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RENORMALISATION GROUP STUDY OF XY AND HEISENBERG MODELS IN TWO DIMENSIONS

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We perform a numerical study of the XY and Heisenberg models with the finite size real space renormalisation group method. We confirm the Berezinskii–Kosterlitz–Thouless picture for the XY model and provide strong evidence against a standard algebraic divergence of the correlation length. We also obtain the most accurate determination of the magnetic exponent. For the Heisenberg model, we find that the scaling law predicted by the asymptotic freedom property of the theory around zero bare coupling is fulfilled, indicating the absence of phase transitions at a non-zero temperature.

1. Introduction

The XY and the Heisenberg models in two dimensions are characterised by a phase transition with an exponential divergence of the correlation length at the critical temperature which is expected to be finite in the former case and zero in the latter one. The first model is relevant to several two dimensional physical systems and in particular it is expected to describe the critical properties of thin films of superfluid helium. In this paper we want to analyse the critical properties of these models within a real space renormalisation group technique. The purpose is twofold: we provide more accurate results for some of their critical indices than previous numerical studies with strong evidence against a conventional algebraic type singularity for the XY model and we demonstrate the effectiveness of our technique in phase transitions with an essential singularity of the correlation length. This may turn out to be useful for the study of four dimensional non-abelian gauge theories which have the same property near their continuum limit. Sects. 2 and 3 contain the presentation of the method and the results for the XY model while sect. 4 reports the results for the O(3) model. Brief conclusions are contained in sect. 5.

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2. The XY model: the method

2.1. GENERALITIES

The two dimensional XY model has recently been the subject of new numerical and analytic studies. According to the analysis of Berezinski, Kosterlitz and Thouless [1], this model has a phase transition at finite temperature characterised by the absence of a spontaneous magnetisation and by an essential singularity for the correlation length. This behaviour is much harder to study by numerical methods than the standard one, as the Ising model, where the singularity is only algebraic. Indeed, a direct fit of the exponential increase of the correlation length near the critical temperature needs very large lattice sizes in order to avoid finite size effects and the use of special algorithms to beat the consequent critical slowing down [2]. In practice, even using optimised techniques and a sizeable computer time, one has always to rely on fitting procedures of data obtained rather far from the critical temperature: this leads to inaccurate estimates of the magnetic exponent.

Other analyses have been using the finite scaling method [3]: in this case some better results are obtained, but the exponential character of the singularity cannot be unambiguously distinguished from a standard algebraic singularity. Some recent studies have in fact challenged the nature of the transition and presented some evidence for a conventional behaviour [4]. An analysis of the high temperature expansion seems to conclude in favour of the original BKT picture on the basis of the stability of the Padé coefficient of the high temperature series [5], which, under the hypothesis of an algebraic singularity, leads to an unstable value for the exponent ν increasing with the order of the approximant used.

We have performed a numerical simulation with the finite size real space renormalisation group method. The basic idea is to study the behaviour of block variables defined at a scale which is a fixed fraction of the total lattice size (L) as a function of the original coupling and for different values of L. The method is a combination of the Monte Carlo renormalisation group [6] – we introduce block variables – and of the finite size scaling ideas – we study their dependence upon the infrared cutoff given by the lattice size [8]. In particular cases, it fully reduces to one of the two latter techniques. If, for example, the block variable is defined as the total energy contained in a block, with a normalisation suitable to the linear blocking, the method becomes a finite size scaling analysis of the specific heat. Instead, a linear blocking of the original variables – not of the energies – performed on lattices of sizes L and $2L$ (L even) and defining block variables at a scale equal to half of the original lattice size can be seen as the $N = L/4$ and $N + 1 = L/2$ iteration steps of a blocking by a scale factor equal to two of the classical MCRG technique developed by Ma, Wilson and Swendsen [6]. In general, for non-linear blocking and for generic values of the lattice sizes, the method does not reduce to previous techniques. In the case of discrete spin models, like the Ising and the three

state Potts model, accurate results were obtained using moderate volumes of the order of twenty lattice spacings in each direction [7]. In that case the total volume of a square of size L was divided into four squares and for each of them a block variable was defined according to the standard majority rule. Given the discrete nature of the variables, it was possible to disentangle all the independent couplings of the hamiltonian for the resulting two-by-two system. The critical indices were obtained by linearising near the fixed point the recursion relation between the block couplings of two different lattice sizes.

In the case of the XY and Heisenberg models the continuous character of the variables does not allow us to extract the exact form of the block hamiltonian: instead of a finite number of couplings one has to deal with a finite number of functions. However, at the fixed point and in the infinite volume limit the whole probability distribution should match and, therefore, any function of the couplings, i.e. any correlation of the block variables, can be considered as a "generalised coupling". From the experience of the discrete models one learns that, given an affordable range of volumes, the best results are obtained from the biggest couplings which are the nearest neighbour in the cases quoted above. The determination of the smaller ones involves important cancellations which make the result statistically unstable. The choice of the generalised couplings in the continuous case should also avoid important cancellations between different regions of the probability distribution. We will compare the results obtained at the critical point with different definitions of the generalised couplings: they are expected to be identical in the infinite volume limit and the discrepancies provide an indication of the systematic errors of the method. In general we will find them to be of the same order of our statistical errors.

The XY model is defined by the following hamiltonian:

$$\beta H = -\beta \sum_{i,j} (\sigma_i \sigma_j), \tag{2.1}$$

where the sum is over all first neighbour pairs and the spins σ_i have fixed modulus and can rotate continuously in a plane.

In order to reduce to the minimum the number of variables to deal with, we have divided the spins of the square into two groups, having $L^2/2$ elements each. The first group contains the variables belonging to a rhombus with a side of length $L/\sqrt{2}$ and the axes parallel to the square sides, the second contains all the remaining variables. The latter are also contained in a rhombus due to the periodic boundary conditions. We define the block spins as the normalised average of the original spins inside each group:

$$\boldsymbol{S}_{A,B} = \frac{\Sigma_{(i \in A,B)} \sigma_i}{|\Sigma_{(i \in A,B)} \sigma_i|} . \tag{2.2}$$

The block hamiltonian will be a function of the only non-trivial O(2) invariant quantity $\boldsymbol{S}_A^* \boldsymbol{S}_B = \cos(\phi_{AB})$. We have used three independent generalised couplings:

$$\text{(i)} \qquad K_1 = \langle \cos(\phi_{AB}) \rangle ,$$

$$\text{(ii)} \qquad K_2 = \frac{\langle \cos(\phi_{AB}) \rangle}{\langle \sin^2(\phi_{AB}) \rangle} ,$$

$$\text{(iii)} \qquad K_3 = 3 \frac{\langle \sin^2(\phi_{AB}) \cos(\phi_{AB}) \rangle}{\langle \sin^4(\phi_{AB}) \rangle} . \tag{2.3}$$

The second and the third would be identical if the block hamiltonian had the same form of the original one, i.e. a *linear* function of $S_A * S_B$ only, and would be equal to the value of its single coupling (K). Indeed, in this case one can simply derive the following Schwinger–Dyson type equations from the couplings:

$$\int_0^{2\pi} \mathrm{d}\phi_{AB} \frac{\mathrm{d}}{\mathrm{d}\phi_{AB}} \{ \sin(\phi_{AB}) \exp[K \cos(\phi_{AB})] \} = 0 ,$$

$$\int_0^{2\pi} \mathrm{d}\phi_{AB} \frac{\mathrm{d}}{\mathrm{d}\phi_{AB}} \{ \sin^3(\phi_{AB}) \exp[K \cos(\phi_{AB})] \} = 0 . \tag{2.4}$$

The first coupling in the same approximation would also be a function of the coupling K:

$$K_1 = \frac{I_1(K)}{I_0(K)} , \tag{2.5}$$

where I_1 and I_0 are Bessel functions.

The critical behaviour of the theory is determined by a thermal (ν) and a magnetic (η) exponent. The first, according to the BKT analysis, is related to the diverging correlation length by

$$\xi = A \exp[B(T - T_c)^{-\nu}] \tag{2.6}$$

where A and B are non-universal constants, while the exponent η relates the magnetic susceptibility to the correlation length:

$$\chi = \xi^{2-\eta} . \tag{2.7}$$

Beyond the critical point there is a line of fixed points which extends to zero temperature and where the correlation length stays infinite.

