Universal Crossover Behavior of a Magnetic Impurity and Consequences for Doping in Spin-1/2 Chains

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We consider a magnetic impurity in the antiferromagnetic spin-1/2 chain which is equivalent to the two-channel Kondo problem in terms of the field theoretical description. Using a modification of the transfer-matrix density matrix renormalization group we are able to determine the crossover function for the impurity susceptibility over a large temperature range, which exhibits universal data collapse. We also calculate the local susceptibilities near the impurity, which show an interesting competition of boundary effects. This results in quantitative predictions for experiments on doped spin-1/2 chains, which could observe two-channel Kondo physics directly. [S0031-9007(98)06869-0]

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Magnetic impurities in low-dimensional antiferromagnets are recently of much theoretical and experimental interest in connection with high temperature superconductivity. We now study an impurity model in the spin-1/2 chain consisting of two altered bonds in the chain, which is known to have an equivalent field theory description to the spin sector of the two-channel Kondo (2CK) model [1,2]. The 2CK model has received much interest in the theoretical physics community [3] since it was first proposed in 1980 [4] and this model is often cited as a standard example of non-Fermi-liquid physics. Bethe ansatz [3] and conformal field theory techniques [5] have led to almost complete understanding. On the other hand it is much less clear to what extent experimental applications exist, although there is some hope that the conductance behavior through metal constrictions can be explained by the 2CK effect [6].

To study the 2CK effect experimentally, site-parity symmetric bond defects could feasibly be created by doping quasi-one-dimensional spin-1/2 compounds, and Knight shift experiments would then be able to observe 2CK physics explicitly. Our goal is therefore to provide quantitative predictions for the local susceptibilities in a range around the impurity, which turn out to exhibit an interesting competition between two boundary effects. Moreover, we are able to explicitly show the expected data collapse of the impurity susceptibility for different coupling strengths. For this purpose we have developed a modification of the transfer-matrix density matrix renormalization group (DMRG) [7].

The model we are considering is the antiferromagnetic spin-1/2 chain with two altered bonds,

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

which is known to have an equivalent field theory description of the 2CK effect as we will outline below. Interestingly, an integrable spin-1 chain with a spin-1/2 impurity is also equivalent to the 2CK problem on the level of the Bethe ansatz equations [8], but we cannot analyze that model in terms of the field theory.

The low-temperature and long-wavelength properties of the unperturbed spin-1/2 chain are well described by a conformal field theory Hamiltonian in terms of 1 + 1 dimensional bosons

$$H = \int dx \, \frac{v}{2} [(\partial_x \phi)^2 + \Pi_\phi^2] , \qquad (2)$$

where Π_ϕ is the conjugate operator to the boson field ϕ. This field theory has been discussed in more detail elsewhere [1], and we will just focus on a more pedagogical description in this Letter. For temperatures and wave vectors well below some cutoff $\Lambda \sim J$ the spin-1/2 chain exhibits critical behavior and scale invariance. Scale invariance means that we get the same physical results for some quantity $\mathcal{O}$ if we rescale the temperature or distances with some factor Γ, as long as we also multiply the physical quantity $\mathcal{O}$ with Γ^d:

$$\mathcal{O}(T) = \Gamma^{-d} \mathcal{O}(\Gamma T) , \qquad (3)$$

where d is referred to as the scaling dimension of $\mathcal{O}$, and the temperature T can also be replaced by the inverse system size $1/L$. For example, operators in the "free" Hamiltonian (2) have a scaling dimension of $d = 1$ (after integration over x). This means that the energy spacing of the spectrum is proportional to $1/L$. "Higher order operators" in the Hamiltonian are operators with $d > 1$, which give small corrections to the spectrum of order $1/L^d$ and are hence termed "irrelevant" and are neglected in Eq. (2). (We have also neglected one marginal operator $\cos\sqrt{8\pi}\,\phi$ which turns out to be justified although the corrections are only logarithmically small.) For the rest of this Letter we will work in the thermodynamic limit $L \to \infty$ and rescale T instead.

