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

Sebastian Eggert,[1] David P. Gustafsson,[1] and Stefan Rommer[2]
[1]Institute of Theoretical Physics, Chalmers University of Technology and Göteborg University, S-412 96 Göteborg, Sweden
[2]Department of Physics and Astronomy, University of California, Irvine, California 92697
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We consider a magnetic $S = 1/2$ impurity in the antiferromagnetic spin chain as a function of two coupling parameters: the symmetric coupling of the impurity to two sites in the chain J_1 and the coupling between the two sites J_2. By using field theory arguments and numerical calculations we can identify all possible fixed points and classify the renormalization flow between them, which leads to a nontrivial phase diagram. Depending on the detailed choice of the two (frustrating) coupling strengths, the stable phases correspond either to a decoupled spin with Curie law behavior or to a non-Fermi-liquid fixed point with a logarithmically diverging impurity susceptibility as in the two-channel Kondo effect. Our results resolve a controversy about the renormalization flow.

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Impurities in low-dimensional magnetic and electronic systems have recently received a lot of attention in the context of mesoscopic systems, quasi-one-dimensional compounds and high temperature superconductivity. Much progress has been made in particular for one-dimensional systems, where quantum impurities are known to renormalize as the temperature is lowered, so that the impurity can be described by an effective boundary condition in the low temperature limit [1]. The temperature dependence of the impurity contributions to the specific heat and the susceptibility can also be predicted. Very often the antiferromagnetic spin-1/2 chain with impurities is taken as the prototype example for this renormalization behavior [2–16], which captures the essential renormalization behavior of many other impurity systems.

A number of different impurity configurations have been considered where typically one coupling parameter is varied. The chain with one altered link is known to renormalize to an effective open boundary condition [2] in analogy with the renormalization of the conductivity in a quantum wire [17]. However, two neighboring altered links renormalize to a periodic boundary condition [2] in analogy with resonant tunneling in quantum wires [18]. This renormalization behavior is also equivalent to the two-channel Kondo effect [1–3]. Equally interesting is the coupling of an external impurity spin to one or two sites in the chain. An impurity spin s coupled to one site in the chain gets screened with a resulting decoupled singlet of spin s-1/2 and an open chain with one site removed [2,4–9]. An impurity spin coupled to two sites in the chain was first considered in Ref. [10], where an equivalence with the two-channel Kondo effect was found on the basis of the field theory description [10,11], which would result in an "overscreened" impurity spin with a logarithmically diverging impurity susceptibility. However, numerical simulation studies later questioned this result and predicted instead a decoupled impurity spin as the stable boundary condition with a Curie law susceptibility [7,8], which is an unresolved controversy.

We now consider a two parameter impurity model. This allows us to consider the different impurity configurations above in a richer phase diagram with a greater number of possible fixed points. By using field theory techniques and advanced numerical results, we are able to map out the phase separation line between an overscreened and a decoupled impurity spin exactly, which not only resolves the controversy but also shows a more complex renormalization behavior.

The Hamiltonian we consider here describes a Heisenberg chain, where two neighboring sites are coupled to an impurity spin-1/2 with strength J_1. The two sites are also coupled to each other with strength J_2, as shown in Fig. 1,

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

In the low temperature limit this system is known to be well described by by a level 1 Wess-Zumino-Witten (WZW) model with a marginal irrelevant operator [19]. A spin operator at position x in the chain can be expressed in terms of the current operators $\vec{J}$ and the WZW field g,

$$\vec{S}(x) \approx \vec{J}_L + \vec{J}_R + (-1)^x \times \text{const} \times \text{tr}\vec{\sigma} g . \quad (2)$$

General values of J_1 and J_2 break the conformal invariance of the effective field theory and introduce perturbing

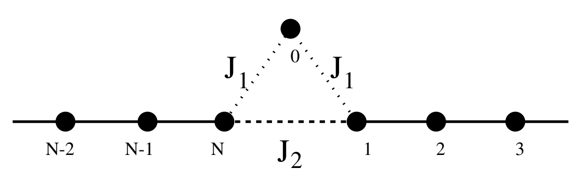

FIG. 1. Impurity model with two parameters J_1 and J_2.