We have performed simulations with three different volumes: $L = 16$, $L = 24$ and $L = 32$. In order to reduce the critical slowing down, we have used an algorithm similar to the one of ref. [2] by alternating a number N_M of standard Metropolis

updates with N_μ microcanonical sweeps. These are obtained by replacing the direction of each spin in a given point with the one symmetric with respect to the direction of the sum of neighbouring spins. By calling ϕ the original angle formed with a reference axis and α (with its sign) the relative angle between a spin and the sum of neighbours, the new angle is $\phi + 2\alpha$ so that the contribution to the total energy of the rotated spin is the same as before. We used a sequence with $N_M = 1$ and $N_\mu = 5$ and we define it as our "iteration unit". This choice is similar to the one adopted by the authors of ref. [2] to obtain a relaxation exponent close to one. We have optimised the choice to obtain a given error with the minimum computer time. The error is estimated from a set of cluster measurements, each grouping several successive spin configurations. The error from the clusters is obtained in two ways. The first is just the standard deviation, the second is with the "jackknife" method. This consists of considering new clusters, each grouping all the original ones but one. It can be shown that the standard deviation obtained from these N highly correlated new clusters should be *multiplied* by N in order to get the usual standard deviation. We determine the optimal values for the number of clusters and their size by requiring the compatibility between the two error estimates. This is expected to hold only if the original clusters are statistically independent. We observe a stability of the results with clusters collecting from 1000 to 8000 iterations. For each point in β we have run a total of 2.5×10^5 iterations including 5×10^4 thermalisation sweeps. We have made a few test runs with 4.8×10^6 total iterations and 8×10^5 thermalisation sweeps for the largest volume. We have observed the expected decrease of the statistical error, but the deviations of the average values from the ones obtained with the "standard" statistics are well inside the error estimates: we have assumed a fortiori the same stability for the smaller volumes.

The location of the critical point can be estimated by the matching of the generalised couplings: figs. 1a and 1b show the ratios of the coupling K_1 at the volume $L = 24$ over the corresponding value at the volume $L = 16$ and for the volumes $L = 32$ and $L = 24$ as a function of the original coupling β respectively. Figs. 2a and 2b show the same quantities for the coupling K_2. Beyond values of β of the order of 1.110 the couplings do match and keep matching also at higher values (lower temperatures), as expected. The critical temperature depends upon the volume and tends to the correct asymptotic value from above.

In the case of an algebraic divergence of the correlation length, the thermal critical index y_T was obtained by linearising the recursion relations between the couplings obtained from two different sizes:

$$y_T = \frac{\ln(\partial K_i(L_1)/\partial K_i(L_2))}{\ln(L_1/L_2)}, \tag{2.8}$$

where $K_i(L)$ indicates a generic coupling "i" normalised at the scale L. The derivatives $\partial K_i(L_1)/\partial K_i(L_2)$ are obtained as a ratio of the derivatives with respect

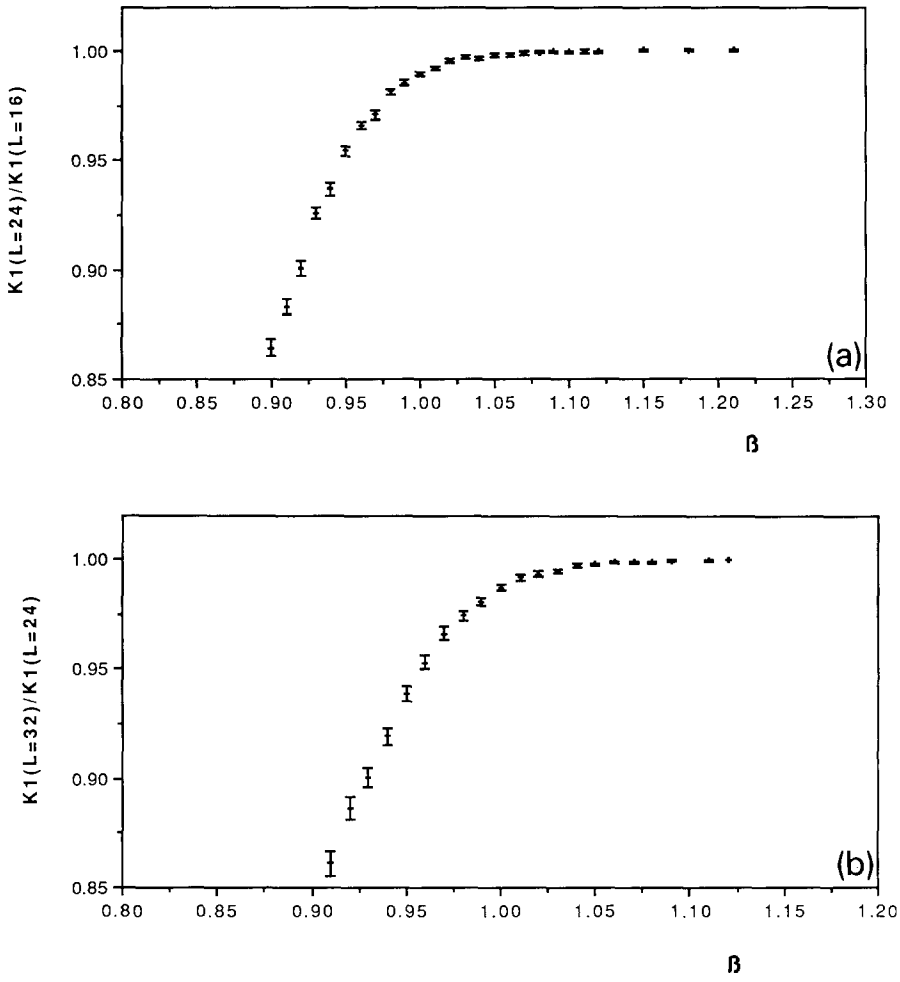

Fig. 1. (a) The ratio of the generalised block coupling K_1 at the scale $L = 24$ over the corresponding one at the scale $L = 16$ as a function of the original coupling β. (b) The same quantity of (a) for the volumes $L = 32$ and $L = 24$.

to the original coupling β which can be evaluated as the connected correlation of the generalised couplings with the total energy of the original system. This way of calculating derivatives of block couplings was introduced for the standard multistep Monte Carlo renormalisation group by Swendsen [6]. We now explain eq. (2.8) more in detail.

2.2. RENORMALISATION AND FINITE SIZE SCALING

Define $\xi_\infty(L)$ the correlation length on an infinite lattice at a scale L, i.e. measured in units of L times the original lattice spacing. Naive dimensional analysis

