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LETTER TO THE EDITOR

Conformal invariance and the phase transition of a spin chain with three-spin interaction

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Abstract. The ground-state properties of a quantum spin chain with three-spin couplings are investigated using finite-size calculations. The results are compared with the predictions of conformal invariance for finite systems at the critical point. The critical exponents η_E and η_S of energy density and spin correlation functions are calculated and estimated to be $\eta_E \simeq 1.30$ and $\eta_S \simeq 0.25$. The results suggest that this model is conformally invariant with a central charge very close to or equal to one.

Recently, models of systems with multibody interactions have received considerable attention. It is known by now that n-body interactions lead to critical behaviour with n-dependent universality classes. In two dimensions (2D) cases in point are the exactly solvable Baxter ($n = 2, 4$) (Baxter 1972) and the Baxter–Wu ($n = 3$) (Baxter and Wu 1973) models.

To study phase transitions systematically as a function of the multiplicity n of interactions a spin model with anisotropic n-spin couplings has been introduced (Penson *et al* 1982, Turban 1982). Here we consider the 1D quantum version (Suzuki 1976) of this model with the Hamiltonian

$$H = -J_n \sum_{l=1}^{L} s_{l+1}^x s_{l+2}^x \dots s_{l+n}^x - h \sum_{l=1}^{L} s_l^z \tag{1}$$

where s^x and s^z are components of spin-$\frac{1}{2}$ operators. Self-duality determines the value of the critical ratio h/J_n exactly, $(h/J_n)_c = 2^{-(n-1)}$. The energy and the transverse field h are measured in units of J_n and we furthermore set $J_n = 1$.

Since the introduction of this model there have been several extensions, including the use of Potts variables, coupling through other spin components and different and competing multiplicities (Turban and Debierre 1982, Penson 1984, Turban 1985, Kolb and Penson 1985). For $n = 3$ there have been attempts to determine the character of the transition. It is generally agreed (Penson *et al* 1982a, b, Turban 1982, Debierre and Turban 1983, Maritan *et al* 1984) that there is a second-order phase transition but there is no consensus as yet concerning the precise values of the critical exponents. For example, the estimates of the exponent ν vary in the range 0.72–0.77 depending on the method used (Igloi *et al* 1983, 1986). The purpose of this letter is to study the finite-size behaviour of this model in the light of the recently developed apparatus based on conformal invariance (Luck 1982a, b, c, Cardy 1986). The question of conformal invariance is particularly intriguing for the present model as the ordered ground state of its 2D classical version is anisotropic in space.

The developments relating conformal invariance and finite systems started with a remarkably simple formula linking finite-size amplitudes to critical exponents. The correlation function exponent η of an infinite 2D classical isotropic system at criticality and the amplitude A of the inverse correlation length, $\xi^{-1} = A/L$, of the same system in a finite strip of width L are related through (Pichard and Sarma 1981, Luck 1982a, b, c, Derrida and de Sèze 1982, Nightingale and Blöte 1983, Cardy 1984a, b)

$$A = \pi\eta. \tag{2}$$

It has been shown that for quantum models (Penson and Kolb 1984) somewhat weaker relations hold. For different operators X and Y the ratios of their respective amplitudes A_X and A_Y are universal and equal to the ratios of their exponents η_X and η_Y

$$A_X/A_Y = \eta_X/\eta_Y. \tag{3}$$

For quantum systems the inverse correlation length is equal to the corresponding gap in the energy spectrum, $\xi_\alpha^{-1} = E_{1\alpha} - E_0$, $\alpha = X, Y$. E_0 is the ground-state energy. In actual calculations one uses for X and Y the spin and energy density operators, respectively (Penson and Kolb 1984, Alcaraz *et al* 1985, Burkhardt and Guim 1985, Guimaraes and Drugowich de Felicio 1986, von Gehlen *et al* 1986, von Gehlen and Rittenberg 1986). For quantum systems equation (3) replaces equation (2) because the Hamiltonian can be multiplied by an arbitrary overall factor without changing its critical properties. This ambiguity is removed if the quantum system is conformally invariant. The spectrum of single-particle excitations then has the form $\varepsilon(k) \equiv E(k) - E_0 = v_s k$ with a sound velocity $v_s = 1$ (Blöte *et al* 1986). In this case equation (2) holds for quantum systems as well. Alternatively, when $v_s \neq 1$ equation (2) takes the form