We can now analyze the perturbation J' on the bonds in Eq. (1) in terms of the scaling dimensions of the local operators, which arise in Eq. (2) due to the broken translational invariance. If the perturbation on the bonds $\delta J = J - J'$ is small, we can use perturbation theory on a chain with periodic boundary conditions. In this case the local operator with the lowest scaling dimension

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which still observes the site-parity symmetry of the problem is known to be $\partial_x \sin\sqrt{2\pi}\,\phi$ of dimension $d = 3/2$ [1]. This operator gives the leading corrections but is still irrelevant. In particular, for a given coupling strength δJ the size of the corrections becomes effectively smaller by a factor of Γ^{d-1} if we rescale T by $\Gamma < 1$. The opposite is also true: If we increase the temperature the effective perturbation strength $\Gamma^{d-1}\delta J$ may become so strong that a systematic expansion fails at some special temperature T_K, called the crossover (or Kondo) temperature. Above T_K we therefore expect a completely different behavior, namely, that of an open chain if $T_K < T < \Lambda$. We say that the system *renormalizes* from an open boundary condition to the infrared fixed point of a healed periodic chain as the temperature is lowered. For small δJ we have *defined* T_K as the temperature at which the product $T_K^{d-1}\delta J$ becomes large, so that we can write $T_K \propto \delta J^{1/(1-d)} = \delta J^{-2}$ in this limit. Hence, rescaling T by Γ is equivalent to changing T_K by $1/\Gamma$, i.e., altering the initial coupling strength δJ by $\Gamma^{d-1} = \Gamma^{1/2}$, which is really the meaning of renormalization.

To compare this system with the 2CK effect it is more instructive to start with open boundary conditions and consider a weak antiferromagnetic coupling $0 < J' \ll J$. In this case the leading operator is $S_0^z[\partial_x\phi(0) + \partial_x\phi(L)]$ with dimension $d = 1$ which turns out to give logarithmically *relevant* contributions as the temperature is lowered. For small J', the Kondo temperature is given by $T_K \propto e^{-b/J'}$, where b is some constant. If we identify the central spin $\vec{S}_0$ with the Kondo impurity and the two ends of the chain with the spin sectors of the two electron channels, it is evident how this scenario is equivalent to the 2CK problem [5]: A small coupling ($J' \ll J$) to the impurity is marginally relevant as we lower the temperature and the system renormalizes to an intermediate coupling ($J' = J$) fixed point, i.e., the periodic chain.

We have chosen the numerical transfer matrix DMRG [7] to test these concepts. The partition function of the spin-1/2 chain can be written in terms of transfer matrices $Z = \mathrm{tr}(\mathcal{T}^{L/2}) \xrightarrow{L\to\infty} \lambda^{L/2}$, where λ is the largest eigenvalue of $\mathcal{T}$. The transfer matrix DMRG constructs a transfer matrix for a finite number of time slices M and then successively increases M by keeping only the most relevant basis states that are necessary to calculate λ. We now extend this method to nonuniform systems by using the eigenstate $|\psi_\lambda\rangle$ corresponding to the highest eigenvalue λ. We can include any impurity interaction which is described by a local matrix $\mathcal{T}_{\mathrm{local}}$ explicitly in the partition function

$$Z = \mathrm{tr}(\mathcal{T}^{L/2-1}\mathcal{T}_{\mathrm{local}}) \xrightarrow{L\to\infty} \lambda^{L/2-1}\langle\psi_\lambda|\mathcal{T}_{\mathrm{local}}|\psi_\lambda\rangle . \tag{4}$$

If the eigenstate $|\psi_\lambda\rangle$ is known to reliable precision from the DMRG, it is straightforward to determine any thermodynamic property (even locally). This method proved to be superior in speed, accuracy, and temperature range compared to Monte Carlo simulations, which we have used for checking purposes.

The first task is to show that our renormalization picture is accurate, i.e., that we can indeed use periodic boundary conditions to describe the system at sufficiently low temperatures. For this purpose we consider the linear response χ_0 of the impurity spin $\vec{S}_0$ to a *local* magnetic field B_0, which is given by the Kubo formula