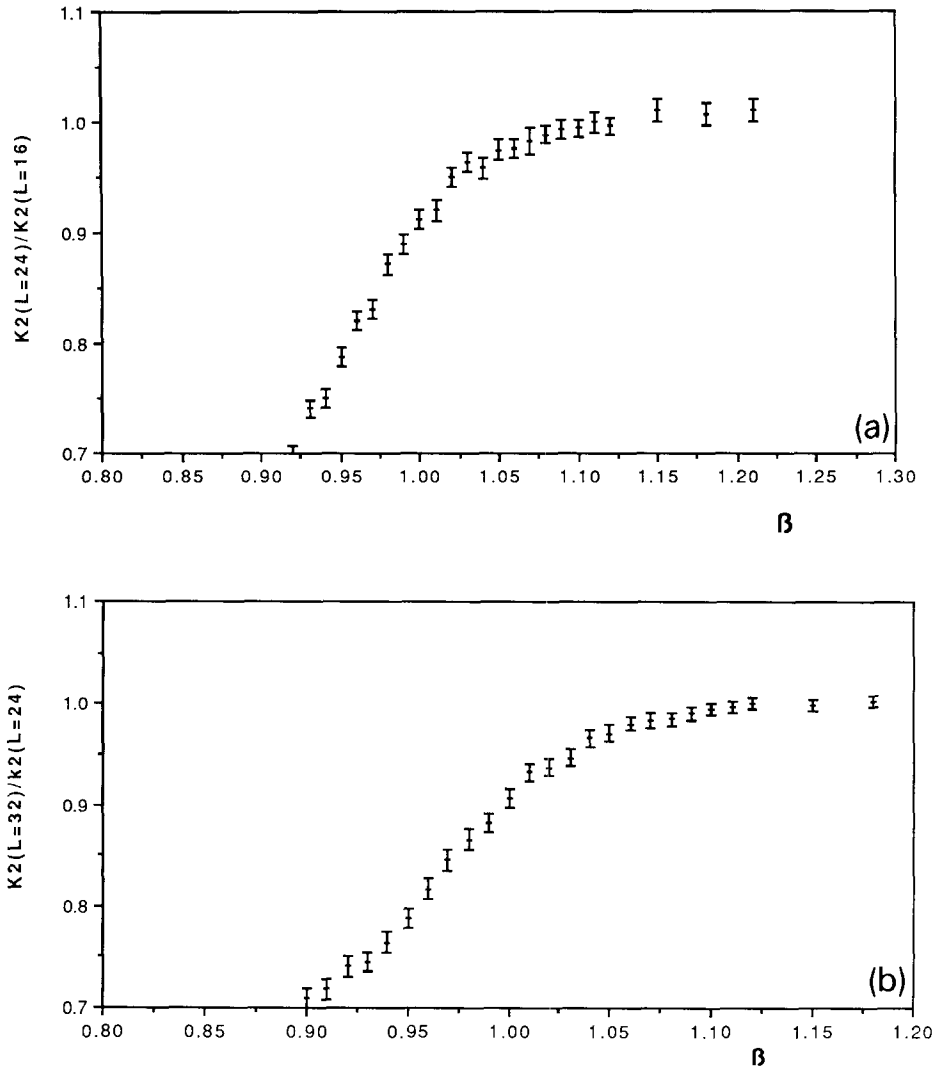

Fig. 2. (a) The same as in fig. 1a for the coupling K_2. (b) The same as in fig. 1b for the coupling K_2.

relates the correlation length measured with two different units:

$$\xi_\infty(L) = \xi_\infty(1)/L\,. \tag{2.9}$$

Following the finite size scaling ansatz [8], on a finite volume of size L the correlation length can be written as

$$\xi_L(1) = LF\left[\xi_\infty(1)/L\right], \tag{2.10}$$

where F is a scaling function with $F[x]_{x\to 0} = x$ and with a maximum at some value v_0 of its argument.

The second property implies that the apparent critical temperature, i.e. the value of the original coupling β where the correlation length has a maximum, shifts to the correct value defined by $\xi_\infty = \infty$ only when the volume goes to infinity. The deviation from the asymptotic value dies as an inverse power of the volume in the algebraic case and as an inverse power of the *logarithm* of the volume in the exponential case. In the following we will neglect violations of the scaling ansatz and some of our formulas should be read under this assumption.

By combining eqs. (2.9) and (2.10) one obtains the behaviour of the correlation length on a finite volume L measured with a length unit L':

$$\xi_L(L') = \frac{L}{L'} F\left[\frac{\xi_\infty(L')}{(L/L')}\right], \tag{2.11}$$

where L/L' is the available volume L measured in the units L'.

Imagine that we perform a simulation with two different volumes, say L_1 and L_2, and define generalised couplings at a scale which is a fixed fraction of the total size in both cases so that the ratio L_1/L_1' is equal to L_2/L_2'. The matching of the generalised couplings is obtained for the same β only at the critical point β_c. Below β_c it occurs for different values depending upon the volume, called $\beta(L_1)$ and $\beta(L_2)$. The matching indicates that the physics is the same on the two volumes, i.e. that they see the same correlation length $\xi_L(L')$. It follows the equation

$$\xi_{L_1}(L_1')_{\beta=\beta(L_1)} = \xi_{L_2}(L_2')_{\beta=\beta(L_2)}. \tag{2.12}$$

There is a solution to the equation obtained by substituting eq. (2.11) into eq. (2.12) which is independent from the explicit form of the function F, provided that this is a monotonic function in the matching region. This excludes regions in β which lie between the critical value for the volume L_1 and the one for the volume L_2. The solution is simply given by

$$\xi_\infty(L_1)_{\beta=\beta(L_1)} = \xi_\infty(L_2)_{\beta=\beta(L_2)}. \tag{2.13}$$

The above relation can be used to fix the thermal exponent.

The general idea of interpreting the ratio of different lattice sizes as renormalisation group scaling factor was developed by Nightingale and called phenomenological renormalisation group. In this approach the test quantities are the specific heat or the susceptibility of the original system and not renormalised quantities like in the method discussed in this paper. It was applied to the study of the XY model by Roomany and Wyld [8] who obtained accurate results for the thermal exponent.

2.3. THE THERMAL EXPONENT

In the algebraic case correlation length diverges at the critical point as

$$\xi_\infty(1) = A(T - T_c)^{-\nu}, \tag{2.14}$$

and eq. (2.13) reads

$$\frac{[\beta(L_1) - \beta_c]^{-\nu}}{L_1} = \frac{[\beta(L_2) - \beta_c]^{-\nu}}{L_2}, \tag{2.15}$$

where we have used eq. (2.14) by replacing the difference of the temperatures with that of their inverse, i.e. of the couplings β's. The two expressions differ by a smooth function of T/T_c which does not alter the exponent for T near T_c. In general we will write expressions containing the couplings instead of the temperatures.

The value of β_c to be used is the one of the infinite volume. A possible phenomenological way of reabsorbing some of the finite size corrections to the scaling formula in eq. (2.13) is to use instead the relative β_c for the two volumes L_1 and L_2 which lies below the asymptotic one and between the critical values of each individual volume. We have not done it and we have used a common value of β_c for the three volumes. The exponent ν, equal to the inverse of the thermal exponent y_T, can be obtained from a fit to eq. (2.15). A more straightforward result is obtained by considering the limit of the same equation at the critical point. To perform such a limit it is convenient to express the shift of the value of a generalised coupling from its fixed point value (ΔK) in terms of the shift of the original β from its critical value ($\Delta\beta$): these are simply proportional close enough to the fixed point:

$$\Delta K = \Delta\beta \frac{\partial K}{\partial \beta}, \tag{2.16}$$

where the derivative is taken at the fixed point. By substituting this expression into eq. (2.15) and remembering that the values of $\beta(L_1)$ and $\beta(L_2)$ were chosen by requiring the corresponding ΔK to be equal, one obtains the relation (2.8).

Eq. (2.13) represents a scaling law for the $\Delta\beta$ shifts. A similar equation can be derived for the ΔK ones. We extend the Kadanoff ansatz for block couplings [9] to our generalised couplings; indeed, close enough to the fixed point a shift in the generalised coupling is linear in the shift of the true underlying block couplings. We therefore assume that the correlation length at the scale L has the same form as the one at the original scale when expressed in terms of the generalised couplings at the scale L.

If the original dependence is according to eq. (2.14), we write

$$\xi_\infty(L) = A'\left[K(L) - K_c\right]^{-\nu}. \tag{2.17}$$

Using eq. (2.9), we get

$$A'\left[K(L) - K_c\right]^{-\nu} = \frac{\xi_\infty(1)}{L}. \tag{2.18}$$

By intersecting horizontally, i.e. for a given value of K, the curves of the generalised couplings for different volumes as a function of β one obtains the $\Delta\beta(L)$ which can be used for the $\Delta\beta$ scaling law of eq. (2.15). The ΔK scaling is obtained by intersecting the same curves vertically, i.e. for a given value of β. There one has the same $\xi_\infty(1)$ for both volumes and the $\Delta K(L)$, defined as the difference between the value of K intersected, for a volume L, by the vertical curve and its fixed point value, should scale from eqs. (2.14) and (2.9) according to

$$\left[\Delta K(L_1)^{-\nu}\right] L_1 = \left[\Delta K(L_2)^{-\nu}\right] L_2. \tag{2.19}$$

The difference with the $\Delta\beta$ scaling law eq. (2.15) is just the exchange of the volumes. By taking the limit to the fixed point one recovers again eq. (2.8).

