



A two-channel Kondo impurity in the spin-1/2 chain: consequences for Knight shift experiments

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Abstract

A magnetic impurity in the spin- $\frac{1}{2}$ chain is a simple realization of the two-channel Kondo problem since the field theoretical descriptions in the spin sector are identical. The correlation functions near the impurity can be calculated. Using a modified version of the numerical transfer matrix DMRG, we are now able to accurately determine local properties close to the impurity in the thermodynamic limit. The local susceptibilities (Knight-shifts) show an interesting behavior in a large range around the impurities. We are able to make quantitative experimental predictions which would allow one to observe two-channel Kondo physics for the first time directly by doping of spin- $\frac{1}{2}$ chain compounds. © 1999 Elsevier Science B.V. All rights reserved.

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We are considering a defect in the antiferromagnetic spin- $\frac{1}{2}$ chain, consisting of two altered bonds in the chain

$$H = J \sum_{i=1}^{L-1} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J'(\mathbf{S}_L + \mathbf{S}_1) \cdot \mathbf{S}_0. \quad (1)$$

Such an impurity could be created in quasi-one-dimensional spin compounds by doping with other spin- $\frac{1}{2}$ ions or substituting suitable non-magnetic neighboring atoms.

From field theory calculations it is known that the model in Eq. (1) is equivalent to the two-channel Kondo problem in terms of the renormalization behavior [1–3]. For a weak coupling J' the impurity spin \mathbf{S}_0 is almost free, but the effective coupling grows logarithmically as the temperature is lowered. The system then renormalizes to a stable intermediate coupling fixed point $J' = J$ which corresponds to the “healed” chain. Our calculations now give quantitative results which can be compared to experiments, so that the two-channel Kondo

physics can be observed directly. For our calculations we have used the numerical transfer matrix renormalization group [4–7], which we have modified to calculate impurity properties directly in the thermodynamic limit.

In particular, we consider the local susceptibilities over a large range around the impurity as a function of site index x

$$\chi(x) = \left. \frac{d\langle S^z(x) \rangle_B}{dB} \right|_{B=0}, \quad (2)$$

where B is a uniform magnetic field on the entire chain. The susceptibility of the impurity spin $\chi(0)$ is a good approximation to the true impurity susceptibility

$$\chi_{\text{imp}} \approx \chi(0) - J'\chi, \quad (3)$$

where we have subtracted the pure susceptibility per site χ to only capture the impurity effects. We find that the impurity susceptibility χ_{imp} is logarithmic divergent with temperature as expected from the two-channel Kondo effect. Moreover, we can explicitly show that the impurity susceptibility indeed follows the scaling form

$$\chi_{\text{imp}}(T) = f(T/T_K)/T_K, \quad (4)$$

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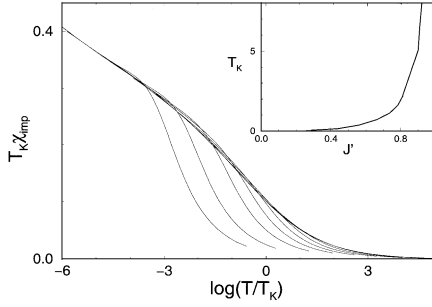


Fig. 1. The scaled impurity susceptibility χ_{imp} , which shows logarithmic behavior and the scaling of Eq. (4) for an appropriate choice of T_K as a function of $J' = 0.1J, \dots, 0.95J$ (inset).

as shown in Fig. 1 up to deviations at higher temperatures which are due to non-universal behavior above the cut-off. Here T_K is the crossover temperature, which is exponentially small near the unstable fixed point $J' \ll J$ and diverges at the stable fixed point with $(J - J')^{-2}$.

More interesting is the spatial dependence of $\chi(x)$ as a function of site index. It is known that open boundary conditions induce a large staggered part which *increases* with the distance from the boundary [8] $\chi(x) \propto (-1)^x x \sqrt{T} / \sqrt{\sinh 4xT}$, where T is measured in units of J . This surprising effect has been confirmed by NMR experiments [9,10].

For the impurity in question we can predict a similar effect which then could again be measured by NMR experiments. The leading operator of the impurity spin also induces a staggered component which we have explicitly calculated to be

$$\chi(x) \propto (-1)^x \log [\tanh(xT)]. \quad (5)$$

For small distances x this formula shows the logarithmic temperature dependence of the impurity susceptibility explicitly. Clearly, for small coupling J' and at larger temperatures we expect the open chain behavior, but as the temperature is lowered (or the coupling is increased) the alternating part in Eq. (5) will start to dominate, which has the opposite sign. This competition between the two contribution is indeed observed in Fig. 2. Moreover, below T_K the total staggered contribution always fits extremely well to a superposition

$$\chi_{total}(x) = c_1 \log [\tanh(xT)] + c_2 \frac{x\sqrt{T}}{\sqrt{\sinh 4xT}}. \quad (6)$$

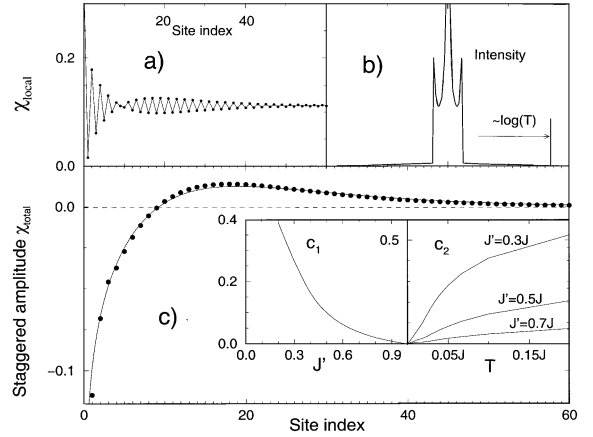


Fig. 2. (a) The local susceptibilities as a function of site index for $T = 0.05J$ and $J' = 0.7J$. (b) The corresponding typical NMR spectrum. (c) The fit of the alternating amplitude to Eq. (6) with the appropriate coefficients (inset).

We have determined the coefficients c_1 and c_2 for all coupling strengths $J' \geq 0.2J$ in Fig. 2, where c_1 is temperature independent and c_2 renormalizes to zero if the temperature is lowered as expected. We have also calculated the corresponding NMR spectrum which shows a logarithmically broad feature and distinctive kinks, which have a unique temperature dependence as determined from Eq. (6) depending on the coupling strength J' . These quantitative predictions should allow experiments to observe two-channel Kondo physics by NMR and susceptibility measurements on doped spin- $\frac{1}{2}$ chain compounds.

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