Universal cross-over 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 (DMRG) we are able to determine local and global properties in the thermodynamic limit. The cross-over function for the impurity susceptibility is calculated over a large temperature range, which exhibits universal data-collapse. We are also able to determine 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.

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 \[7\]. The 2CK model has received much interest in the theoretical physics community \[7\] since it was first proposed in 1980 \[7\] and this model is often cited as a standard example of non-Fermi-liquid physics. Bethe ansatz \[7\] and conformal field theory techniques \[7\] have lead to almost complete understanding. On the other hand it is much less clear to what extend experimental applications exist, although there is some hope that the conductance behavior through metal constrictions can be explained by the 2CK effect \[7\].

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, and calculate the resulting cross-over function over a large temperature range. For this purpose we have developed a modification of the transfer-matrix DMRG \[7\].

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

\[ H = J \sum_{i=1}^{L-1} \vec{S}_{i} \cdot \vec{S}_{i+1} + J' (\vec{S}_{L} + \vec{S}_{1}) \cdot \vec{S}_{0}, \]

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 known to be equivalent to the 2CK problem on the level of the Bethe ansatz equations \[3\], but we are not able to 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

\[ H = \int dx \frac{\nu}{2} \left[ (\partial_{x} \phi)^{2} + \Pi_{x}^{2} \right], \]

where \( \Pi_{x} \) is the conjugate operator to the boson field \( \phi \). This field theory has been discussed in more detail elsewhere \[6\], 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 \( \Gamma \), as long as we also multiply the physical quantity \( \mathcal{O} \) with \( \Gamma^{d} \),

\[ \mathcal{O}(T) = \Gamma^{-d} \mathcal{O}(\Gamma T), \]

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...
The linear response of the impurity spin to a local magnetic field. Inset: the data-collapse for 14 different \( J' = 0.1 J, \ldots, J \) and the effect of a finite field \( B_0 = \Lambda_{\text{eff}} \).

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 \( \chi_0 \) of the impurity spin \( S_0 \) to a local magnetic field \( B_0 \), which is given by the Kubo formula

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

For open boundary conditions the impurity spin will be asymptotically free and the response is given by a Curie law \( \chi_0 \propto 1/4T \). On the other hand, for periodic boundary conditions the auto-correlation functions will be determined by the leading field theory operator which obeys the same symmetry transformations as \( S_0 \). We found this operator to be \( \cos \sqrt{2\pi \phi} \) with dimension \( d = 1/2 \) and an auto-correlation function proportional to \( 1/\tau \), which should lead to a logarithmic divergence as \( T \to 0 \). As can be seen in Fig. (b), we indeed find a cross-over from Curie law to logarithmic behavior at an effective cutoff \( \Lambda_{\text{eff}} = \min(\Lambda, T_K) \), depending on the coupling strength \( J' \) with a scaling behavior of the form \( \chi_0(T) = g(T/\Lambda_{\text{eff}})/\Lambda_{\text{eff}} \) (inset). The logarithmic behavior was observed before at one coupling only by other methods (c). Note, however, that the response \( \chi_0 \) is only an indication of the auto-correlation functions, but it must not be confused with the impurity susceptibility, since we have only applied the magnetic field at one

\( \delta J = J - J' \) 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 which still observes the site-parity symmetry of the problem is known to be \( \partial_x \sin \sqrt{2\pi \phi} \) of dimension \( d = 3/2 \). This operator gives the leading corrections, but is still irrelevant. In particular, for a given coupling strength \( \delta J \) the size of the corrections becomes effectively smaller by a factor of \( \Gamma^{d^{-1}} \) 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 cross-over (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 \( \delta J \) we have defined \( T_K \) as the temperature at which the product \( T^{d-1} \delta J \) 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 \( \Gamma \) is equivalent to changing \( T_K \) by \( 1/\Gamma \), i.e. altering the initial coupling strength \( \delta J \) 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 \( 0 < J' < J \). 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 \( S_0 \) 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 (b): 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 (5) to test these concepts. The partition function of the spin-1/2 chain can be written in terms of transfer matrices \( Z = \text{tr}(T^{L/2}) \) \( \xrightarrow{L \to \infty} \lambda^{L/2} \), where \( \lambda \) is the largest eigenvalue of \( T \). 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 \( \lambda \). We now extend this method to non-uniform systems by using the eigenstate \( |\psi_\lambda \rangle \) corresponding to the highest eigenvalue \( \lambda \). We can include any impurity interaction which is described by a local matrix \( T_{\text{local}} \) explicitly in the partition function

\[
Z = \text{tr}(T^{L/2-1} T_{\text{local}}) \xrightarrow{L \to \infty} \lambda^{L/2-1} \langle \psi_\lambda | T_{\text{local}} | \psi_\lambda \rangle. \tag{4}
\]

If the eigenstate \( |\psi_\lambda \rangle \) is known to reliable precision from

the DMRG, it is straightforward to determine any thermodynamic property from this expression (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.
spin. In fact every spin in the periodic chain shows a logarithmic response to a local magnetic field.

