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Essential singularity in the *XY* spin-1 chain with uniaxial anisotropy

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Abstract. We have performed finite-cell calculations on the one-dimensional spin-1 *XY* model with transverse anisotropy. Infinite size extrapolation of the results shows strong evidence for a transition at $T = 0$ by increasing the strength of the anisotropy with peculiar scaling properties characteristic of an essential singularity. Thus, this quantum chain, which is a simple truncated version of the quantum formulation of the classical $2d$ *XY* model, behaves very similarly to its classical analogue.

1. Introduction

There has been a growing interest in the theory of phase transitions in two dimensions since the discovery by Kosterlitz and Thouless (1973) of a 'line of fixed points' in the planar Heisenberg model (the O(2) model) in two dimensions. In such a model, the susceptibility diverges at a characteristic temperature as the temperature is lowered, remaining infinite in the whole low-temperature phase. The nature of the singularity near the characteristic temperature is very peculiar: just above the critical point the coherence length is predicted to diverge more rapidly than any power law (Kosterlitz 1974). This behaviour is characteristic of a so called 'essential singularity'.

Recently an interesting quantum formulation of the O(n) model has been derived (Hamer and Kogut 1979, Kogut 1979). Using a continuous time, discrete spatial lattice, the d-dimensional classical model is shown to be equivalent to a $(d-1)$-dimensional quantum Hamiltonian of coupled rotators. Approximate methods on the quantum version of the O(2) model, such as strong coupling series expansions (Hamer and Kogut 1979) as well as very recent finite-cell scaling calculations (Hamer and Barber 1981) confirm the existence of a transition with an essential singularity.

Here we are concerned by a very simple one-dimensional quantum Hamiltonian which can be interpreted as a truncated version (by retaining only the three lowest levels of each rotator) of the quantum formulation of the O(2) model. This model consists in an *XY* spin-one chain with a uniaxial transverse anisotropy and is described by the following Hamiltonian

$$\mathcal{H} = -J \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + D \sum_i (S_i^z)^2 \qquad (1)$$

where S^x, S^y, S^z are usual spin-one Pauli matrices and where J and D ($D > 0$) represent

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the strength of the XY coupling and the anisotropy, respectively. By considering the limiting cases $x = D/J = 0$ and $x = D/J = \infty$ in which the ground state of the system is respectively degenerate and non-degenerate, we expect a transition at $T = 0$ by increasing the strength of the anisotropy. By continuity from the $D = 0$ limiting case, we expect that in the low-D phase there is no spontaneous magnetisation (i.e. $\langle S_i^x \rangle = 0$), as in the $2d$ O(2) model. It is, however, not obvious that the transition would occur at a non-zero $x_c = (D/J)_c$ value and that the critical behaviour would be characteristic of an essential singularity since, due to the truncation, the Hamiltonian is not strictly equivalent to the O(2) model.

Hamiltonian (1) has been already considered by Luther and Scalapino (1977) as a simple representation of the classical planar $2d$ model. However, their treatment which consists in replacing a spin-1 by two spins-$\frac{1}{2}$ is doubtful, as confirmed to us by one of the authors (D Scalapino, private communication). Also, by considering this model as a truncated representation of a more complicated Hamiltonian of coupled spin-$\frac{1}{2}$ chains we have done real-space renormalisation group calculations on Hamiltonian (1) and we were unable to recover the essential singularity (Jullien *et al* 1979).

In this paper, we present the results of finite-cell scaling calculations on Hamiltonian (1) similar to those performed by Hamer and Barber (1980) on the more general coupled rotator Hamiltonian. From the present calculations there is strong evidence for an essential singularity, showing that the truncation in energy does not affect the general properties of the O(2) model. Thus, Hamiltonian (1) constitutes a very simple and very useful representation of the O(2) model. We, however, cannot study the precise form of the essential singularity and we cannot show that it is exactly the same as for the $2d\,XY$ model.

2. Method

Finite-cell scaling, as introduced by Fisher and Barber (1972), asserts that in a finite system of size N the physical quantities follow the same scaling equations near the critical point as in the infinite system. For example, in the case of the gap $G(D/J, N)$ between the ground state and the first excited level, we set

$$G \sim N^{-z} f(N^{1/\nu} \Delta x) \tag{2}$$

where

$$\Delta x \sim D/J - (D/J)_c \tag{3}$$

and where f is a given (regular) scaling function. The exponent ν appearing in (2) describes the divergence of the coherence length at the transition:

$$\xi \sim \Delta x^{-\nu}. \tag{4}$$

The exponent z defined by (2) is the 'dynamical' exponent which tells us how the gap scales with size at the critical point. For a quantum Hamiltonian derived directly from a classical model, z must be strictly equal to one since in the correspondence with the classical system, G^{-1} corresponds to the coherence length in the extra (time) dimensionality (Kogut 1979). Considering that, here, the Hamiltonian is not strictly equivalent to a classical system (due to the truncation in energy) the equality $z = 1$ must be checked.

