_c(n))]$$
 (3.1)

where α is the same exponent as in equation (2.16), ν is the correlation length exponent characterising the bulk (i.e. $n \to \infty$) behaviour and Q(w) is a scaling function of the variable $w = n^{1/\nu}(g - g_c(n))$. (Strictly speaking, the above ansatz is only valid for very large n and for g near the 'pseudocritical' coupling $g_c(n)$.)

As $\lim_{n\to\infty} g_c(n) = g_c$ (Fisher 1971), we can have a crude estimate of g_c from a quadratic extrapolation to $n \to \infty$. This yields $g_c = 4.5$, which should be compared with the series result $g_c = 4.77$ (Yanase *et al* 1976). Also, the ratio α/ν can be estimated from a log-log plot of $C_n[g_c(n)]$ as a function of n, according to equation (3.1):

$$\left(\frac{\alpha}{\nu}\right)_{n} \equiv \ln\left(\frac{C_{n}[g_{c}(n)]}{C_{n-1}[g_{c}(n-1)]}\right) \left(\ln\left(\frac{n}{n-1}\right)\right)^{-1}.$$
(3.2)

Furthermore, the scaling law

$$2/\nu = \alpha/\nu + d^* \tag{3.3}$$

with $d^* = d + 1 = 3$ for the TIM[2] at zero temperature (Pfeuty and Elliott 1971, Young 1975, Hertz 1976, Suzuki 1976) provides us with an estimate of ν , once α/ν is given. In table 1 we show successive estimates $(\alpha/\nu)_n$ and ν_n calculated from (3.2) and (3.3), respectively, together with the series results of Yanase (1977).

In spite of these rather encouraging results, the 'specific heat' at zero temperature yields meaningless results within a FSRT approach with small clusters. In fact, since

Table 1. Successive estimates of α/ν and ν as given by equations (3.2) and (3.3), respectively, for the triangular clusters in figure 1, together with the series results (Yanase 1977).

n	$(\alpha/\nu)_n$	ν _n	
3 4	0.55 0.38	0.56 0.59	
Series	0.194	0.64	

 $b^{-\alpha/\nu} \sim 1$, a non-trivial fixed point is roughly where two successive plots of $C_n(g)$ intersect. However, figure 2 shows that for the three simplest triangular clusters this point would correspond to a negative eigenvalue because the slopes $(dC_n/dg)|_{g^*(n)}$ have opposite signs.

3.2. FSRT results and discussion

As we can calculate both $\Delta_n(g)$ and $\chi_n(g)$ for the three clusters in figure 1, we can use two successive scalings to determine p as in § 2. In order to test the overall accuracy of the method, we also calculate the critical properties of the TIM[2] using the energy gap with $p = s/\nu = -1$ (Young 1975, Hertz 1976) and the susceptibility with $p = \gamma/\nu \approx$ 1.944 (Yanase *et al* 1976). These results are shown in table 2, together with other RG estimates.

Table 2. Estimates of the critical field (g^*) and the correlation length exponent (ν) for the TIM at zero temperatures on a triangular lattice, calculated through the scaling of the energy gap (Δ) and the susceptibility (χ) . Other RG results are also shown.

Sc	aling	g*	ν	Remarks
	(3, 2)	3.09	1.02	<i>p</i> taken to be -1 (Young 1975, Hertz 1976,
Δ	(4, 3) (4, 2), (2, 2)	3.74	0.93	Sneddon and Stinchcombe 1979) n (calculated) = -1.27
	(4, 3); (3, 2) (3, 2)	3.28 2.95	0.72	p (calculated) = -1.37 $p \equiv v/v$ taken to be 1.94
X	(4, 3)	3.62	0.71	from series (Yanase <i>et al</i> 1976)
O	her RG	3.43	0.92	Perturbative RG (Friedman 1976)
re	sults	4.73	0.95	Truncated basis states (Penson et al 1979)
Se	ries	4.77	0.64	(Yanase 1977)

Unfortunately, the calculations with the susceptibility and two successive scalings yielded very inaccurate values for g^* and p. This reflects the fact that the functions $g_n^*(p)$ (see § 2) obtained from (3, 2) and (4, 3) scalings with the susceptibility do not vary much over a wide range of values of p. If calculations with n = 5 could be performed one could possibly obtain very good results in this case.

Nevertheless, the present method is able to give overall better estimates for ν than other RG schemes, although estimates for g^* are no better.

4. Results for the square lattice

4.1. Square clusters

As mentioned at the end of § 2, we cannot obtain the eigenvalues of the Hamiltonian (1.1) for a cluster with n = 4 (N = 16) within acceptable computer times. Thus, if we only consider square clusters, we cannot calculate p from two successive scalings, and we have to use the energy gap and the susceptibility simultaneously.

These two quantities were calculated for the two square clusters in figure 3, where periodic boundary conditions (PBC) were imposed for two reasons. Firstly, for a square cluster with PBC the symmetry group is now the space group, instead of only the point



Figure 3. Clusters used in calculations on the square lattice, where the spins are represented by open circles. \tilde{n} and \bar{n} are the effective sizes calculated from simple and quadratic harmonic means, respectively.

group D_4 . In this way the Hamiltonian matrix is cast in block form with smaller blocks than in the case of free ends. Secondly, quantities like the energy gap, susceptibility, specific heat, etc, calculated for systems of finite size *n*, converge faster to their large-*n* limit when PBC are imposed than for free ends (Fisher 1971, dos Santos 1980). The reason for this probably lies in the fact that a system with PBC has the space group as the symmetry group, as does the infinite lattice.