With an essential singularity one has two parameters to determine (B and ν). In this case, the $\Delta\beta$ scaling law of eq. (2.15) is replaced by

$$\exp\left(B\left\{\left[\Delta\beta(L_1)\right]^{-\nu} - \left[\Delta\beta(L_2)\right]^{-\nu}\right\}\right) = L_1/L_2, \tag{2.20}$$

where $\Delta\beta(L) = \beta(L) - \beta_c$ and the ΔK scaling law by

$$\exp\left(B'\left\{\left[\Delta K(L_1)\right]^{-\nu} - \left[\Delta K(L_2)\right]^{-\nu}\right\}\right) = L_2/L_1. \tag{2.21}$$

Notice that in the latter case one has in general a new parameter (B') depending upon the generalised coupling replacing the parameter B.

The index ν can be formally obtained by using two pairs of volumes and by eliminating B' from the corresponding equations. The result is

$$\frac{\left[\Delta K(L_1)\right]^{-\nu} - \left[\Delta K(L_2)\right]^{-\nu}}{\left[\Delta K(L_1)\right]^{-\nu} - \left[\Delta K(L_3)\right]^{-\nu}} = \frac{\ln(L_1/L_2)}{\ln(L_1/L_3)}. \tag{2.22}$$

Contrary to the algebraic case, the limit of this equation at the fixed point leads to a trivial result: indeed, by replacing $\Delta\beta$ with ΔK times the appropriate derivative one obtains

$$\frac{1 - D_{21}^{-\nu}}{1 - D_{31}^{-\nu}} = \frac{\ln(L_1/L_2)}{\ln(L_1/L_3)}, \tag{2.23}$$

where quantities D_{ij} are the derivatives of the generalised coupling at the volume L_i with respect to the corresponding coupling at the volume L_j. In the limit of small $\Delta\beta$ they all go to one, independently from the volume. This is a consequence of the following ΔK scaling ansatz from which eq. (2.22) has been derived:

$$\exp\left[B'(\Delta K)^{-\nu}\right] = C\frac{\exp\left[B(\Delta\beta)^{-\nu}\right]}{L}, \tag{2.24}$$

where C is some constant. This equation leads to

$$\lim_{\Delta\beta\to 0}\left(\frac{\Delta K(L_1)}{\Delta K(L_2)}\right)^{-\nu} = 1 - \frac{(\Delta\beta)^{\nu}}{B}\ln\left(\frac{L_1}{L_2}\right). \tag{2.25}$$

The expression in eq. (2.23) reduces in the limit $\Delta\beta \to 0$ to a trivial identity and cannot be used to extract the value of ν.

3. The *XY* model: the results

3.1. THE THERMAL EXPONENT

In the case of the XY model we have performed runs at $L = 16$, 24 and 32. The critical temperature is estimated to be

$$T_c = 0.899 \pm 0.002, \tag{3.1}$$

in agreement with the results of refs. [2, 3], and the critical values of K couplings:

$$K_1^c = 0.9485 \pm 0.0015, \qquad K_2^c = 10.1 \pm 0.1, \qquad K_3^c = 10.1 \pm 0.1, \tag{3.2}$$

where the error comes both from the volume dependence of the critical temperature and from the statistical accuracy of our results.

Although we have not attempted an exhaustive analysis to determine the exact form of the fixed point finite volume hamiltonian, we know from our result that it is dominated by the simple first neighbour interaction like in the original hamiltonian. In fig. 3 we plot the values of $K_1 - K_1(K_2)$ and of $K_1 - K_1(K_3)$ as a function of β, where $K_1(K)$ is the value that K_1 would have if there were a single first neighbour coupling K in the hamiltonian. Both differences are very small and go to zero at the fixed point, demonstrating the first neighbour coupling dominance. In the following we will restrict to the results for the coupling K_1 and K_2 only.

The values of ν are obtained from a χ^2 fit to the $\Delta\beta$ and to the ΔK scaling laws of eqs. (2.20) and (2.21). We have found that a fit with the temperatures, i.e. obtained by replacing β and K with their inverse in the quoted equations, leads to a

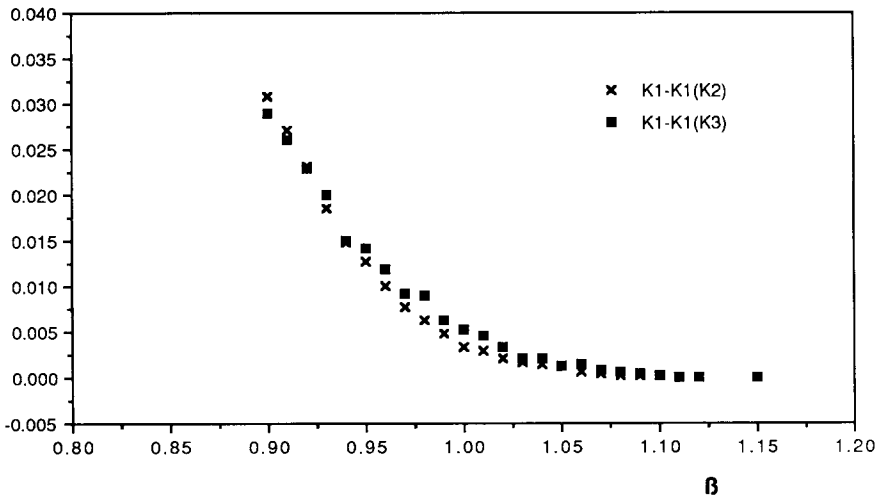

Fig. 3. The dependence upon β of the difference between the coupling K_1 and $K_1(K)$, i.e. its value if there was a single first neighbour interaction coupling in the block hamiltonian.

better χ^2. Our final results are quoted from such a fit. Tables 1 and 2 report the values of the generalised couplings K_1 and K_2 at different values of β and for different volumes which formed the basis of our fits. Fig. 4 shows the data for K_2 for β around β_c. The result of the fit to the ΔK scaling law are

$$\nu = 0.52 \pm 0.04 \quad \text{from the coupling } K_1\,, \tag{3.3}$$

and

$$\nu = 0.49 \pm 0.04 \quad \text{from the coupling } K_2\,, \tag{3.4}$$

with a χ^2 per degrees of freedom of 0.5 and 0.4, respectively. The quality of the fit is shown in fig. 5 where it is superimposed to the data points.

The error estimates includes both the statistical accuracy and the uncertainty in the value of the critical coupling. The latter dependence is shown in fig. 6 for the coupling K_2.

We have also checked the stability of our results for K_2 to the region of β values used for the fit. In the regions $1.07 \geqslant \beta > 1.01$ and $1.01 \geqslant \beta \geqslant 0.97$ we get $\nu = 0.50$ and $\nu = 0.49$ respectively, i.e. a difference in the results within our final error.

The fit to the $\Delta\beta$ scaling law is more unstable, mainly because, as can be seen from fig. 4, the higher the volume, the closer one gets to the critical value of β. In the case of the ΔK scaling things go the other way round. The simultaneous fit to both B and ν gives

$$B = 1.9 \pm 0.3\,, \qquad \nu = 0.46 \pm 0.04\,, \tag{3.5}$$

TABLE 1
The values of the generalised coupling K_1 for different volumes and as a function of β

