Comment on "Phase Diagram of an Impurity in the Spin-1/2 Chain: Two-Channel Kondo Effect versus Curie Law"

In a recent Letter [1] an antiferromagnetic (AF) Heisenberg (J > 0) spin- $\frac{1}{2}$ chain with a two-parametric (J_1, J_2) spin- $\frac{1}{2}$ impurity (at site 0) has been considered [using renormalization group (RG), bosonization, and numerical studies] with the Hamiltonian

$$H = J \sum_{i=1}^{N-1} \vec{S}_i \vec{S}_{i+1} + J_1 \vec{S}_0 (\vec{S}_N + \vec{S}_1) + J_2 \vec{S}_N \vec{S}_1.$$
 (1)

The authors claimed that they identified all possible fixed points and classified the renormalization flow between them. Four fixed points were studied: $O_N \otimes \frac{1}{2}$ with $J_1 = J_2 = 0$; P_{N+1} with $J_1 = J$, $J_2 = 0$; $P_N \otimes \frac{1}{2}$ with $J_1 = 0$, $J_2 = J$, and $O_{N-2} \otimes \frac{1}{2}$ with $J_2 = \infty$. It turns out that the analysis [1] is incomplete. There exist several other fixed points (e.g., at $J_2 = -\infty$, $J_1 = -\infty$, etc.). The most interesting behavior is in the AF sector $J_1, J_2 \geq 0$. Here at least one additional fixed point (which can be called $O'_{N-2} \otimes \frac{1}{2}$) exists with $J_1 = \infty$. The impurity spin and two neighboring spins are effectively decoupled from the rest of the chain by an infinite AF interaction. Therefore this fixed point is stable.

However, it was claimed that the P_{N+1} fixed point is also stable. There are two possibilities to resolve this controversy: (i) there exists some other (unstable) fixed point between P_{N+1} and $O'_{N-2} \otimes \frac{1}{2}$ or (ii) the fixed point P_{N+1} is not stable. Really, one can see that a weak AF coupling J_2 is frustrating. According to [2] a frustrated state should always be unstable since renormalization typically occurs towards a state with lower ground state degeneracy. Here we can use the same approach as in [1]. Using the non-Abelian bosonization $S(x) \approx$ $\vec{J}_L + \vec{J}_R + (-)^x \times \text{const} \times tr \vec{\sigma}g$ [1] the effective part of the impurity Hamiltonian near P_{N+1} can be approximated as $H_{\text{imp}} = \gamma_2'(J_L + J_R)\dot{S}_0 + \gamma_3'\partial_x tr \vec{\sigma}g\dot{S}_0 + \dots,$ where the first term is marginal and the second is irrelevant [1], and to the lowest order $\gamma'_{2,3} \sim (J_1 - J)$. Related RG equations are $\partial_t \gamma'_2 = (\gamma'_2)^2 - \frac{3}{4}(\gamma'_3)^2 + \dots$ and $\partial_t \gamma'_3 = -\frac{1}{2}\gamma'_3 + 2\gamma'_2\gamma'_3 + \dots$ (with t being the logarithm of the RG cutoff). Clearly here (as well as for $P_N \otimes \frac{1}{2}$) the irrelevant coupling constant plays an important role. The right hand sides of RG equations can be negative or positive depending on values of $\gamma'_{2,3}$. Hence the P_{N+1} fixed point can be not stable (saddle) and the renormalization can be directed from this point to $O'_{N-2} \otimes \frac{1}{2}$.

It turns out that for $0 \le J_1 \le J$ at $J_2 = J - J_1 \ge 0$ the Hamiltonian Eq. (1) with the additional term

 $\pm 2\sqrt{J_1J} - J_1^2 \vec{S}_0[\vec{S}_N \times \vec{S}_1]$ (square brackets denote a vector product) is exactly solvable [3]. This latter term does not change classical equations of motion of spins (total time derivative). Using the above mentioned bosonization [1] one can show that it should be irrelevant from the usual RG viewpoint (its dimension is larger than 1). However, the zero-temperature (T = 0) susceptibility of an impurity for N odd is [3] finite $\chi_{\text{imp}} \propto \hat{T}_K^{-1} \sim (4\sqrt{e}/\pi^{7/2}J) \exp[\pi\sqrt{(J-J_1)/J_1}].$ For the same impurity situated at the edge of an open Heisenberg chain (without three-spin term) there exists an additional divergent contribution to the T = 0 susceptibility due to <u>open</u> edges of the chain $\chi_{\rm edge} \sim \sqrt{\pi^3/e}/4H \ln^2(H/\sqrt{\pi^3/e})$ in an external magnetic field H. At low $T(H \rightarrow 0)$ such a contribution is also T-divergent (cf. [4]), reminiscent of a two-channel Kondo behavior. For N even the impurity susceptibility is Curie-like (with logarithmic corrections). Finite impurity susceptibility at $T \rightarrow 0$ can also be obtained for an impurity with arbitrary J_1 and $J_2 = 0$ in the simpler XX model [5] (it is well-known that the "easy-plane" anisotropy of a XX model is irrelevant). This is also in contrast to the results [1,6]. We determine susceptibilities as derivatives of the magnetizations of impurities and free edges with respect to H (with $H \rightarrow 0$ then). Probably the reason for such a discrepancy is the different definition used in [6] $\chi_{\rm imp} = \lim_{N \to \infty} (\chi_{\rm system} - N\chi)$ because the order of limits $T \to 0$, $H \to 0$, and $N \to \infty$ is crucial for such problems.

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Received 18 January 2001; published 12 July 2001 DOI: 10.1103/PhysRevLett.87.059701

PACS numbers: 75.10.Jm, 75.20.Hr

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