$$\chi_0(T) = \int^{1/T} \langle S_0^z(\tau)S_0^z(0)\rangle\, d\tau . \tag{5}$$

For open boundary conditions the reponse of the free impurity spin is given by the Curie law $\chi_0 \propto 1/4T$. For periodic boundary conditions the autocorrelation function is determined by the leading field theory operator which obeys the same symmetries as $\vec{S}_0$. We found this operator to be $\cos\sqrt{2\pi}\,\phi$ with $d = 1/2$ and an autocorrelation function proportional to $1/\tau$, which leads to a logarithmic divergence as $T \to 0$. In Fig. 1 we show this crossover from Curie law to logarithmic behavior at an effective cutoff $\Lambda_{\mathrm{eff}} = \min(\Lambda, T_K)$, depending on the coupling strength J' with a scaling behavior of the form $\chi_0(T) = g(T/\Lambda_{\mathrm{eff}})/\Lambda_{\mathrm{eff}}$ (Fig. 1 inset). The logarithmic behavior was observed before at one coupling only by other methods [9]. Note, however, that the response χ_0 is only an indication of the autocorrelation functions, but it must not be confused with the impurity susceptibility, since we have only applied the magnetic field at one spin. In fact every spin in the periodic chain shows a logarithmic response to a *local* magnetic field.

From an experimental point of view it is much more interesting to look at the impurity susceptibility, which can be defined as the size independent contribution to the total system susceptibility $\chi_{\mathrm{imp}} = \lim_{L\to\infty}(\chi_{\mathrm{system}} - L\chi)$, where χ is the susceptibility per site far away from any boundary. While our method is, in principle, capable of extracting the impurity susceptibility directly, we were

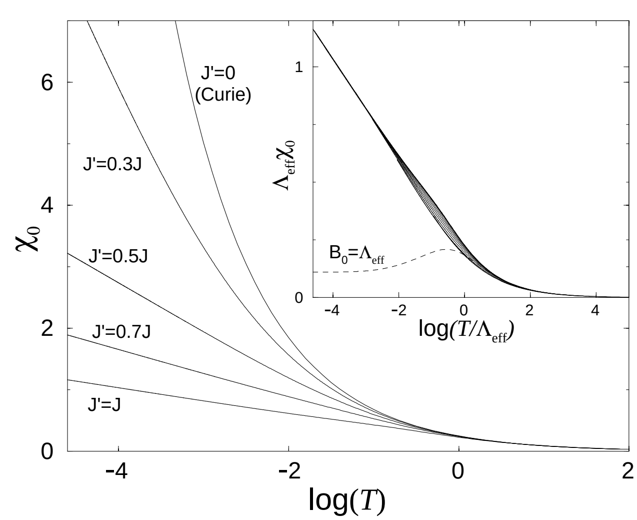

FIG. 1. The linear response of the impurity spin to a local magnetic field. Inset: The data collapse for 14 different $J' = 0.1J, \ldots, J$ and the effect of a *finite* field $B_0 = \Lambda_{\mathrm{eff}}$.

able to obtain results at much lower temperatures by considering the linear response of the impurity spin to a *uniform* field B instead:

$$\chi_{\mathrm{imp}} \approx \frac{d\langle S_0^z\rangle_B}{dB} - J'\chi\,, \tag{6}$$

which gives a good indication of the true impurity susceptibility [in contrast to χ_0 in Eq. (5), where we considered only a *local* field B_0]. From the 2CK effect it is known that the impurity susceptibility is logarithmically divergent below T_K while it shows a Curie-law behavior above [3,5]. Interestingly, this crossover shows a universal data collapse, because changing the coupling strength (i.e., T_K) is equivalent to rescaling the temperature, i.e., there is only one independent variable T/T_K

$$\chi_{\mathrm{imp}}(T) = f(T/T_K)/T_K\,, \tag{7}$$

where $f(x)$ is a universal function (ignoring higher order operators). This data collapse is clearly seen in Fig. 2 with an appropriate choice of T_K as a function of J' (inset), showing the predicted logarithmic scaling at low T. The nonuniversal deviations of some of the curves at higher T/T_K are due to the fact that in those cases T_K was so large that regions above the cutoff have been included.