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operators in the field theory Hamiltonian, which in turn can be classified by their renormalization behavior. As the temperature is lowered the system must always approach a fixed point that restores conformal invariance [1]. For the spin-$1/2$ chain in Eq. (1) the possible fixed points are always given in terms of simple boundary conditions on the spin chain (open or periodic). In addition there may be completely decoupled impurity spins present. The possible fixed points for this system are shown in Fig. 2. (i) $J_1 = J$, $J_2 = 0$. A periodic chain with $N + 1$ sites and no impurity spin. The impurity spin has been absorbed. We denote this fixed point by P_{N+1}. (ii) $J_1 = 0$, $J_2 = 0$. An open chain with N sites and a decoupled $s = 1/2$ impurity spin. We denote this fixed point by $O_N \otimes \frac{1}{2}$. (iii) $J_1 = 0, J_2 = J$. A periodic chain with N sites and a decoupled $s = 1/2$ impurity spin, denoted by $P_N \otimes \frac{1}{2}$. (iv) $J_1 = 0$, $J_2 = \infty$. An open chain with $N - 2$ sites and a decoupled impurity $s = 1/2$. The two end sites at 1 and N have locked into a singlet state. We denote this fixed point by $O_{N-2} \otimes \frac{1}{2}$.

The renormalization behavior in the vicinity of each of those fixed points is determined by the operator content of the impurity Hamiltonian according to the perturbation of J_1 and J_2 around the corresponding fixed point values. Typically the operators with the lowest scaling dimensions (leading operators) can be determined by either a straightforward symmetry analysis or by direct application of Eq. (2). Local operators become relevant when their scaling dimension is less than one $d < 1$.

In the vicinity of the periodic fixed point P_{N+1} the leading irrelevant operator is given by $\partial_x \operatorname{tr} g$ because site parity symmetry does not allow more relevant operators [2]. We therefore immediately conclude that this fixed point is stable in all directions in the $J_1 - J_2$ phase diagram; i.e. small perturbations on both J_1 and J_2 are irrelevant, as indicated in the phase diagram Fig. 3.

In the vicinity of the fixed point $O_N \otimes \frac{1}{2}$, the fields in the perturbing Hamiltonian are given by boundary operators. This stems from the analytic continuation of the left moving fields in terms of right moving fields in order to restore the conformal invariance at an open boundary. The leading operator $[\vec{J}_L(0) + \vec{J}_L(N)] \cdot \vec{S}_{\text{imp}}$ of scaling dimension $d = 1$ is created by the coupling J_1 to the impurity spin from the open ends. This operator is marginally relevant for an antiferromagnetic sign and marginally irrelevant for a ferromagnetic sign analogous to the Kondo effect [2]. The coupling between the end spins J_2 can only produce the irrelevant operators [2] $\vec{J}_L^2(0)$, $\vec{J}_L^2(N)$, and $\vec{J}_L(0) \cdot \vec{J}_L(N)$ with scaling dimension $d = 2$. Hence the coupling J_2 is always irrelevant in the vicinity of $O_N \otimes \frac{1}{2}$. We therefore conclude that the fixed point $O_N \otimes \frac{1}{2}$ is stable for $J_1 \leq 0$, but for $J_1 > 0$ the effective coupling to the impurity spin increases under renormalization and flows towards the stable fixed point P_{N+1}, corresponding to a "healing" of the chain [2] as indicated in the phase diagram (Fig. 3). This effect is in fact completely analogous to the renormalization flow and overscreening of the spin excitations in the two-channel Kondo problem [1–3], resulting in a logarithmically diverging impurity susceptibility.

Near the fixed point $O_{N-2} \otimes \frac{1}{2}$ the impurity spin is separated by a locked singlet in the limit $J_2 \to \infty$ which is effectively decoupled from the rest of the chain (unless we introduce additional coupling constants). Therefore the fixed point $O_{N-2} \otimes \frac{1}{2}$ appears to be stable in all directions in our $J_1 - J_2$ phase diagram in Fig. 3.

A more interesting scenario can be found near the fixed point $P_N \otimes \frac{1}{2}$ since a small coupling J_1 of either sign is frustrating. Here the most relevant operator $\operatorname{tr} g$ corresponds to a slight modification of one link in the chain J_2. If the impurity spin is absent this operator is responsible

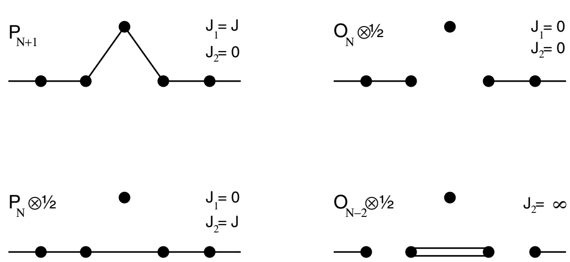

FIG. 2. The four possible fixed points.

