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LETTER TO THE EDITOR

Varying exponent of the impurity magnetisation in the Ising chain with a transverse field

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Abstract. Using a $T=0$ real-space renormalisation-group method, the spontaneous magnetisation is calculated on an impurity site of the quantum spin-$\frac{1}{2}$ Ising chain in a transverse field. Two kinds of impurities are considered: either a transverse field or a bond is different from its host value. In both cases the magnetisation vanishes at the critical field with an exponent β_0 different from the host exponent and varying continuously with the impurity field (or impurity bond). These results agree with recent exact investigations of equivalent classical two-dimensional models.

It is of interest to study the influence and the role of different kinds of defects or impurities on the properties of a system that undergoes a second-order phase transition. In the case of an isolated impurity, it is well known that the *global* characteristics of the transition are not affected. However, the *local* properties in the vicinity of the impurity site could be greatly different from the host properties. We have chosen to study this problem in the case of the spin-$\frac{1}{2}$ Ising chain in a transverse field described by the Hamiltonian

$$\mathcal{H} = -\sum_i (J_i S_i^x S_{i+1}^x + h_i S_i^z) \tag{1}$$

where

$$S_i^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad S_i^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2}$$

In the uniform case ($J_i \equiv J$, $h_i \equiv h$) this quantum system undergoes at $T=0$ a second-order phase transition by increasing the transverse field. Exact results (Pfeuty 1970) show that below a critical value $(h/J)_c = 1$, the ground state is degenerate with a non-zero ground-state magnetisation $\langle S_i^x \rangle \neq 0$, which vanishes at the critical field with exponent $\beta = \frac{1}{8}$ while for $h/J > (h/J)_c$ the ground state is a singlet, in which $\langle S_i^x \rangle = 0$. This $d=1$ quantum model at $T=0$ maps onto the $d=2$ classical Ising model (Suzuki 1971) with horizontal (i.e. in the direction of the quantum chain) Ising constants J_1 and vertical Ising constants J_2 in the limit $J_1 \to 0$, $J_2 \to \infty$ with

$$(J_1/kT)^{-1} \exp(-2J_2/kT) \to h/J. \tag{3}$$

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The characteristics of the transition have recently been well reproduced by a real-space renormalisation-group approach (Drell *et al* 1976, Jullien *et al* 1978) well adapted to study quantum lattice systems at $T = 0$. The purpose of this Letter is to present an extension of this renormalisation-group approach in the case where a local defect is included. We will consider two simple cases (see the upper part of figure 1): (*a*) the bond between sites $i = 0$ and $i = 1$ is different from the others, i.e. $J_0 = J' \neq J$ while $J_i \equiv J$ for $i \neq 0$ and $h_i \equiv h$ everywhere; (*b*) the field on site $i = 0$ is different from the others, i.e. $h_0 = h' \neq h$, while $h_i \equiv h$ for $i \neq 0$ and $J_i \equiv J$ everywhere. In both cases we have calculated the x component of the magnetisation $\langle S_0^x \rangle$ in the ground state on the impurity site $i = 0$. As a main result of our calculations, we find that the magnetisation vanishes at the host transition, i.e. for $h/J = (h/J)_c$, with an exponent β_0 different from the host exponent β and varying continuously with J'/J in case (*a*) and h'/h in case (*b*). The classical two-dimensional equivalent problems (lower part of figure 1) have recently been intigated by Bariev (1979) and also by McCoy and Perk (1980). Our approximate results agree with their exact predictions in the limit of the Suzuki equivalence.

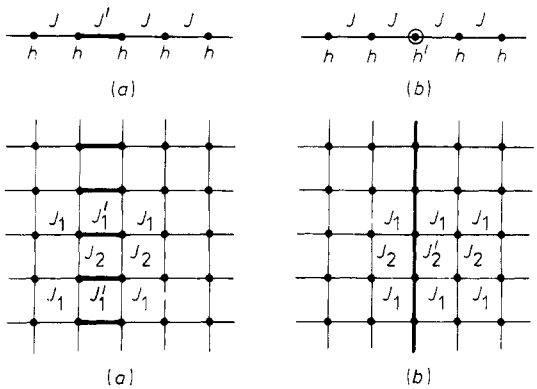

Figure 1. Sketch of the two kinds of impurities in the quantum chain (upper part): (*a*) a local bond is different from the others; (*b*) a local transverse field is different from the others. The corresponding classical equivalent two-dimensional Ising models are shown in the lower part of the figure.