$$A = \pi\eta v_s. \tag{4}$$

Conformal invariance actually tells us much more than this (Cardy 1986). The structure of higher-lying energy levels is given by the formula (Cardy 1986, Rittenberg 1986)

$$\begin{aligned} \varepsilon_\alpha(k) &= (2\pi/L)(x_\alpha + r + x'_\alpha + r')v_s \qquad r, r' = 0, 1, 2, \ldots \\ k &= (2\pi/L)(x_\alpha + r - x'_\alpha - r') \end{aligned} \tag{5}$$

for periodic boundary conditions where, in our case, $x_\alpha = x'_\alpha = \eta_\alpha/4$. α labels the different symmetries of the excitations—here we distinguish between spin- (η_S)- and energy- (η_E)-type excitations. Equation (4) follows from equation (5) setting $r = R' = 0$. The x_α are anomalous dimensions of irreducible representations of an operator algebra. For unitary theories the characteristic central charge or conformal anomaly c, as well as the x_α, is quantised ($c < 1$) (Belavin *et al* 1984, Friedan *et al* 1984, Huse 1984). Additional consequences of the conformal invariance have recently been analysed (Itzykson *et al* 1986, Saleur 1986).

Now we want to apply these concepts to the Hamiltonian system given by equation (1). The transition separates a disordered phase from an ordered phase with a fourfold degenerate ground state. The strategy is to calculate critical exponents by conventional finite-size methods and compare the results with the predictions of the amplitude exponent relations, equation (4). Equation (5), furthermore, provides a number of consistency tests.

We have diagonalised the Hamiltonian matrix of equation (1) numerically using standard methods for periodically bounded chains up to length $L = 15$. The Lanczos tridiagonalisation scheme has been used and the symmetries of the Hamiltonian were explored. The Hamiltonian commutes with the translation operator T (which shifts the chain by one lattice spacing) and with the parity operators $P_f = \prod_{m=1}^{L/3} s^x_{3m+f-2} s^x_{3m+f-1}$, $f = 1, 2, 3$, which satisfy $P_f P_{f+1} = P_{f+2}$ (modulo 3). These parities do not commute with the translation operator, but the projection operator $P = (1 + P_1 + P_2 + P_3)/4$ does. Accordingly, the states can be classified by their wavevector and into either singlet or triplet states. The triplet states have wavevectors k and $k \pm 2\pi/3$. This can be seen directly from applying the operator $P^{\pm} = \sum_{f=1}^{3} e^{\pm 2\pi i f} P_f$ to a state with a given wavevector k, $|k\rangle = \sum_{l=1}^{L} e^{2\pi i k l} T^l |0\rangle$. $P^{\pm}|k\rangle$ yields—if it does not vanish—a vector of wavevector $k \pm 2\pi/3$. For finite systems the classification in a singlet subspace and a triplet subspace only holds for $L = 3, 6, 9, \ldots$. Therefore we restrict our study to these values.

We first use the phenomenological renormalisation group (PRG) (Barber 1983) to determine the energy density correlation function exponent $\eta_E = 4 - 2/\nu$ from ν (the correlation length exponent) and then the spin correlation function exponent η_S from η_E and the amplitude ratios, equation (3). The excitations of energy type are singlets (as is the ground state with wavevector $k = 0$) and the excitations of spin type are triplets. The PRG is performed between sizes L and $L - 3$ for $L = 6, 9, 12, 15$. The amplitude ratios for η_S are estimated from size L at the fixed point of the PRG. In figure 1 the calculated values for η_E and η_S are plotted as a function of $1/L$. They yield—if extrapolated to $L \to \infty$—the estimates $\eta_E \simeq 1.30$ and $\eta_S \simeq 0.25$.