In the following we will also consider the derivative of the gap with respect to the dimensionless parameter $x = D/J$. From (2), G' obeys the scaling relation:

$$G' \sim N^{-z+1/\nu} g(N^{1/\nu} \Delta x). \tag{5}$$

It follows from (2) and (5) that the decay of G/G' with size at the transition ($\Delta x = 0$) is simply governed by the exponent $1/\nu$:

$$G/G' \sim N^{-1/\nu}. \tag{6}$$

We have calculated G and G' by diagonalising exactly Hamiltonian (1) for finite cells of N spins with periodic boundary conditions. The diagonalisation has been done in each subspace corresponding to integer values of ΣS_i^z ranging from $-N$ to $+N$. In each subspace we have constructed the ground state iteratively by using the Lanczos method (Whitehead 1980) which appears to be really powerful for such finite-cell calculations (Roomany *et al* 1980, Hamer and Barber 1981). We have observed that

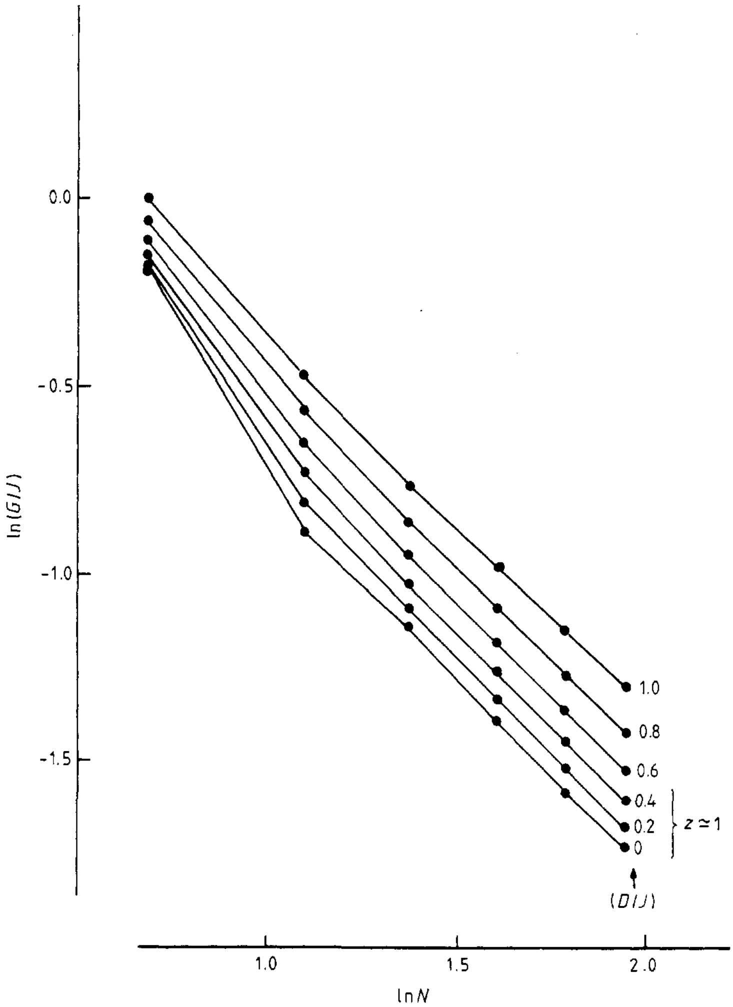

Figure 1. Plot of $\ln(G/J)$ as a function of $\ln N$ for different D/J values.

the absolute ground state of the chain always corresponds to $\Sigma S_i^z = 0$, while the first excited states (a doublet) correspond to $\Sigma S_i^z = \pm 1$. We have been able to calculate the gap $G(D/J, N)$ as well as its first derivative with respect to $x = D/J$, for any value of x and for N varying up to $N = 7$. The results are now analysed in the next section in view of the scaling equations (2) and (6).

3. Results

In order to estimate the exponent z we have first plotted $\ln G$ as a function of $\ln N$ (figure 1) for several values of $x = D/J$. For ordinary phase transitions the relation must be asymptotically ($N \to \infty$) linear only for $x = x_c$, the slope giving $-z$ at the transition. Here we observe that the linearity is asymptotically verified, leading to $z = 1$, in an extended range of low D/J values from 0 up to $D/J \simeq 0.4$. This is already a first indication for a line of fixed points, but it does not allow us a precise evaluation of $(D/J)_c$.

Assuming $z = 1$, we have used equation (2) as in the phenomenological renormalisation group (Nightingale 1976, Sneddon 1978). Comparing adjacent sizes N and $N+1$, we have determined the location of the transition x_c by the implicit equation:

$$NG(x_c, N) = (N+1)G(x_c, N+1) \tag{7}$$

and ν by linearising the RG equation at the fixed point:

$$\nu = \ln \frac{N}{N+1} \Big/ \ln \left(\frac{NG'(x_c, N)}{(N+1)G'(x_c, N+1)} \right). \tag{8}$$

In figures 2 and 3 we have reported the results as a plot of $(D/J)_c$ and $1/\nu$ respectively as a function of $1/N$. Despite odd–even size oscillations, the critical value extrapolates quite well for $N \to \infty$ to a non-zero value $(D/J)_c \simeq 0.4$ while $1/\nu$ seems to converge to zero or to an extremely small value. This last result ($\nu \simeq \infty$) is a strong argument for an essential singularity at $(D/J)_c$.