The method is an iterative and approximate construction of the ground state of the whole chain. At each iteration the chain is divided in adjacent blocks of n_s sites. All the blocks are equivalent except the block containing the impurity. The Hamiltonian is solved exactly for both the impurity block and the host block. Then a subset of n_L low-lying levels is retained to rewrite the original interblock couplings and we obtain a new Hamiltonian dealing with blocks, on which we repeat the procedure until the parameters reach 'fixed-point' values. Details of the procedure were explained in the treatment of the homogeneous problem (Jullien *et al* 1978). The only difference here is the number n_L of levels retained. There the two lowest levels were sufficiently separated so that taking $n_L = 2$ was sufficient to obtain reliable results. This is no longer the case here, where a larger number of levels must be considered. We have performed calculations for $n_L = 3$ and $n_L = 4$ (with $n_s = 3$) and we present here the more precise calculations performed with $n_L = 4$.

At step (n) the Hamiltonian takes the general form

$$\mathscr{H}^{(n)} = \sum_i D_i^{(n)} - \sum_i A_i^{(n)} B_{i+1}^{(n)}. \tag{4}$$

$D_i^{(n)}$ is a diagonal matrix of order $n_L = 4$ containing the energy levels E_1, E_2, E_3, E_4 for the host sites and $E_1' E_2', E_3', E_4'$ for the impurity site. $A_i^{(n)}$ and $B_i^{(n)}$ are matrices of order $n_L = 4$ containing the coupling parameters, the elements of which are different for the host sites and for the impurity site. Initially, we group the sites two by two, in order to have two spins per site and the four levels considered are exact. We solve exactly the blocks of three sites (at the first step this corresponds to solving exactly a chain of six spins), then we retain the four lowest levels, etc. Computer diagonalisations are performed at each step using the symmetries at maximum. The different matrix elements of D_i, A_i, B_i on both the host sites and the impurity site are followed during the iterative process. The results depend numerically on the choice for the location of the impurity in the impurity block. This artifact can be avoided by averaging at each step the new matrix elements for the impurity block over the $n_s = 3$ possibilities of location for the impurity site.

As in the two-level scheme, we observe that the two lowest states become degenerate when $n \to \infty$ for h/J lower than a critical value $(h/J)_c$, while a gap opens for $h/J > (h/J)_c$. Here, for $n_s = 3$, $n_L = 4$, we find the more precise result $(h/J)_c = 0{\cdot}969997\ldots$.

The magnetisation is calculated by following the 4×4 matrix representation of an initial operator S_i^x through the iterations, up to the fixed point, the magnetisation then being represented by the element (1, 2) of the matrix. As previously observed (Jullien *et al* 1978), the results depend on the site i. This artifact is avoided by renormalising instead an averaged operator over the block. We have preferred this procedure instead of that used previously (Jullien *et al* 1978), which consists of considering a site located at the centre, or near the centre, of the block, because with $n_L = 4$ one of the levels is block-antisymmetric and the average gives a more correct result. For the host magnetisation (far away from the impurity site) we follow an averaged operator always for an host block. We find for the host magnetisation an exponent $\beta = 0{\cdot}124 \pm 0{\cdot}002$, which, accidentally, is extremely good (the exact result is $\beta = 0{\cdot}125$). In order to compare with the previous results for the pure chain (Jullien *et al* 1978), let us give the results for the other exponents: $z = 1{\cdot}10$, $\eta_x = 0{\cdot}286$, $s = 0{\cdot}95$, $\nu = 0{\cdot}87$ (exact: $z = s = \nu = 1$, $\eta_x = 0{\cdot}25$).

For the magnetisation on the impurity site, we also follow an averaged operator which, now, always refers to the impurity site, but is averaged over the three possible positions of the impurity in the block.

The results for the impurity magnetisation are given as a function of h/J in figure 2 for different values of J'/J (case (a)) or h/h' (case (b)). For a given value of h/J the magnetisation increases with J'/J (case (a)) or h/h' (case (b)) and tends to 1 when J'/J or h/h' tends to infinity. This upper limit can easily be understood, since in case (a) $h/h' = \infty$ corresponds to $h' = 0$, where the impurity spin has no local constraint and aligns completely in the field of neighbouring spins, while in case (b) $J'/J = \infty$ corresponds to the consideration of a molecule of two sites in the ground state of which $\langle S_0^x \rangle = \langle S_1^x \rangle = \pm 1$. However, the lower limits when $h/h' \to 0$ or $J'/J \to 0$ are different in the two cases: in case (a) $h/h' \to 0$ corresponds to $h' \to \infty$ where the impurity spin is forced to be completely aligned in the direction and thus $\langle S_0^x \rangle \to 0$, while in case (b),

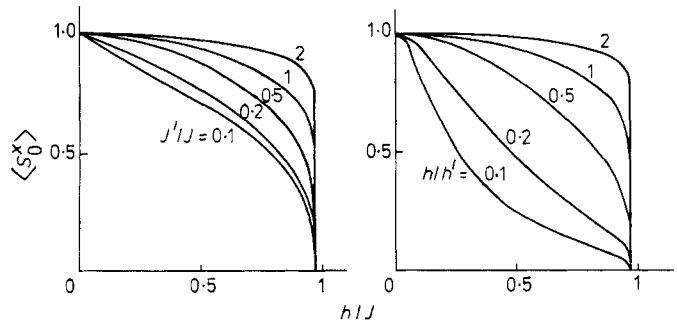

Figure 2. Results for the impurity magnetisation $\langle S_0^x \rangle$ as a function of h/J for different values of J'/J (case (a)) or h/h' (case (b)).

when $J'/J \to 0$, $\langle S_0^x \rangle$ tends to a non-zero limit which corresponds to the edge magnetisation.