In order to calculate the exponents directly using conformal invariance, we first have to calculate the sound velocity v_s. This is done from equation (5) (von Gehlen

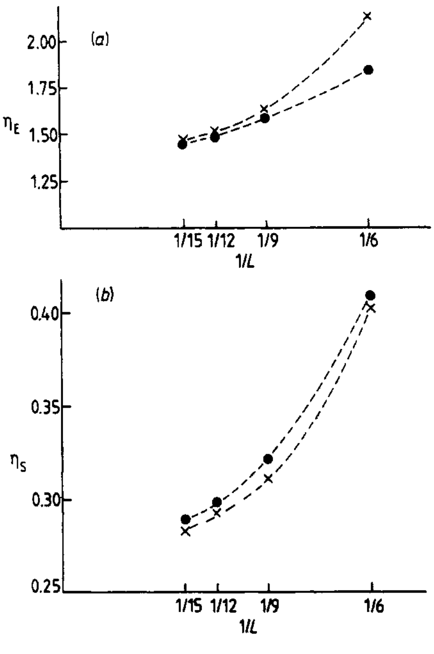

Figure 1. Critical exponents η_E and η_S against $1/L$ calculated from the PRG (sizes L and $L-3$) and using the amplitude exponent relations. In (a) the exponent $\eta_E = 4 - 2/\nu$ is calculated (i) from ν obtained by the PRG (●) and (ii) using $\varepsilon_E(0) = (2\pi/L)(\eta_E/2)v_s$ (×) where v_s is obtained from $\varepsilon_S(2\pi/L) - \varepsilon_S(0) = (2\pi/L)v_s$. In ($b$) the exponent η_S is calculated (i) from η_E and the amplitude ratio $A_S/A_E = \eta_S/\eta_E$ (●) and (ii) is obtained from $\varepsilon_S(0) = (2\pi/L)(\eta_S/2)v_S$ with the same V_s as in (a) (×).

and Rittenberg 1986, Cardy 1986):

$$\varepsilon_\alpha(k=2\pi/L)-\varepsilon_\alpha(k=0)=(2\pi/L)v_s \tag{6}$$

both for energy (singlet) and for spin (triplet) excitations. In this and all subsequent analyses of the energy spectrum, the ratio (h/J_3) was set to the exact critical value of the infinite system, $(h/J_3)_c=0.25$. The results for v_s are presented in figure 2. Both the series from the singlet and the triplet levels appear to converge towards a value of $v_s\simeq 0.42$. This is our first indication that the system is conformally invariant.

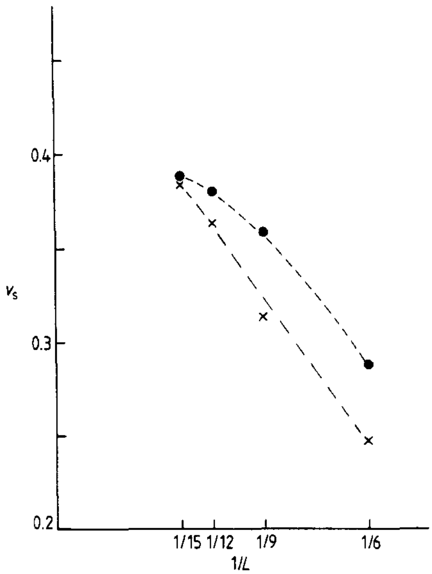

Figure 2. The sound velocity v_s of a conformally invariant system can be determined from $\varepsilon_\alpha(2\pi/L)-\varepsilon_\alpha(0)=(2\pi/L)v_s$ where α stands either for triplet (spin) (●) or singlet (energy) (×) excitations. The finite-size estimates at the critical point $h/J_3=0.25$ are shown for both types of excitation. They converge towards a limiting value $v_s\simeq 0.42$.

The central charge c, which for $c<1$ determines the quantised set of x_α can be determined from the finite-size correction of the ground-state energy (Blöte *et al* 1986, Affleck 1986):

$$E_0=[Le_0-\pi c/6L]v_s \tag{7}$$

where e_0 is the energy density of the infinite system. In order to eliminate e_0 the difference $E_0^L/L-E_0^{L'}/L'$ with $L'=L-3$ is calculated. For v_s the L-dependent values shown in figure 2 are used, both from the singlet and the triplet spectrum. The resulting series for the central charge c are shown in figure 3. Both curves suggest that c is very close to 1.