In table 3 we show the FSRT results for the TIM[2] at zero temperature on a square lattice, together with series (Pfeuty and Elliott 1971) and other RG results. The first two rows show the results obtained with p taken from other sources: $p = -s/\nu = -1$ (Young 1975, Hertz 1976) and $p = \gamma/\nu = 1.94$ (Pfeuty and Elliott 1971), respectively. The third row shows the results obtained using Δ and χ simultaneously where, as happened for the linear chain (dos Santos 1980), ν is of satisfactory accuracy, but not g^* . In this

Table 3. Estimates of the critical field (g^*) and of the correlation length exponent (ν) for the TIM at zero temperature on a square lattice calculated through the (3, 2) scaling of the energy gap (Δ) and the susceptibility (χ) using only the square clusters of figure 3, with periodic boundary conditions. Other RG results are also shown.

Quantity used	g*	ν	Remarks
Δ	3.16 0.	0.80	p taken to be -1 (Young 1975, Hertz 1976, Sneddon and Stinchcombe 1979)
χ Δ, χ	3.18 2.42	0.66 0.52	<i>p</i> taken to be 1.944 (Pfeuty and Elliott 1971) s/ν (calculated) = 2.5; γ/ν (calc) = 4.2
Series results	3.04	0.63	(Pfeuty and Elliott 1971)
Other RG results	3.09 2.63 1.55	0.72 1.1 0.50	Cluster approximation (Friedman 1976) Truncated basis states (Penson <i>et al</i> 1979) Cluster decimation (dos Santos 1981)

case $s/\nu = 2.5$ and $\gamma/\nu = 4.2$, which are very poor compared with the values quoted above.

4.2. Rectangular clusters

An alternative approach, which allows us to use two successive scalings, consists in using the rectangular clusters in figure 3. The difficulty in this case, however, lies in a rather loose definition of the effective size n.

Within the context of finite-size scaling, Fisher (1971) pointed out that the effective size of a *d*-dimensional hypercubic system of volume $v = n_1 \times n_2 \times \ldots \times n_d$ (in units of (lattice spacing)^{*d*}) can be given either as a simple harmonic mean

$$\tilde{n} = \frac{d}{1/n_1 + 1/n_2 + \ldots + 1/n_d}$$
(4.1)

or by a quadratic harmonic mean

$$\bar{n} = \left(\frac{d}{(1/n_1^2 + 1/n_2^2 + \ldots + 1/n_d^2)}\right)^{1/2}.$$
(4.2)

Although the difference between \tilde{n} and \bar{n} should be immaterial for very large systems, this is not the case for systems of fairly small sizes, such as the ones considered in this work. This effect can be assessed through a finite-size scaling ansatz for the energy gap similar to (3.1),

$$\Delta_n(g) \approx n^{-1} R(n^{1/\nu} (g - g_c)), \tag{4.3}$$

where we should note the appearance of the unshifted coupling $(g - g_c)$ (Fisher 1971). While calculations for the one-dimensional model (Hamer and Barber 1981, dos Santos and Stinchcombe 1981) indicated that $\Delta_n(g_c) \rightarrow 1/n$ monotonically as *n* increases from 2, this monotonic behaviour is only verified for the clusters in figure 3 (using the series value $g_c = 3.04$ (Pfeuty and Elliott 1971)) if the quadratic harmonic mean (4.2) is used. For this reason, in FSRT calculations we shall adopt the definition (4.2) for the effective size of the rectangular clusters.

The results of FSRT calculations using the energy gap and the clusters in figure 3 are shown in table 4. Although the results oscillate around the series estimates (Pfeuty and Elliott 1971), the values of g^* and p are usually more accurate than those using Δ and χ simultanously (cf table 3). Also, this method provides us with reasonable estimates for ν , especially if we consider an average of the two values obtained when two successive scalings are used simultaneously.

It is worth stressing that the oscillation of the results appears to be entirely due to the loose definition of the effective size, since it was not present in the calculations for the linear chain (dos Santos and Sneddon 1981). Also, these oscillations are worse when the simple harmonic definition is used.

5. Conclusion

The critical behaviour of the Ising model with a transverse field at zero temperature on both square and triangular lattices was investigated by means of a finite-size rescaling transformation.

Scaling used	<i>g</i> *	р	ν
(2.35, 2) (2.53, 2.35) (3, 2, 53)	3.21 3.15 3.14	-1^+ -1^+ -1^+	0.77 0.69 0.98
(2.53, 2.35) (2.35, 2)	3.03	-1.19	0.55 0.69
(3, 2.53) (2.53, 2.35)	3.17	-0.965	1.00 0.63

Table 4. Estimates of the critical point g^* , the constant p and the correlation length exponent ν using the energy gap and the finite systems of figure 3 with the quadratic harmonic definition of the effective size. When two successive scalings are used we show the two corresponding estimates of ν .

[†] Young (1975), Hertz (1976), Sneddon and Stinchcombe (1979).

Unlike the one-dimensional case, numerical calculations are very involved already for the smallest clusters. Although the adjustable parameter of the FSRT can still be determined, the results obtained are not as accurate as those for the linear chain. Nevertheless, the overall accuracy is still comparable to other RG schemes. If fast numerical methods, like Monte Carlo techniques, are used to calculate the macroscopic quantities, it is very likely that the present approach will yield extremely accurate results.

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