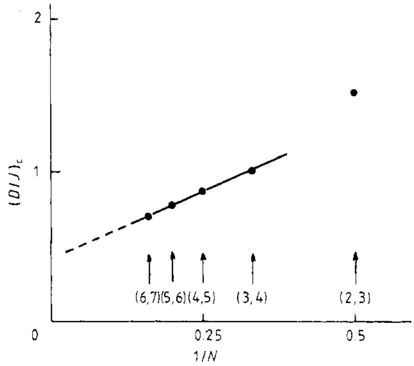

Figure 2. Results of the phenomenological renormalisation group calculations when comparing sizes N and $N+1$: plot of $(D/J)_c$ as a function of $1/N$.

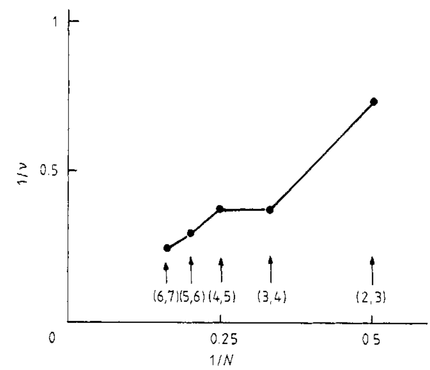

Figure 3. Results of the phenomenological renormalisation group calculations when comparing sizes N and $N+1$: plot of $1/\nu$ as a function of $1/N$.

In order to make this last point precise, in figure 4 we have reported $\ln(G/G')$ as a function of $\ln N$ for several $x = D/J$ values. We again observe odd–even size oscillations in the low D/J phase. But let us focus on the asymptotic slope of the curves which can be reasonably estimated to be strictly zero in the whole range $D/J \leqslant 0.4$, while the curve starts to deviate from this behaviour (and the oscillations disappear) for larger anisotropies. Here also, we cannot deduce any precise value for $(D/J)_c$. However, all these results are consistent with a transition at about $(D/J) \simeq 0.4$ with an essential singularity. Any further scaling analysis, in particular any attempt to extract the essential singularity index σ (assuming $\xi \sim \exp(b/\Delta x^{\sigma})$) would be really doubtful.

An interesting point is the existence of size oscillations for low D/J values which could be an indication for oscillating correlation functions in this low anisotropy phase, as in the low-field phase of the spin-$\frac{1}{2}$ XY chain in a transverse field (Barouch and McCoy 1970).

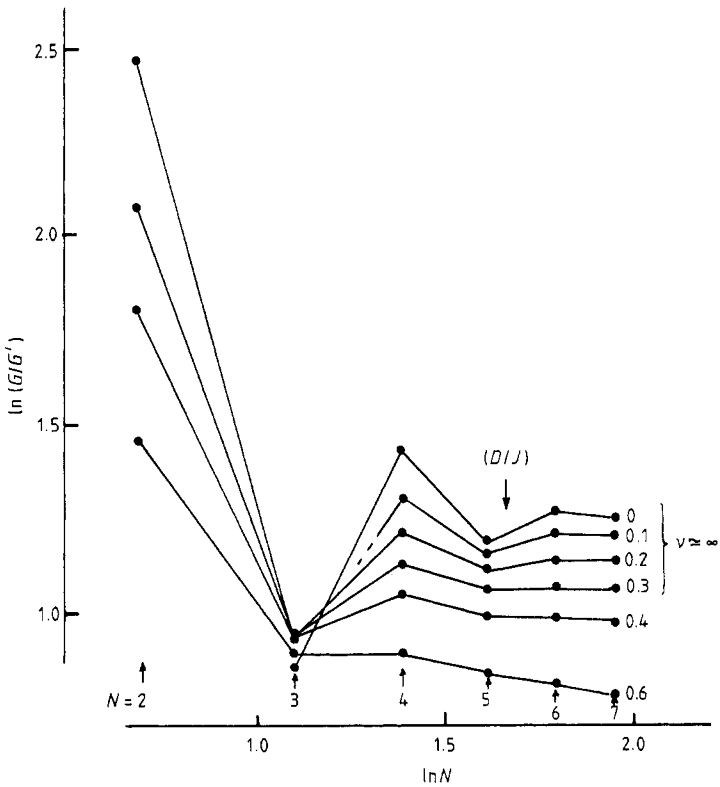

Figure 4. Plot of $\ln(G/G')$ as a function of $\ln N$ for different D/J values.

4. Conclusion

From finite-size scaling calculations we have presented strong evidence for a transition with an essential singularity in the spin-1 XY chain with anisotropy. This quantum model, which is an approximate representation of the $2d$ classical XY model, seems to behave as its classical analogue. The main conclusion from this calculation is that the truncation in energy has no dramatic effect on the main properties. It would be interesting to extend these calculation to the other truncated representations of the O(n) models for $n > 2$ in two dimensions which consist of spin-$\frac{3}{2}$, spin-2 . . . chains.

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