β	$K_1(16)$	$K_1(24)$	$K_1(32)$
0.90	0.806(1)	0.697(2)	0.586(2)
0.91	0.827(1)	0.730(2)	0.629(2)
0.92	0.844(1)	0.760(2)	0.674(2)
0.93	0.860(1)	0.795(1)	0.716(2)
0.94	0.8742(9)	0.819(1)	0.753(2)
0.95	0.8848(8)	0.844(1)	0.793(2)
0.96	0.8947(7)	0.864(1)	0.824(2)
0.97	0.9034(7)	0.877(1)	0.848(1)
0.98	0.9103(6)	0.8932(9)	0.870(1)
0.99	0.9164(6)	0.9031(7)	0.886(1)
1.00	0.9225(5)	0.9129(6)	0.9013(9)
1.01	0.9267(5)	0.9196(5)	0.9119(7)
1.02	0.9301(4)	0.9260(4)	0.9199(5)
1.03	0.9332(4)	0.9306(3)	0.9257(5)
1.04	0.9362(4)	0.9332(4)	0.9310(4)
1.05	0.9381(4)	0.9365(3)	0.9345(4)
1.06	0.9409(3)	0.9394(3)	0.9381(2)
1.07	0.9428(4)	0.9418(3)	0.9408(2)
1.08	0.9446(3)	0.9440(2)	0.9430(2)
1.09	0.9460(3)	0.9457(2)	0.9452(2)
1.10	0.9474(2)	0.9471(1)	0.9469(1)
1.11	0.9486(4)	0.9487(1)	0.9484(2)
1.12	0.9501(2)	0.9499(2)	0.9499(2)
1.15	0.9528(3)	0.9533(1)	0.9532(2)
1.18	0.9555(3)	0.9559(1)	0.9559(1)

while, by imposing the value of ν obtained from the ΔK fit, we get for B

$$B = 1.65 \pm 0.2. \tag{3.6}$$

We consider this our best estimate of the parameter B. The analysis of Kosterlitz and Thouless and later studies based on analytic renormalisation group recursion relations give $\nu = 0.5$ exactly and a value for the non-universal parameter B around 1.6. Our results confirm their estimates within the errors. They are more precise than those of ref. [2] and are obtained using sizes typically smaller by a factor four to ten. The results of ref. [3] appear to be much more precise than ours but their error estimates are not explicitly explained.

Some of the past analyses have tried to argue in favour of a conventional algebraic type singularity at the fixed point. Already the matching of the couplings K beyond the critical temperature is a confirmation of the BKT picture. If we make

TABLE 2
The values of the generalised coupling K_2 for different volumes and as a function of β

β	$K_2(16)$	$K_2(24)$	$K_2(32)$
0.90	3.43(2)	2.28(1)	1.61(1)
0.91	3.76(2)	2.56(2)	1.84(1)
0.92	4.09(2)	2.86(2)	2.12(1)
0.93	4.43(2)	3.28(2)	2.44(2)
0.94	4.84(3)	3.64(2)	2.79(2)
0.95	5.19(3)	4.09(2)	3.23(2)
0.96	5.55(3)	4.56(2)	3.72(2)
0.97	5.93(3)	4.93(3)	4.17(3)
0.98	6.29(3)	5.49(3)	4.75(3)
0.99	6.63(3)	5.90(3)	5.21(3)
1.00	7.03(4)	6.42(3)	5.82(3)
1.01	7.40(4)	6.81(3)	6.35(3)
1.02	7.66(4)	7.28(3)	6.82(3)
1.03	7.95(4)	7.66(3)	7.25(3)
1.04	8.30(4)	7.96(3)	7.69(3)
1.05	8.51(5)	8.29(3)	8.05(4)
1.06	8.82(5)	8.61(3)	8.44(2)
1.07	9.09(7)	8.94(4)	8.79(3)
1.08	9.34(4)	9.23(3)	9.09(3)
1.09	9.58(5)	9.51(3)	9.41(4)
1.10	9.81(4)	9.75(3)	9.70(2)
1.11	10.02(7)	10.01(2)	9.99(4)
1.12	10.30(5)	10.26(3)	10.26(3)
1.15	10.85(7)	10.96(3)	10.95(3)
1.18	11.50(8)	11.58(3)	11.60(3)

a fit to our data using a behaviour like in eq. (2.15), we get the following result:

$$\nu_{\text{algebraic}} = 1.35 \pm 0.35, \tag{3.7}$$

with a χ^2 per degrees of freedom of ...10! This clearly shows the inadequacy of such an interpretation.

Fig. 7 reports the value of $\nu_{\text{algebraic}}$ estimated from different regions of β: the steady increase with increasing β is inconsistent with a constant value of a conventional algebraic type singularity. The increasing ν is the way the data indicate a singularity stronger than algebraic. This behaviour was never clearly seen in previous numerical analyses and agrees with the recent analytic estimates based on a high temperature expansion and discussed in ref. [5].

3.2. THE MAGNETIC EXPONENT

The exponent η relates the correlation length ξ with the magnetic susceptibility χ according to eq. (2.7) and is connected to the magnetic exponent y_H governing the

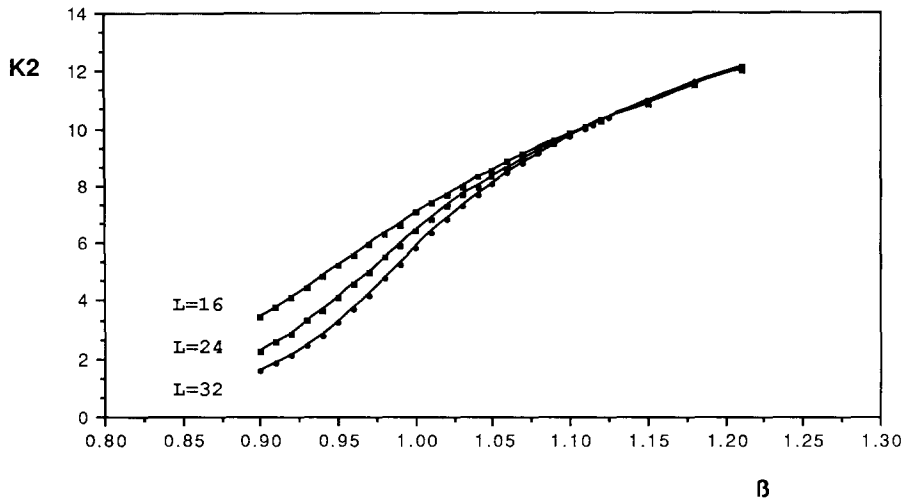

Fig. 4. The behaviour of $K_2(L)$ for different values of L near $\beta = \beta_c$.

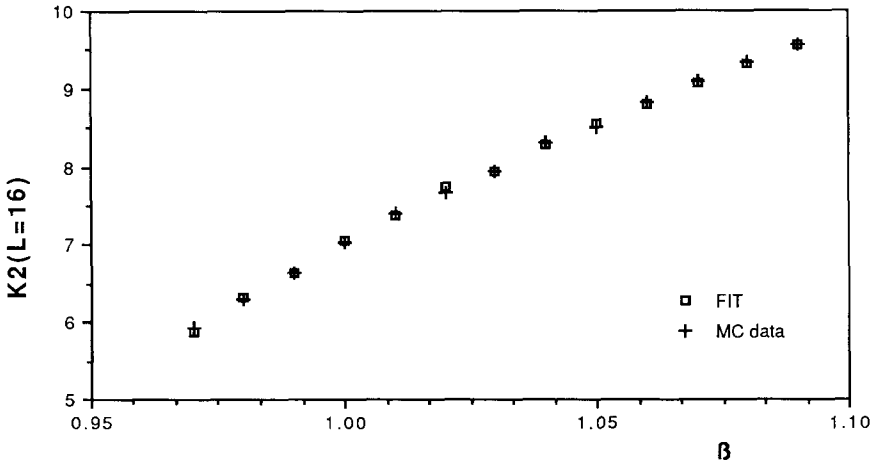

Fig. 5. The ΔK shift superimposed to the data for K_2 at $L = 16$ as a function of β: the statistical errors have a size of the order of the data points.

behaviour of the free energy F in the presence of an external magnetic field h in the scaling region:

$$F = A\xi^{-d} G\left[\frac{\xi}{h^{-\mu}}\right], \tag{3.8}$$

where $\mu = 1/y_H$. The relation between η and y_H is

$$\eta = 2 + d - 2y_H = 4 - 2y_H. \tag{3.9}$$

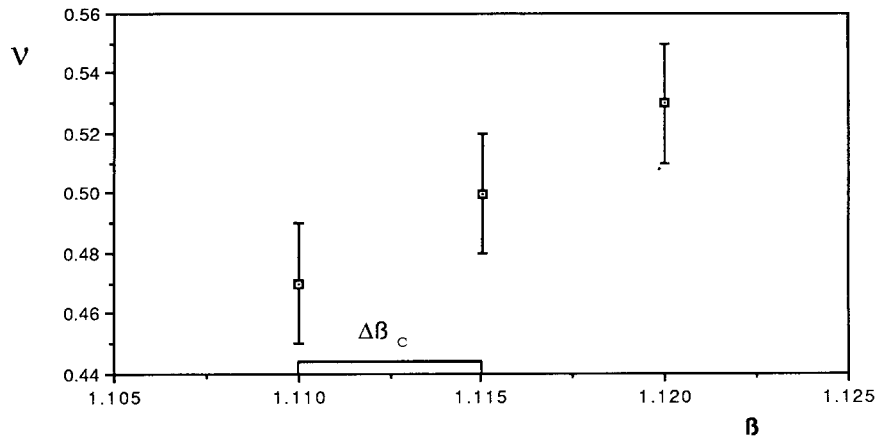

Fig. 6. The dependence of ν extracted from the ΔK fit upon the value of the critical temperature.