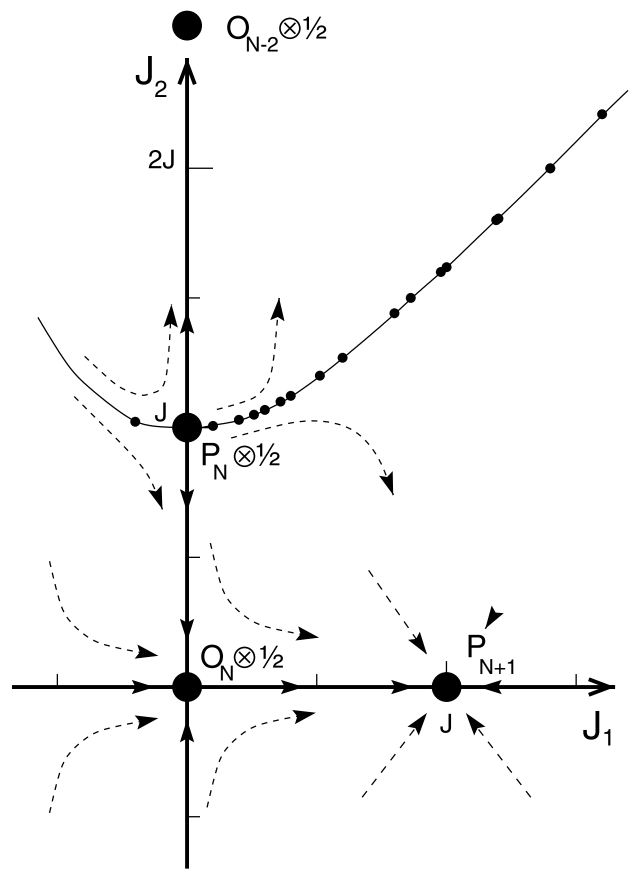

FIG. 3. The full phase diagram of the $J_1 - J_2$ impurity model. The possible fixed points are indicated by the thick solid dots. The points on the phase separation line have been estimated numerically by analyzing $\langle \mathbf{S}_1 \cdot \mathbf{S}_N \rangle$ as in Fig. 4 for 132 different values for J_1 and J_2.

for the breaking of the chain [2], but the frustrating coupling J_1 must now also be considered. In particular, a small coupling to the impurity spin J_1 produces the operator $(\vec{J}_L + \vec{J}_R) \cdot \vec{S}_{\rm imp}$ which is marginally relevant/irrelevant for antiferromagnetic/ferromagnetic sign respectively. The irrelevant operator $\partial_x {\rm tr}\vec{\sigma} g \cdot \vec{S}_{\rm imp}$ of dimension $d = 3/2$ is also created by J_1. In summary we may express the impurity Hamiltonian at the fixed point $P_N \otimes \frac{1}{2}$ as

$$H_{\rm imp} = \gamma_1 {\rm tr} g + \gamma_2 (\vec{J}_L + \vec{J}_R) \cdot \vec{S}_{\rm imp} + \gamma_3 \partial_x {\rm tr}\vec{\sigma} g \cdot \vec{S}_{\rm imp}\,, \tag{3}$$

where, to lowest order,

$$\gamma_1 \propto (J_2 - J), \qquad \gamma_2 \propto J_1, \qquad \gamma_3 \propto J_1\,. \tag{4}$$

The renormalization group equations can then be determined by using the operator product expansion. We find that

$$\begin{aligned} \dot{\gamma}_1 &= \tfrac{1}{2}\gamma_1 - \tfrac{3}{2}\gamma_2\gamma_3\,, \\ \dot{\gamma}_2 &= \gamma_2^2 - \tfrac{3}{4}\gamma_3^2\,, \\ \dot{\gamma}_3 &= -\tfrac{1}{2}\gamma_3 + 2\gamma_2\gamma_3\,. \end{aligned} \tag{5}$$

where the dot indicates the derivative with respect to the logarithm of the cutoff. The renormalization flow is dominated by the relevant coupling constant γ_1, so that it is crucial to determine if $\dot{\gamma}_1$ is initially negative or positive. Interestingly, the irrelevant coupling constant γ_3 plays an important role in defining the corresponding phase separation line along $\gamma_1 = 3\gamma_2\gamma_3$, which, together with Eq. (4), gives a parabolic shape in the $J_1 - J_2$ phase diagram $J_2 - J \propto J_1^2$, as indicated in Fig. 3. Indeed if the irrelevant coupling constant γ_3 is neglected, one might erroneously come to the conclusion that the relevant backscattering γ_1 is exactly zero along the line $J_2 = J$ resulting in just a marginal renormalization flow as postulated in Refs. [10,11], which is not the case.