![Graph](image)

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

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 $\chi_{\text{imp}} = \lim_{L \to \infty} (\chi_{\text{system}} - L \chi)$, where $\chi$ 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 able to obtain results at much lower temperatures by considering the linear response of the impurity spin to a uniform field $B$ instead

$$\chi_{\text{imp}} \approx \frac{d\langle S_x^z \rangle_B}{dB} - J' \chi,$$

which gives a good indication of the true impurity susceptibility (in contrast to $\chi_0$ in Eq. (1), where we only considered 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 $T_K$. Interestingly, this cross-over 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 $T/T_K$

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

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 non-universal 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 $C_{\text{imp}}/T$. However, we find that the critical scaling of the specific heat occurs at lower $T$ and instead $C_{\text{imp}}$ shows a more complex behavior in the intermediate range. Moreover, the numerical method is known to produce larger errors for $C$ at low $T$ which may be due to the second derivative involved. Therefore, we could not fully reproduce the corresponding data collapse of $C_{\text{imp}}/T$, but our data is nonetheless consistent with a cross-over to logarithmic scaling as $T \to 0$. Just like 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 cross-over to a constant susceptibility below some temperature $T_{KL}$ as shown in inset of Fig. 2. 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 $T_{KL} \propto B^2_0$, which has already been demonstrated in Ref. [3].

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

$$\chi_{\text{local}}(x) = \frac{d\langle S_x^z(x)B \rangle_B}{dB} \bigg|_{B=0}$$

In Ref. [1] the most dramatic effect of an open boundary condition on the Knight shifts was found to be a staggered component $\chi_{\text{open}} = \chi_{\text{local}} - \chi$ in the response to a uniform magnetic field $B$, which actually increases with site index $x$

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

where $T$ is measured in units of $J$.

The staggered part in Eq. (8) 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 $\chi_{\text{periodic}}$, but with opposite sign, i.e. the induced response at the first site $S_1$ is negative. The alternating response as a function of site index $x$ is now

$$\chi_{\text{periodic}}(x) = (-1)^x \frac{1}{T} \int dy \langle S_{alt}^z(x)S_{uni}^z(y) \rangle \propto (-1)^x \frac{1}{T} \int dy \int d\tau g(x, y, \tau).$$
where $S_{\text{alt}}^z$ and $S_{\text{uni}}^z$ 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

$$g(x, y, \tau) \propto \left( \cos \sqrt{2\pi} \phi(x) \right) \left( \cos \sqrt{2\pi} \phi(y) \right) \sin^2 \frac{\sqrt{2\pi} \phi(0, \tau)}{T^2}, \quad (11)$$

where we have used standard field theory techniques (e.g. the boson mode expansion). The integral of the second factor over the spatial coordinate $y$ is the same that determines the unperturbed susceptibility per site and simply gives a $\tau$-independent contribution proportional to $T$. The integral of the first factor over the imaginary time variable can then easily be done, giving

$$\chi_{\text{local}}(x) \propto (-1)^x \log [\tanh (xT)]. \quad (12)$$

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 $xT \to \infty$ (i.e. with the same exponential as observed for the open chain response). As $J'$ is increased, the alternating part changes from the behavior of Eq. (11) to the behavior of the stable fixed point in Eq. (12), which is always logarithmically dominant as $T \to 0$. However, even very close to the periodic chain fixed point we observe an interesting and complex competition of both contributions (see Fig. (2a)), which is nonetheless completely understood. In particular, below $T_K$ the total amplitude of the staggered part of $\chi_{\text{local}}$ always fits very well to a superposition

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

This formula gave excellent results as can be seen for a typical fit in Fig. (3c), 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 $T \to 0$.

To see these effects experimentally, it will be necessary to induce site-symmetric bond defects into quasi one-dimensional spin-1/2 compounds like Sr$_2$CuO$_3$, 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 non-magnetic ions can be doped in order to create a suitable lattice deformation. The effect of open boundaries has already been seen in NMR experiments [3], 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. (3b)).

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[1] S. Eggert, I. Affleck, Phys. Rev. B 46, 10866 (1992)
[2] D.G. Clarke, T. Giamarchi, B.I. Shraiman, Phys. Rev. B 48, 7070 (1993).
[3] For a review see P. Schlottmann, P.D. Sacramento, Adv. Phys. 42, 641 (1993).
[4] P. Nozières, A. Blandin, J. Phys. (Paris) 41, 193 (1980).
[5] For a review see I. Affleck, Acta Physica Polonica B 26, 1869 (1995); preprint cond-mat/9512099.
[6] D.C. Ralph, et. al., Phys. Rev. Lett. 69, 2118 (1992); ibid. 72, 1064 (1994); Phys. Rev. B 51, 3554 (1995); N.S. Wingren et. al. Phys. Rev. Lett. 75, 769 (1995).
[7] R.J. Bursill, T. Xiang, G.A. Gehring, J. Phys. C 8, L583 (1996); X. Wang, T. Xiang, Phys. Rev. B 56, 5061 (1996); N. Shibata, J Phys. Soc. Jpn. 66, 2221 (1997); S.R. White, Phys. Rev. B 48, 10345 (1993).
[8] P. Schlottmann, J. Phys.: Condens. Matter 3, 6617 (1991).
[9] W. Zhang, J. Igarashi, P. Fulde, J. Phys. Soc. Japan 66, 1912 (1997).
[10] C.L. Kane, M.P.A. Fisher, Phys. Rev. B 46, 15233 (1992).
[11] S. Eggert, I. Affleck, Phys. Rev. Lett. 75, 934 (1995).
[12] S. Eggert, A.E. Mattsson, J.M. Kinaret, Phys. Rev. B 56, R15537 (1997).
[13] S. Eggert, I. Affleck, M. Takahashi, Phys. Rev. Lett. 73, 332 (1994).
[14] M. Takigawa, N. Motoyama, H. Eisaki, S. Uchida, Phys. Rev. B 55, 14129 (1997); Phys. Rev. Lett. 76, 4612 (1996).