In principle, a similar logarithmic scaling should be observable for the impurity specific heat C_{imp}/T. However, we find that the critical scaling of the specific heat occurs at lower T and instead C_{imp} shows a more complex behavior in the intermediate range. Moreover, the numerical method is known to produce larger errors for C at low T [7], which may be due to the second derivative involved. Therefore, we could not fully reproduce the corresponding data collapse of C_{imp}/T, but our data is nonetheless consistent with a crossover to logarithmic scaling as $T \to 0$. Just as in the 2CK effect we also find that a *finite* magnetic field (local or global) will change the logarithmic non-Fermi-liquid behavior and produce a crossover to a constant susceptibility below some temperature T_{FL} as shown in the inset of Fig. 1. The different renormalization behavior can be traced to the broken spin-flip symmetry, which allows the relevant operator $\cos\sqrt{2\pi}\,\phi$ with $d = 1/2$ at the periodic chain fixed point. This will result in a quadratic field dependence $T_{\mathrm{FL}} \propto B_0^2$, which has already been demonstrated in Ref. [3]. In experiments, however, fields are expected to be small compared to J and T_K, so that in most cases only the non-Fermi-liquid behavior will be observed. The effect of a finite B_0 is analogous to violating the symmetry condition in the resonant tunneling scenario for electrons [10].

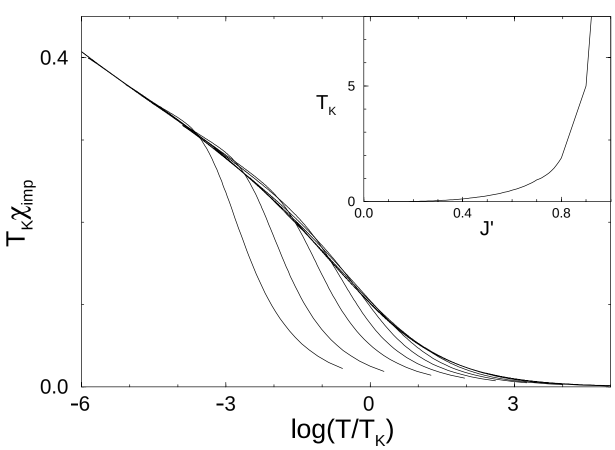

FIG. 2. The scaled impurity susceptibility $T_K\chi_{\mathrm{imp}}$ for an appropriate choice of T_K as a function of $J' = 0.1J, \ldots, 0.95J$ (inset).

Finally, we consider the local susceptibilities (the Knight shift) of the individual spin sites in a region around the impurity as a function of site index x

$$\chi_{\mathrm{local}}(x) = \frac{d\langle S^z(x)\rangle_B}{dB}\bigg|_{B=0}\,. \tag{8}$$

In Ref. [11] the most dramatic effect of an open boundary condition on the Knight shifts was found to be a *staggered* component $\chi_{\mathrm{open}} = \chi_{\mathrm{local}} - \chi$ in response to a *uniform* magnetic field B, which *increases* with site index x:

$$\chi_{\mathrm{open}}(x) \propto (-1)^x \frac{x\sqrt{T}}{\sqrt{\sinh 4xT}}\,, \tag{9}$$

where T is measured in units of J.

The staggered part in Eq. (9) arises due to open boundary conditions and hence it will be diminished as the system renormalizes to the periodic chain fixed point. However, there will be a whole new effect due to the leading irrelevant operator $\partial_x \sin\sqrt{2\pi}\,\phi$ at the periodic chain fixed point. This operator also induces a staggered part χ_{periodic}, but with opposite sign; i.e., the induced response at the first site $\vec{S}_1$ is *negative*. The alternating response as a function of site index x is now

$$\chi_{\mathrm{periodic}}(x) = (-1)^x \frac{1}{T}\int dy\,\langle S_{\mathrm{alt}}^z(x) S_{\mathrm{uni}}^z(y)\rangle$$
$$\propto (-1)^x \frac{1}{T}\int dy \int^{1/T} d\tau\, g(x,y,\tau)\,, \tag{10}$$

where S_{alt}^z and S_{uni}^z refer to the leading operators which describe the alternating ($\cos\sqrt{2\pi}\,\phi$) and uniform ($\partial_x\phi$) parts of the spin z component, respectively. The correlation function $g(x,y,\tau)$ is therefore given by

$$g(x,y,\tau) \propto \langle \cos\sqrt{2\pi}\,\phi(x)\,\partial_x\phi(y)\,\partial_x \sin\sqrt{2\pi}\,\phi(0,\tau)\rangle$$
$$\propto \frac{T}{\sin T(\pi\tau - i2x)}\,\frac{T^2}{\sin^2 T(\pi\tau - i2y)}\,, \tag{11}$$

where we have used standard field theory techniques (e.g., the boson mode expansion [12]). The integral of the second factor over the spatial coordinate y is the same that determines the unperturbed susceptibility per site [13] and simply gives a τ-independent contribution proportional to T. The integral of the first factor over τ gives