In both cases, the variation in the shape of $\langle S_0^x \rangle$ is also accompanied by a variation of the exponent β_0 defined in the vicinity of $(h/J)_c$ by

$$\langle S_0^x \rangle \sim [(h/J)_c - (h/J)]^{\beta_0}. \tag{5}$$

The results for both cases (a) and (b) are given in figure 3 as a plot of β_0 as a function of J'/J (case (a)) or h/h' (case (b)). The two curves are almost superposed, and β_0 varies from about 0·32 (for $J'/J = 0$ or $h/h' = 0$) to zero (for $J'/J \to \infty$ or $h/h' \to \infty$). Note that the edge exponent, which is known exactly to be 0·5, is here only approximately recovered for $J'/J = 0$. This is due to the fact that for $J' = 0$, the impurity block is cut in two parts; this corresponds to considering a smaller block, thus increasing the error.

The same behaviour was found in the equivalent two-dimensional Ising model studied by Bariev (1979) and McCoy and Perk (1980). Our cases (a) and (b) correspond to the cases (a) and (b) of Bariev (1979) sketched in the lower part of figure 1: a line of horizontal bond defects is located between two neighbouring columns (case (a)) or a line of vertical defects lies inside one column (case (b)). Bariev derived the exact formula

$$\beta_0 = \frac{1}{2\pi^2}(\cos^{-1}(-x))^2 \tag{6}$$

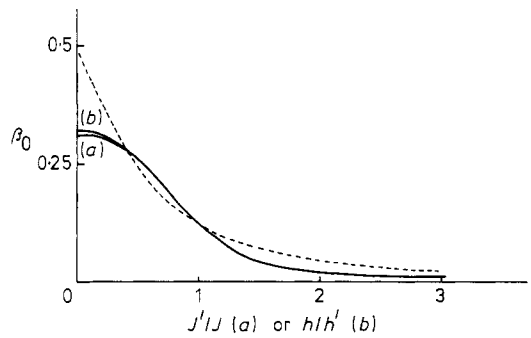

Figure 3. Exponent β_0 of the impurity magnetisation as a function of J'/J (case (a)) or h/h' (case (b)). The exact formula (8) is represented by the broken curve.

where

$$x = \frac{\cosh(2J_1/kT) - \cosh(2J_1'/kT)}{\cosh(2J_1/kT)\cosh(2J_1'/kT) - 1} \qquad \text{(case } (a)\text{)}$$

$$x = \tanh[2(J_2 - J_2')/kT] \qquad \text{(case } (b)\text{).} \tag{7}$$

In Suzuki's (1971) equivalence given by formula (3), the following correspondence holds between Bariev's notations and ours:

$$J_1'/J_1 \rightarrow J'/J \qquad \text{case } (a)$$

$$\exp[2(J_2' - J_2)] \rightarrow h/h' \qquad \text{case } (b). \tag{8}$$

Then formula (6) corresponds to

$$\beta_0 = \frac{1}{2\pi^2}\left(\cos^{-1}\left(\frac{(J'/J)^2 - 1}{(J'/J)^2 + 1}\right)\right)^2 \qquad \text{case } (a) \tag{9}$$

and exactly the same formula holds in case (b) if J'/J is replaced by h/h'. Formula (8) is represented by the broken curve of figure 3, which starts from the exact edge value 0·5 for $J'/J = 0$, goes through the exact host value 0·125 for $J'/J = 1$ and tends to zero when $J'/J \rightarrow \infty$. One can see from figure 3 that, considering the approximations used, our calculations reproduce quite well the predictions of formula (8), except for the shape near $J' = 0$.

It would be interesting to extend the present calculations to a study of the variation of the magnetisation with distance from the impurity site or to a study of other kinds of defects. We are presently studying a 'grain boundary' in the Ising chain with a transverse field, i.e. a model where $J_i = J$ for $i < 0$ and $J_i = J'$ for $i > 0$, while $h_i = h$ everywhere. These studies are performed in the context of analysing the different types of effects introduced by disorder, when treating a completely disordered quantum Ising chain by the same kind of techniques (Uzelac *et al* 1980).

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