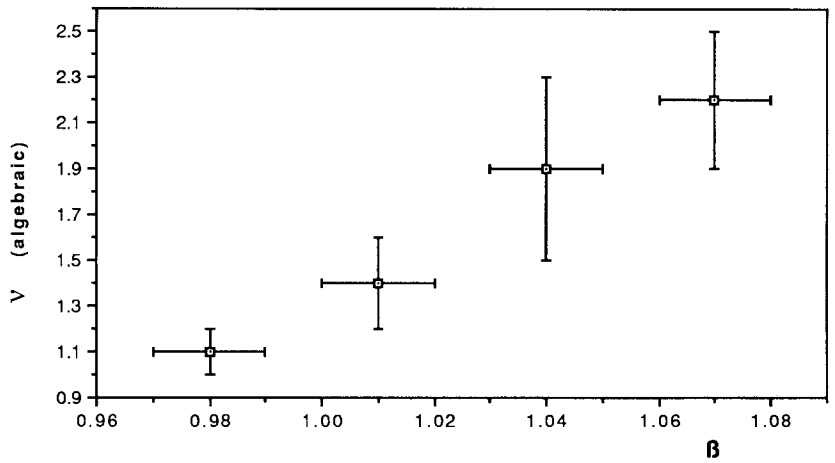

Fig. 7. The value of $\nu_{\text{algebraic}}$ estimated from different regions of β.

Eq. (3.8) fixes the dynamic dimensions of the magnetic field h in correlation length units and states that in the limit $\xi \to \infty$ and $h \to 0$, i.e. close to the phase transition at zero magnetic field, the physics stays the same along the lines of constant $\xi/h^{-\mu}$. This remains true also if both the correlation length and the magnetic field are defined at a scale length L:

$$\ln[\xi(L)] = -\mu \ln[h(L)] + \text{constant}. \tag{3.10}$$

Using eq. (2.9) relating the correlation length at two different scales for a fixed value of β, one obtains a simple scaling law for the magnetic field at the scales L_1

and L_2:

$$\ln\left(\frac{L_1}{L_2}\right) = \mu \ln\left(\frac{h(L_1)}{h(L_2)}\right). \tag{3.11}$$

Since the critical value for h is zero, one can interpret $h(L)$ as $\Delta h(L)$, i.e. the difference between the coupling and their fixed point values and replace the ratio in eq. (3.11) with the corresponding derivative taken at the critical value of β and at h, the original magnetic field at scale 1, set equal to 0. We obtain the equation fixing y_H:

$$\ln\left(\frac{L_1}{L_2}\right) = \frac{1}{y_H}\ln\left(\frac{\partial h(L_1)}{\partial h(L_2)}\right) = \frac{1}{y_H}\ln\left(\frac{\partial h(L_1)/\partial h}{\partial h(L_2)/\partial h}\right)_{h=0}. \tag{3.12}$$

One can replace the block magnetic fields with any correlation which is odd under the operation of spin reflection: we have chosen the most straightforward, the total block magnetisation defined as

$$\boldsymbol{M}(L) = \boldsymbol{S}^A(L) + \boldsymbol{S}^B(L). \tag{3.13}$$

The derivative of the block magnetisation with respect to the original magnetic field h taken at $h = 0$ of eq. (3.12) is just the connected part of its scalar product with the original total magnetisation (*not* averaged over the spins) at zero magnetic field and at the critical β. This quantity is even under spin reflection and does not vanish at zero magnetic field.

The results for η are reported in fig. 8 for T near T_c and in fig. 9 for T around zero, where they successfully compare with the expected linear decrease with the

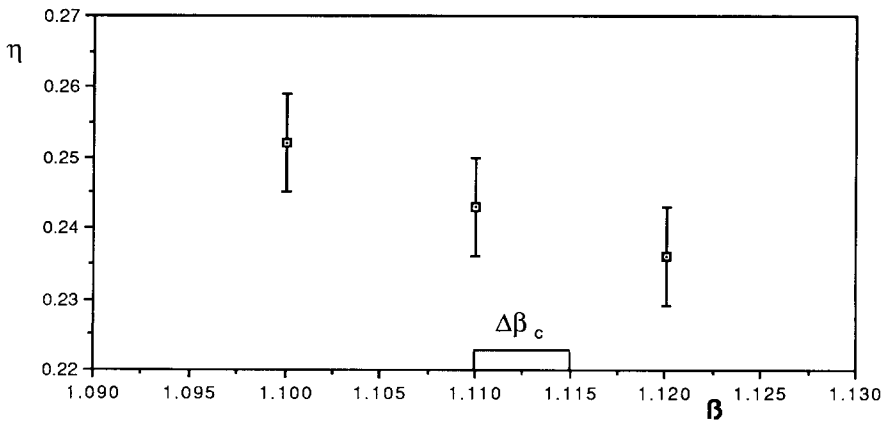

Fig. 8. The exponent η around the critical temperature.

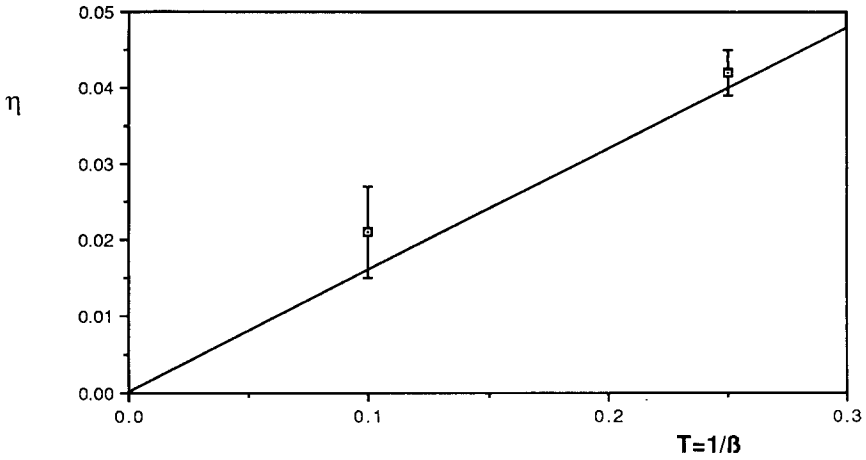

Fig. 9. The exponent η near $T = 0$: the full line is the theoretical expectation.

temperature [1]

$$\eta_{T\to 0} = \frac{T}{2\pi} . \tag{3.14}$$

At the critical temperature we get

$$\eta = 0.243 \pm 0.007 . \tag{3.15}$$

These results are in perfect agreement with the BKT prediction and with the experimental results obtained from thin films of superfluid helium [10]. They are far better than those of refs. [2, 3].