If $\dot{\gamma}_1 > 0$ the effective coupling J_2 increases quickly so that the two end spins lock into a singlet independent of the value of J_1. Therefore, the stable fixed point is $O_{N-2} \otimes \frac{1}{2}$ above the phase separation line. If, however, $\dot{\gamma}_1 < 0$ the effective coupling J_2 decreases towards zero and the stable fixed point now depends on the marginal coupling J_1. For $J_1 \leq 0$ the stable fixed point is $O_N \otimes \frac{1}{2}$ while for $J_1 > 0$ the healing process towards the fixed point P_{N+1} takes place again. The leading irrelevant operators close to P_{N+1} will again produce a logarithmically divergent impurity susceptibility [1], but the renormalization flow is not completely analogous to the two-channel Kondo effect since the operator content near the unstable fixed point is quite different. In particular, the relevant operator ${\rm tr}g$ is completely absent in the ordinary Kondo problem. The impurity susceptibility in the phases characterized by the fixed points $O_N \otimes \frac{1}{2}$ and $O_{N-2} \otimes \frac{1}{2}$ is a Curie law behavior as $T \to 0$ from the decoupled impurity spin degrees of freedom.

We have now determined the basic shape of the phase diagram, but to quantitatively map out the phase separation line it is necessary to resort to numerical methods. We therefore choose the transfer matrix renormalization group method for impurities, which can determine local correlation functions directly in the thermodynamic limit [9]. One obvious order parameter is the correlation between the two end spins which takes well-defined values at each fixed point in the zero temperature limit

$$\begin{array}{ll} P_{N+1} & \langle \vec{S}_1 \cdot \vec{S}_N \rangle = \frac{1}{4} - 4\ln 2 + \frac{9}{4}\zeta(3) \\ O_N \otimes \frac{1}{2} & \langle \vec{S}_1 \cdot \vec{S}_N \rangle = 0 \\ P_N \otimes \frac{1}{2} & \langle \vec{S}_1 \cdot \vec{S}_N \rangle = \frac{1}{4} - \ln 2 \\ O_{N-2} \otimes \frac{1}{2} & \langle \vec{S}_1 \cdot \vec{S}_N \rangle = -\frac{3}{4}\,, \end{array} \tag{6}$$

where ζ is the Riemann Zeta function. The values at the periodic chain fixed points correspond to the first and second nearest neighbor correlations in the ordinary Heisenberg chain [20], while the open chain fixed point values correspond to two uncorrelated spins and a spin singlet, respectively. Numerical simulations can never reach zero temperature in the thermodynamic limit, but it is quite possible to determine if the correlation between the spins renormalizes towards larger or smaller values as the temperature is lowered and thereby determines the stable fixed point.

In particular we postulated that above the phase-transition line in Fig. 3 the two end spins effectively lock into a singlet so that the correlation should *decrease* with decreasing temperature. Below the phase-transition line, however, the two spins will only be weakly correlated at $O_N \otimes \frac{1}{2}$ or ferromagnetically correlated at P_{N+1} so that the correlation should *increase* with decreasing temperature.

This behavior is shown in Fig. 4 for $J_1 = 0.8J$ and different values of J_2. As $T \to 0$ the correlation clearly decreases for larger values of $J_2 \gtrsim 1.5J$ but increases for smaller values $J_2 \lesssim 1.2J$ so that the phase transition occurs somewhere between those two values. We can identify the critical value of J_2 more closely by considering the slope and absolute value of $\langle \vec{S}_1 \cdot \vec{S}_N \rangle$ as $T \to 0$. The critical value can be defined as the point where the slope is zero or the absolute value is $1/4 - \ln 2$, which gives approximately the same result $J_2 \approx 1.44J$. We have made a similar analysis for many different points in the $J_1 - J_2$ parameter space and thereby mapped out the exact numerical location of the phase separation line as shown in Fig. 3. As $J_1, J_2 \to \infty$ the phase transition occurs at $J_1 = J_2$ which can be determined by analyzing the ground state of the three coupled spins $\vec{S}_N$, $\vec{S}_0$, and $\vec{S}_1$.