Higher-lying energy levels of the three-spin system can be compared with the predictions of equations (5) as well. Figure 4 shows all the low-lying excitations up to $\varepsilon_L\simeq 6/L$. We have selected all singlet and triplet levels with wavevectors $k=0$ and $k=2\pi/L$. The extrapolation of the finite-L estimates are consistent with the theoretical values of equation (5). Levels above $L\varepsilon_L\simeq 6$ are difficult to analyse because the convergence is much more slow and because the Lanczos method becomes less reliable.

We conclude that the spectrum of the quantum Ising model with three-spin interaction is consistent with predictions of conformal invariance, equation (5). Using this

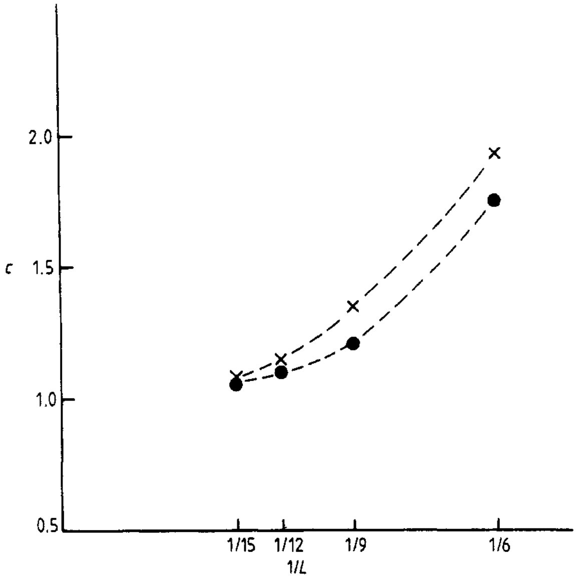

Figure 3. The central charge c calculated from the finite-size corrections to the ground-state energy. Equation (7) is used for two sizes, L and $L-3$, and v_s is taken from figure 2 (●, spin), (×, energy). The $L\to\infty$ estimate for c is very close to $c=1$.

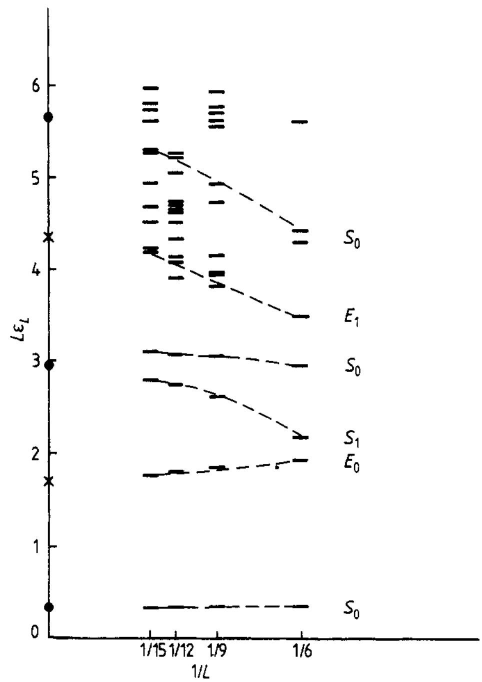

Figure 4. Spectrum of all low-lying excitations $L\varepsilon_L$ ($L\varepsilon_L<6$) at the critical point. The broken lines connect the singlet (energy) excitations with wavevector $k=0$, $2\pi/L(E_0, E_1)$ and the triplet (spin) excitations with $k=0$, $2\pi/L(S_0, S_1)$. The levels predicted from equation (5) for r, $r'=0$, 1 are indicated for singlet (×) and triplet (●) excitations. The value $v_s=0.42$ is used, as estimated from extrapolating the finite L values of figure 2 to $L=\infty$.

fact the exponents η_E and η_S are calculated. The value of η_E is consistent with the direct estimate from the PRG. The central charge c is estimated to be very close to 1 (multispin models which are known to have $c = 1$ are the Baxter and the Baxter–Wu models). While the convergence of the data is sufficient to draw qualitative conclusions, it is not accurate enough to clearly identify the universality class for this model.

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Note added. After completion of this work, we received a preprint by F C Alcaraz and M N Barber on the three-spin Ising model. Their results differ from ours numerically because they calculate v_s from excitations in the $k = 0$ sector, but their conclusions are very similar to ours.

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