4. The Heisenberg model

With the same method we have analysed the Heisenberg model in two dimensions defined by the hamiltonian in eq. (2.1) where, however, the spins lie on a sphere instead of a circle. The divergence of the correlation length is expected to be of the same type as for the XY model, but the fixed point is at zero temperature. Borrowing the terminology of gauge theories, the model is asymptotically free and one can calculate the values of B and ν appropriate to this case from a weak coupling expansion. The result is [11]

$$B = 2\pi \quad \text{and} \quad \nu = 1 . \tag{4.1}$$

Two loop calculations also allow us to determine the next to leading contribution to the asymptotic scaling law for the correlation length [11], which reads

$$\xi_\infty(\beta) = \text{const.} \frac{\exp(2\pi\beta)}{1 + 2\pi\beta} . \tag{4.2}$$

Following the same procedure adopted for the XY model, we define block spins $\boldsymbol{S}_A$ and $\boldsymbol{S}_B$ which are the generalisation to the O(3) case of eq. (2.2). The generalised couplings J_1 and J_2 are the analog of K_1 and K_2 and are defined by

$$J_1 = \langle \cos \theta_{AB} \rangle , \qquad J_2 = 2 \frac{\langle \cos \theta_{AB} \rangle}{\langle \sin^2 \theta_{AB} \rangle} , \tag{4.3}$$

where θ_{AB} is the relative angle between the two block spins. If the effective hamiltonian had the same form as the original one, J_2 would be its coupling, as can be seen from the following Schwinger–Dyson equation:

$$\int_1^{-1} \mathrm{d} \cos \theta_{AB} \frac{\mathrm{d}}{\mathrm{d} \cos \theta_{AB}} \left[\sin^2 \theta_{AB} \exp(J_2 \cos \theta_{AB}) \right] = 0 . \tag{4.4}$$

We have performed runs between $\beta = 1.6$ and $\beta = 2.3$ on squares with $L = 20$, 26 and 32 using also in this case an algorithm obtained by alternating one standard Metropolis sweep with five microcanonical sweeps where, in the plane identified by a given spin and the resultant of its first neighbours, one performs the same operation already defined for the XY model. We have used statistics similar to those for the XY model, by performing a total of 3.6×10^5 iterations including 10^5 thermalisation sweeps (TS) for the volume $L = 20$, of 4×10^5 iterations with 2×10^5 TS for $L = 26$ and of 4.4×10^5 iterations with 2×10^5 TS for $L = 32$. We get a relative statistical error on the generalised block couplings of the order of 10^{-4} for J_1 and of 10^{-3} for J_2. The error analysis has been done as in the previous case.

TABLE 3
The values of the generalised coupling J_1 for different volumes and as a function of β

β	$J_1(20)$	$J_1(26)$	$J_1(32)$
1.600	0.8788(3)		
1.646		0.8796(3)	
1.682			0.8803(3)
1.800	0.9198(2)		
1.845		0.9200(2)	
1.881			0.9205(2)
2.000	0.9371(2)		
2.045		0.9373(2)	
2.080			0.9373(2)
2.100	0.9425(2)		
2.145		0.9429(1)	
2.180			0.9432(1)
2.200	0.9475(1)		
2.245		0.9475(1)	
2.280			0.9479(1)

TABLE 4
The values of the generalised coupling J_2 for different volumes and as a function of β

β	$J_2(20)$	$J_2(26)$	$J_2(32)$
1.600	2.101(5)		
1.646		2.109(5)	
1.682			2.118(5)
1.800	3.123(7)		
1.845		3.127(7)	
1.881			3.146(7)
2.000	3.98(1)		
2.045		4.00(1)	
2.080			3.99(1)
2.100	4.36(1)		
2.145		4.37(1)	
2.180			4.39(1)
2.200	4.76(1)		
2.245		4.77(1)	
2.280			4.79(1)

The fixed point is expected at infinite β. We have identified the onset of the scaling region between $\beta = 1.6$ and $\beta = 1.8$. The effective hamiltonian tends to the simple first neighbour form of the original hamiltonian as one moves closer to the fixed point. Fig. 10 shows the quantity $J_1 - J_1(J_2)$ as a function of β, where $J_1(J_2)$ is the value of J_1 if J_2 was the sole coupling and is given by

$$J_1(J_2) = \operatorname{cotanh}(J_2) - \frac{1}{J_2}. \tag{4.5}$$

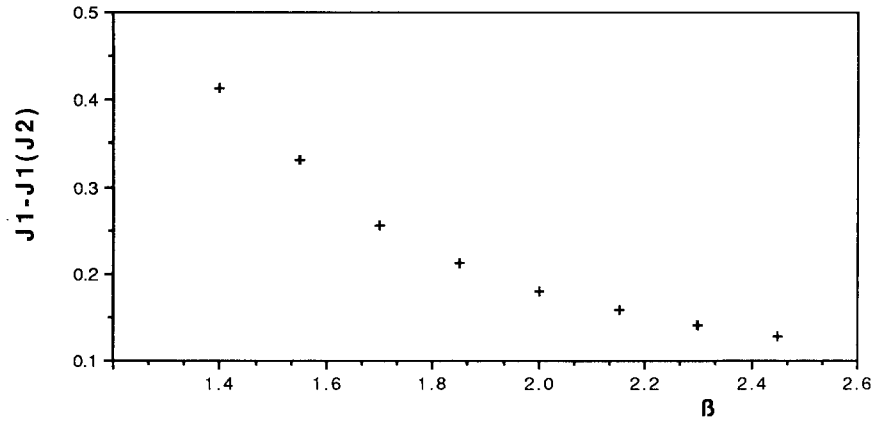

Fig. 10. The same as in fig. 3 for the J block couplings of the Heisenberg model.

Like in the XY case, the relevance of extra couplings vanishes with β approaching β_c. Using the results of refs. [2, 11], one can see that, in the region of β that we have explored, the typical infinite volume correlation length for this model is of the same order as the one we have been dealing with in the region of β near β_c that we have analysed for the XY model, i.e. of about 600 lattice units.

From the behaviour of J_1 and J_2 between $\beta = 1.6$ and $\beta = 2.3$ on the volumes $L = 20$, 26 and 32 we could determine the values of B and ν using the assumptions already discussed for the XY model. The $\Delta\beta$ scaling from two different volumes L_1 and L_2 leads to the equation

$$2\pi\left[\beta(L_1) - \beta(L_2)\right] = \ln\left(\frac{1 + 2\pi\beta(L_1)}{1 + 2\pi\beta(L_2)}\right) + \ln\left(\frac{L_1}{L_2}\right), \tag{4.6}$$

which essentially predicts a constant shift in β for the curves referring to couplings normalised at two different scales.

The ΔJ scaling (what we called before the ΔK scaling), neglecting the two loops corrections, leads to

$$\text{const.}\left[J(L_1) - J(L_2)\right] = \ln\left(\frac{L_2}{L_1}\right), \tag{4.7}$$

where the constant is unknown and varies with the choice of the generalised coupling.

Fig. 11 shows that the predicted constant shift in $\Delta\beta$ *and* ΔJ is indeed realised in the scaling region. We have therefore decided to compare directly in figs. 12a and

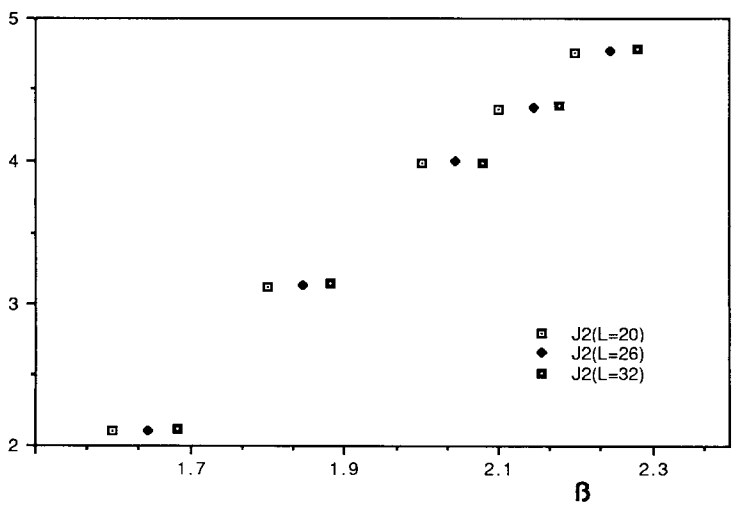

Fig. 11. The behaviour of J_2 for different volumes as a function of β.

