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COMMENT

Critical properties of the XXZ chain in an external staggered magnetic field

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Abstract. We comment on the recent work of Alcaraz and Malvezzi on the critical properties of the $S = \frac{1}{2} XXZ$ chain in staggered magnetic field. The method of determining the phase boundary from the finite-size numerical data is also discussed.

Recently Alcaraz and Malvezzi (AM) [1] studied the ground-state phase diagram of the $S = \frac{1}{2} XXZ$ spin chain in external homogeneous and staggered magnetic fields described by

$$H(\Delta, h, h_s) = -\frac{1}{2} \sum_{i=1}^{M} \{\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z + 2[h + (-1)^i h_s]\sigma_i^z\} \tag{1}$$

where σ_i^x, σ_i^y and σ_i^z are Pauli matrices, Δ is the anisotropy parameter and h (h_s) is the uniform (staggered) magnetic field. They found that the ground-state phase diagram is composed of the antiferromagnetic (AF) phase, the massless (ML) phase and the ferromagnetic (FE) phase. Although we agree with their schematic phase diagram of $H(\Delta, h, h_s)$ (figure 5 of [1]), we want to comment on the nature of the ground-state phase transition and also on the method to determine the phase boundary from the finite-size numerical data.

First we discuss the nature of the ground-state phase transition. When $h \neq 0$, the uniform magnetic field breaks the spin-reversal symmetry held in the $h = 0$ case, so that the nature of the phase transition may be different from that in the $h = 0$ case. Throughout this comment we restrict ourselves to the $h = 0$ case on which AM focused. Figure 1 shows the schematic phase diagram of $H(\Delta, h = 0, h_s)$, which is essentially the same as AM's figure 3. They stated that the phase transition between the AF phase and the ML phase (path 1) is of second order. We believe, however, that it is of infinite order, i.e. of Kosterlitz–Thouless (KT) type. The operator coupled to the staggered magnetic field is irrelevant in the ML region and is relevant in the AF region. The excitation spectrum is either massless or massive depending on whether this operator is irrelevant or relevant. This mass-generating mechanism is the same as that of the sine–Gordon model, as AM

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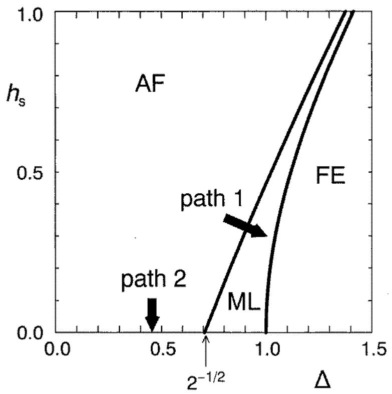

Figure 1. Schematic ground-state phase diagram of the Hamiltonian $H(\Delta, h = 0, h_s)$. The antiferromagnetic, massless and ferromagnetic phases are indicated by AF, ML and FE, respectively. The AF–ML transition along path 1 is of the KT type and that along path 2 is of second order. The transition to the FE state is of first order.

themselves noted. Thus the AF–ML transition of path 1 is of the KT type, which is seen from the well known properties of the sine–Gordon model [2].

We can also observe the AF–ML transition along path 2. This transition is different from that of path 1, because it is due to the vanishing of the coefficient (which is proportional to the magnitude of the staggered field) of the relevant operator coupled to the staggered magnetic field. Thus this transition is of second order and its critical exponents vary continuously.

Next we discuss the method to determine the AF–ML phase boundary from the finite-size numerical data obtained by the numerical diagonalization of the Hamiltonian. AM used the $M \to \infty$ extrapolation of the sequences $(\Delta^{(M)}, h^{(M)}, h_s^{(M)})$ $(M = 2, 4, \ldots)$ obtained by solving the so-called phenomenological renormalization group (PRG) equation

$$MG_M(\Delta, h, h_s) = (M-2)G_{M-2}(\Delta, h, h_s) \tag{2}$$

where $G_M(\Delta, h, h_s)$ is the gap of the Hamiltonian (1) with M sites. At the fixed point of the PRG equation (2), the gap G_M behaves as

$$G_M \sim M^{-1} \tag{3}$$

in the lowest order of M^{-1}. If the transition is of second order, the PRG method leads to the correct transition point because the system is massless and equation (3) holds only at the transition point. In the case of the KT transition, on the other hand, care must be taken for the application of the PRG method. Since the present system is massless not only at the AF–ML transition line but also in the whole of the ML region, the PRG relation (2) is satisfied in the lowest order of M^{-1} in the whole of the ML region. Where is the fixed point of the PRG equation? It is controlled by the lowest-order correction to equation (3) which may come from the operator coupled to the staggered magnetic field. Thus the fixed point of the PRG equations located at the point where the staggered field vanishes. If this is the case, the transition point obtained through the PRG method is brought over from the AF–ML point to the $h_s = 0$ line. Then the simple application of the PRG method to the KT transition is dangerous. In the present problem, of course, there may be other corrections which make the situation more complicated.

Let us demonstrate that the PRG solution may lead to an incorrect critical point for the KT transition [3]. When $h = h_s = 0$, as is well known, the Hamiltonian (1) is exactly solvable by the use of the Bethe ansatz method. Its ground state is either the AF state or the ML state depending on whether $\Delta < -1$ or $-1 \leqslant \Delta < 1$. The excitation gap in the AF state behaves as [4, 5]

$$G(\Delta) \simeq 8\pi \exp\left(-\frac{\pi^2}{2\sqrt{2(|\Delta|-1)}}\right) \qquad (\Delta \to -1-0) \tag{4}$$

which indicates that this AF–ML transition at $\Delta = -1$ is of the KT type. If we apply the PRG method to the finite-size numerical data of the excitation gap, we obtain $\Delta_c = -0.507\,06$ ($M = 10, 12$) and $\Delta_c = -0.475\,64$ ($M = 18, 20$). Therefore the critical value of Δ_c obtained from the PRG equation goes far off from the exact value $\Delta_c = -1$ as M increases. Where is the fixed point of the PRG equation in this case? Since the mass in the AF state is generated by the operator coming from the Umklapp scattering between the Jordan–Wigner fermions originated from the $S_i^z S_{i+1}^z$ term in the spin Hamiltonian, the fixed point is the XY point ($\Delta = 0$) where there is no $S_i^z S_{i+1}^z$ term resulting in the vanishing of the interaction between fermions. Thus the PRG solution is brought over from the true transition point $\Delta_c = -1$ to the XY point. This example was also noticed by Bonner and Müller [6] and by Sólyom and Ziman [7].

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