$$\chi_{\mathrm{periodic}}(x) \propto (-1)^x \log[\tanh(xT)]\,. \tag{12}$$

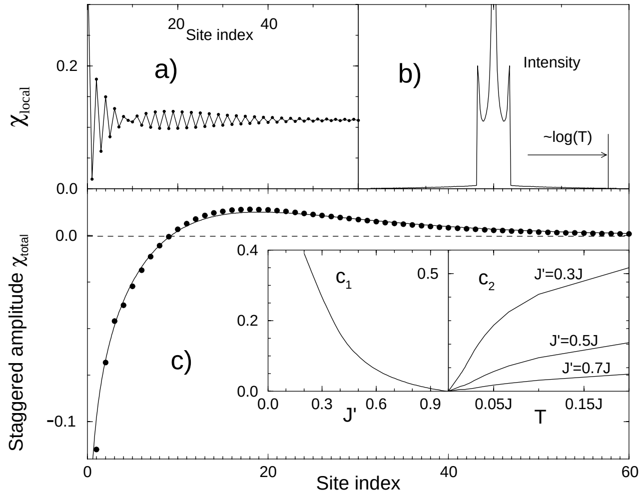

FIG. 3. (a) The local susceptibilities as a function of site index for $T = 0.05J$ and $J' = 0.7J$. (b) The corresponding typical NMR spectrum with a distinct feature (kink). (c) The fit of the alternating amplitude to Eq. (13) (solid line) with the appropriate coefficients (inset).

This expression shows the logarithmic divergence with T explicitly for small x at the impurity, and the response then drops off with $\exp(-2xT)$ as $xT \longrightarrow \infty$ [i.e., with the same exponential as in Eq. (9)].

As J' is increased, the alternating part changes from the behavior of Eq. (9) to the behavior of the stable fixed point in Eq. (12), which is always logarithmically dominant as $T \longrightarrow 0$. However, even very close to the periodic chain fixed point we observe an interesting and complex competition of *both* contributions [see Fig. 3(a)], which is nonetheless completely understood. In particular, below T_K the total amplitude of the staggered part of χ_{local} always fits very well to a superposition

$$\chi_{\mathrm{total}}(x) = c_1 \log[\tanh(xT)] + c_2 \frac{x\sqrt{T}}{\sqrt{\sinh 4xT}} . \qquad (13)$$

This formula gave excellent results as can be seen for a typical fit in Fig. 3(c), and the coefficients have been determined for all values of $J' \geq 0.2J$ and T (inset). The coefficient c_1 is T independent, while c_2 renormalizes to zero as $T \longrightarrow 0$.

To see these effects experimentally, it will be necessary to induce site-symmetric bond defects into quasi-one-dimensional spin-$1/2$ compounds as, e.g., Sr_2CuO_3, $KCuF_3$, or copper pyrazine nitrate. A simple doping with another effective spin-$1/2$ ion for Cu^{2+} may be possible, but more likely the surrounding nonmagnetic ions can be doped in order to create a suitable lattice deformation. The effect of open boundaries has already been seen in NMR experiments [14], by observing a unique feature that broadened with $1/\sqrt{T}$ and had the predicted shape derived from Eq. (9). For site-symmetric perturbations we can now predict a broadening with $\log T$ of the NMR spectrum. In addition, there will be a feature (kink) at smaller Knight shifts which comes from the relative maximum in the alternating response [see Fig. 3(b)]. This feature has a distinctive shape and temperature dependence which can be calculated from the constants c_1 and c_2 with the help of Eq. (13) for any coupling strength J'. Ordinary susceptibility measurements should be able to identify the impurity contribution as predicted by the crossover function in Fig. 2. In a more exotic twist we can even imagine muon spin rotation experiments, where the muon itself may play the role of an impurity; i.e., depending on the preferred muon location in the lattice, the muon could feasibly induce a site-symmetric lattice distortion and at the same time measure the logarithmically divergent response at the impurity site.

In summary, we have shown the crossover of a two-channel Kondo impurity explicitly, which confirmed the renormalization picture and demonstrated the expected data collapse explicitly. Moreover, we were able to predict the response to a uniform magnetic field of individual spin sites in a large region around the impurity, which led to quantitative predictions for Knight-shift experiments on doped spin-$1/2$ compounds.

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