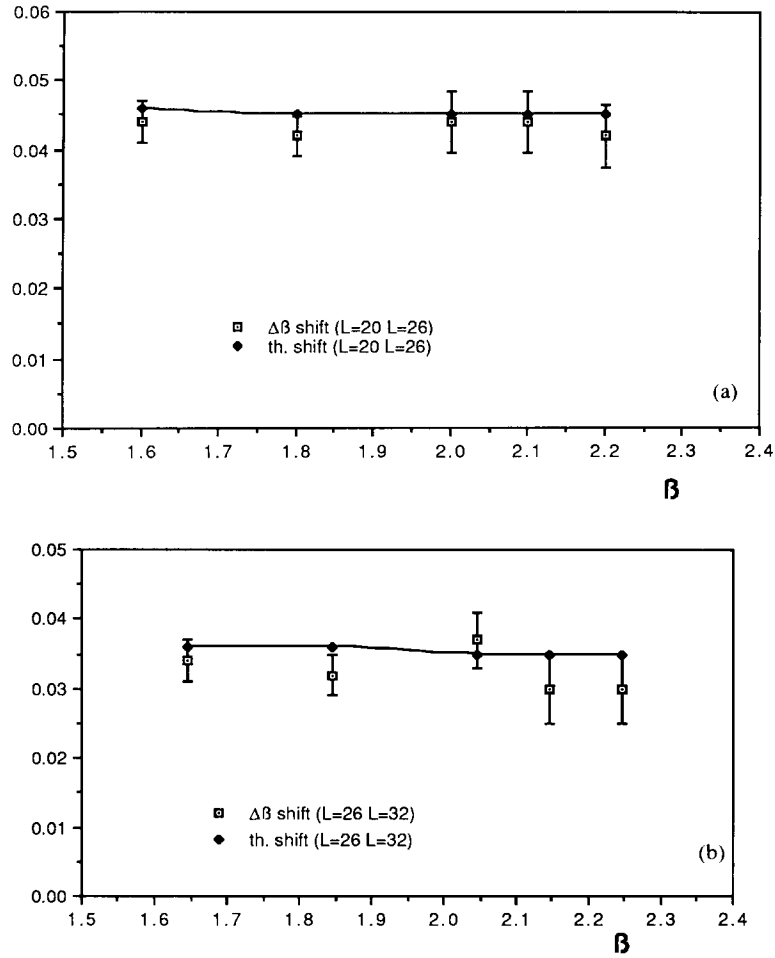

Fig. 12. (a) The $\Delta\beta$ shift is compared with the theoretical asymptotic scaling law (full line) for the volumes $L = 20$ and $L = 26$ and the coupling J_2. (b) The $\Delta\beta$ shift is compared with the theoretical asymptotic scaling law (full line) for the volumes $L = 26$ and $L = 32$ and the coupling J_2.

12b the $\Delta\beta$ obtained by imposing the matching of J_2 between the $L = 20$ and $L = 26$ and between $L = 26$ and $L = 32$ respectively with the prediction of eq. (4.6). With three volumes one can eliminate the constant in eq. (4.7) and check the ΔJ shift for J_2 at the same β: this is shown in fig. 13. The choice of the β points at different volumes has been made according to the $\Delta\beta$ shift expected theoretically: when used for the test of the ΔJ shift these points need interpolations which increase the size of the final error. The figures for the coupling J_1 are of similar quality: the data for both couplings are collected in tables 3 and 4. The $\Delta\beta$ tends to be smaller than expected at small β because of a peak in the specific heat [12]

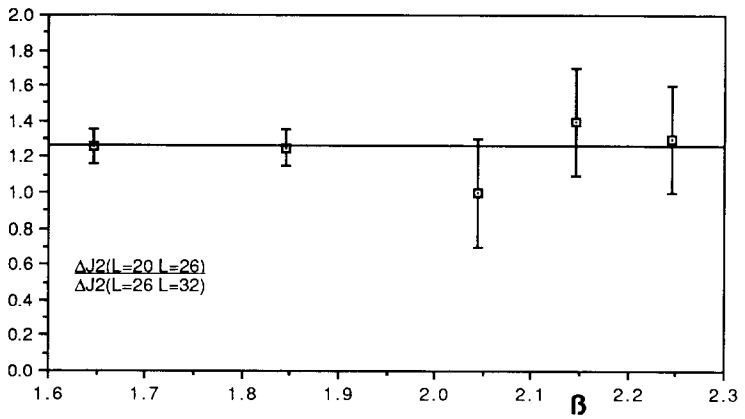

Fig. 13. The ΔJ_2 shift between volumes $L = 20$ and $L = 26$ compared with the one between $L = 26$ and $L = 32$ as a function of β.

around $\beta = 1.5$ which, on volumes smaller than the ones we have used, produces even a fictitious matching of the block couplings, i.e. $\Delta\beta = 0$. The decrease of $\Delta\beta$ at the highest values of β can be justified with a shift of the critical temperature from zero to a finite value which is expected to occur on finite volumes.

The results we have obtained exhibit the scaling behaviour predicted by the asymptotic freedom of the theory which implies the existence of a fixed point only at $\beta = \infty$.

5. Conclusions

The XY and the Heisenberg model in two dimensions are both characterised by an essential singularity in the correlation length at the critical temperature. We have investigated their properties with the real space finite size renormalisation group method. The results confirm for the XY model the BKT analysis and in particular we obtain accurate determinations of the exponents ν and η. The possibility of a conventional algebraic transition turns out to be inconsistent and is excluded from our analysis. For the Heisenberg model the validity of the scaling law predicted by a weak coupling renormalisation group improved expansion is established, ruling out the existence of a phase transition at finite temperature. The results have been obtained on lattices by one–two order of magnitude smaller than those needed in previous analyses for reaching a comparable accuracy: actually, in the case of the η exponent for the XY model, our results are the most precise. The renormalisation group study of a finite size hamiltonian has proven an efficient and economical way of investigating the critical properties of theories with logarithmic scaling violations.

The numerical calculations described in this paper amount to about one hundred CPU hours of the CRAY XMP/48 at CERN. We are grateful to the CERN theory and computer divisions for the time allocated to us and in particular to Eric McIntosh for its assistance. One of us (R.P.) thanks the CERN theory division for the hospitality extended to him when this work was started.

References

[1] V.L. Berezinskii, Sov. Phys. JETP 32 (1970) 493;
J.M. Kosterlitz and D.J. Thouless, J. Phys. C6 (1973) 1181;
J.M. Kosterlitz, J. Phys. C7 (1974) 1646

[2] J. Tobochnik and G.V. Chester, Phys. Rev. B20 (1979) 3761;
J. Fernandez, M. Ferreira and J. Stankiewicz, Phys. Rev. B34 (1986) 292

[3] R. Gupta et al., The phase transitions in the 2-d *XY* model, Los Alamos National Laboratory preprint LA-UR-88-2021

[4] E. Seiler, I.O. Stamatescu, A. Patrasciou and V. Linke, Phys. Rev. Lett. 60 (1988) 875

[5] P. Butera, M. Comi and G. Marchesini, Critical behaviour of the 2-d *XY* model: an analysis of extended high temperature series, preprint IFUM-399/FT, UPRF-88-225 (July 1988)

[6] S.K. Ma, Phys. Rev. Lett. 37, (1976) 471;
K. Wilson, unpublished;
for a review of further references, see R.H. Swendsen, *in* Real space renormalisation, ed. T.W. Burkhardt and J.M.J. van Leeuwen (Springer, Berlin, 1982); Phys. Rev. Lett. 42 (1979) 856

[7] R. Benzi and R. Petronzio, Finite size real space renormalisation group, MPI-PAE/PTH 44/88

[8] M.N. Barber, *in* Phase transitions and critical phenomena, Vol. VIII, ed. C. Domb and J. Lebowitz (Academic Press, New York, 1984);
M.P. Nightingale, Physica 83A (1976) 561;
H.H. Roomany and H.W. Wyld, Phys. Rev. D21 (1980) 3341

[9] K. Wilson and J. Kogut, Phys. Rep. 12 (1974) 75

[10] I. Rudnick, Phys. Rev. Lett. 40 (1978) 1454;
D.J. Bishop and J. Reppy, Phys. Rev. Lett. 40 (1978) 1727

[11] See for example A.M. Polyakov, *in* Gauge fields and strings, Contemporary Concepts in Physics, Vol. 3 (Harwood Academic Publishers, Chur, 1987)

[12] G. Martinelli, G. Parisi and R. Petronzio, Phys. Lett. B100 (1981) 485;
G. Fox, R. Gupta, O. Martin and S. Otto, Nucl. Phys. B205 [FS5] (1982) 188;
M. Fukugita and Y. Oyanagi, Phys. Lett. B123 (1983) 71