We now wish to relate our results to previous numerical studies of this impurity model by Zhang *et al.* [6–8], where three points in the phase diagram were analyzed at ($J_1 = 0.4J$, $J_2 = J$), ($J_1 = 0.4J$, $J_2 = 0$), and ($J_1 = 1.5J$, $J_2 = J$), which led to a controversy with the predictions in Refs. [10,11]. In particular, the numerical studies found no logarithmically diverging impurity susceptibility at ($J_1 = 0.4J$, $J_2 = J$). As mentioned above the analytic studies in Refs. [10,11] failed to consider the leading relevant operator ${\rm tr}g$ at the unstable fixed point $P_N \otimes \frac{1}{2}$, but the logarithmic impurity susceptibility is created by the leading irrelevant operator $\partial_x\, {\rm tr}g$ near the *stable* fixed point

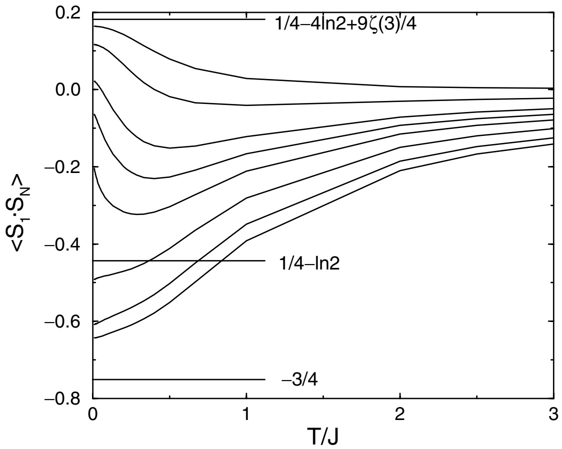

FIG. 4. The correlation $\langle \vec{S}_1 \cdot \vec{S}_N \rangle$ as a function of T for $J_1 = 0.8J$ and $J_2 = 0$, 0.4, 0.8, 1, 1.2, 1.5, 1.8, and $2J$ from above. By analyzing the slope or absolute value compared to $\frac{1}{4} - \ln 2$, the phase transition can be estimated to be at $J_2 \approx 1.44J$ in this case.

P_{N+1} [1], so that we also postulate a logarithmic divergence below some crossover temperature T_K. However, by looking at the phase diagram in Fig. 3 we see that the point ($J_1 = 0.4J$, $J_2 = J$) lies very close to the phase-transition line, so that the crossover temperature T_K must be extremely small and cannot be reached by any numerical method today, which explains the controversy. On the other hand, the points ($J_1 = 1.5$, $J_2 = J$) and ($J_1 = 0.4$, $J_2 = 0$) are farther from the phase separation and the crossover temperature is larger. Therefore, the logarithmic divergence can indeed be observed [3,6,8]. In Ref. [8] the end spin correlation $\langle \vec{S}_1 \cdot \vec{S}_N \rangle$ was also determined, which is consistent with our results, but with a different interpretation. Because the overall value of $\langle \vec{S}_1 \cdot \vec{S}_N \rangle$ is negative, it was concluded in that work that the point ($J_1 = 0.4J$, $J_2 = J$) produces a Curie law susceptibility from frustration, i.e., an effectively decoupled impurity spin. However, the temperature dependence clearly shows a renormalization towards an increasing correlation as $T \to 0$, so that P_{N+1} is the correct stable fixed point with an absorbed impurity spin and a logarithmically diverging susceptibility below an extremely small crossover temperature T_K. Interestingly, there is an integrable spin-1 chain model with a spin-$1/2$ impurity which can also reproduce this two-channel Kondo renormalization behavior near the fixed point P_{N+1} [21]. However, the interesting boundary fixed points that were recently discovered in this integrable model [22] have no analogous expression in our parameter space.

In conclusion we have analyzed a complex impurity model in the spin-$1/2$ chain which shows a rich phase diagram. We were able to identify three different stable phases that are attracted to well-defined fixed points under renormalization. The three phases are separated by the unstable fixed point $P_N \otimes \frac{1}{2}$ which shows a high sensitivity to the detailed choice of couplings due to frustration. By using field theory arguments and numerical techniques, we were able to map out the phase diagram exactly and also resolve a controversy in the literature [7,8,10,11]. Interestingly, an irrelevant operator plays a crucial rule in determining the shape of the phase separation line. It would be interesting to see if the current findings can be generalized to other systems, where a frustrated state may separate more stable phases (e.g., in a ladder system with a zigzag geometry). In general, a frustrated state should always be unstable since it has been postulated that renormalization typically occurs towards a state with a lower ground state degeneracy [23]. The system we considered here is a typical example of this behavior.

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