"Anomalous Fixed Point Behavior" of Two Kondo Impurities: A Reexamination

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We consider the existence of "anomalous fixed point behavior" for the Kondo two-impurity Hamiltonian. This "anomalous" behavior is predicted by calculations which use the "energy-independent coupling constants" (ECC) approximation. Using well-controlled quantum Monte Carlo methods without the ECC approximation, we find no evidence for "anomalous" behavior. We then show that the ECC approximation is, in general, either inconsistent or uninteresting. These results together strongly suggest that the predicted "anomalous" behavior of two Kondo impurities is simply the result of an unphysical approximation rather than an intrinsic property of the model itself.

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There has been great interest in recent years in the properties of two interacting magnetic impurities in a metal [1-11]. This is largely because the understanding of two such impurities is a first step towards understanding the magnetic properties of the "heavy fermion" materials [12,13], materials which appear to consist of a lattice of magnetic moments interacting with a conduction band. In the two-impurity system, there are two effects which can compete against each other: The Kondo effect [14] and the RKKY interaction [15]. The RKKY interaction at low temperatures will by itself tend to lock the two-impurity spins into a singlet or a triplet, depending on the sign of the RKKY coupling constant. The Kondo effect involves the screening of the individual impurity spins by the conduction electron spins, with the accompanying formation of a many-body (impurity)-(conduction-electron) singlet. The competition between the two effects arises because the Kondo effect can inhibit the development of RKKY spin correlations between the impurities. This general competition may offer an explanation for the different varieties of magnetic behavior observed in the heavy fermion materials [12,13,16].

Earlier theoretical work [1-5] on the two-impurity system, for two spin-$\frac{1}{2}$ impurities with an antiferromagnetic RKKY interaction, qualitatively supported the above picture of competition between the RKKY interaction and the Kondo effect. However, numerical renormalization group [6] (NRG) and "exact critical theory" [10] calculations predicted in addition an unexpected "anomalous fixed point" with striking behavior: Certain normally finite quantities diverge as the temperature $T \rightarrow 0$. Well-controlled quantum Monte Carlo simulations [8], however, have so far given no indication of any such divergence. In this Letter, we explore the reasons for this discrepancy.

The model which we consider is the two-impurity spin-$\frac{1}{2}$ Kondo model [1-11]

$$H = H_0 + H_I, \tag{1}$$

where

$$H_0 = \sum_s \int d^{\mathcal{D}} k \, e_{\mathbf{k}} \psi^\dagger_{\mathbf{k},s} \psi_{\mathbf{k},s} \tag{2}$$

and

$$H_I = J \sum_j \mathbf{S}_j \cdot \mathbf{S}_c(\mathbf{R}_j) \,. \tag{3}$$

H_0 refers to the conduction electron band and H_I to the interactions between the spins and the conduction electrons. Specifically, $\mathcal{D}$ is the dimensionality of the system, $s = \uparrow, \downarrow$ refers to spin, $j = 1,2$ refers to the two impurities, $[\psi^\dagger_{\mathbf{k},s}, \psi_{\mathbf{k}',s'}] = \delta_{s,s'} \delta(\mathbf{k} - \mathbf{k}')$,

$$\mathbf{S}_c(\mathbf{R}_j) = \sum_{s,s'} c^\dagger_{js} (\tfrac{1}{2} \boldsymbol{\sigma}_{ss'}) c_{js'} \tag{4}$$

is the normalized conduction electron spin at $\mathbf{R}_j$, with

$$c_{js} = \eta^{-1/2} \int d^{\mathcal{D}} k \, e^{i\mathbf{k}\cdot\mathbf{R}_j} \psi_{\mathbf{k},s} \,, \tag{5}$$

where $\eta = \int d^{\mathcal{D}} k$ so that $[c^\dagger_{js}, c_{j's'}] = \delta_{s,s'} \delta_{j,j'}$, the $\epsilon(\mathbf{k})$'s are the conduction electron energy levels, the $\mathbf{S}_j$'s are the impurity spins, and J is the Kondo coupling constant. For small ρJ, where ρ is the total conduction electron density of states at the Fermi level (spin $\uparrow$ plus spin $\downarrow$), the Kondo temperature T_K at which Kondo screening occurs is given by [14]

$$T_K = D(\rho J)^{1/2} e^{-1/\rho J} \,, \tag{6}$$

where D is here the conduction electron bandwidth. To lowest order in ρJ, the RKKY coupling constant $\mathcal{J}$, associated with the effective Hamiltonian

$$H_{\text{eff}} = \mathcal{J} \mathbf{S}_1 \cdot \mathbf{S}_2 \tag{7}$$

is given by [15]

$$\mathcal{J} = \left(\frac{J}{2\pi} \right)^2 \mathcal{P} \int_{\epsilon(\mathbf{k}) < \epsilon_F} d^{\mathcal{D}} k \int_{\epsilon(\mathbf{k}') > \epsilon_F} d^{\mathcal{D}} k' \frac{\cos[(\mathbf{k} - \mathbf{k}') \cdot (\mathbf{R}_1 - \mathbf{R}_2)]}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}} \,, \tag{8}$$

where $\mathcal{P}$ denotes "principal part" and ϵ_F is the Fermi energy.

Setting $\mathbf{R}_1 = -\mathbf{R}/2$ and $\mathbf{R}_2 = \mathbf{R}/2$, one can rewrite the interaction term H_I of the Hamiltonian of Eq. (1) as

$$H_I = \eta^{-1} J \sum_{p,p'} \sum_{s,s'} (\tfrac{1}{2} \boldsymbol{\sigma}_{ss'}) [\mathbf{S}_1 + (-1)^{(p-p')} \mathbf{S}_2] \left(\int dE \, g_p(E) \psi^\dagger_{ps}(E) \right) \left(\int dE' \, g_{p'}(E') \psi_{p's'}(E') \right) . \tag{9}$$

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Here, $p=0,1$,

$$g_p(E)=\left\{\int d^{\mathcal{D}}k\,\delta[E-\epsilon(\mathbf{k})][h_p(\mathbf{k})]^2\right\}^{1/2}, \quad (10)$$

$$h_0(\mathbf{k})=\cos\left[\frac{\mathbf{k}\cdot\mathbf{R}}{2}\right], \quad (11)$$

$$h_1(\mathbf{k})=\sin\left[\frac{\mathbf{k}\cdot\mathbf{R}}{2}\right], \quad (12)$$

and

$$\psi_{ps}(E)=i^p\{g_p(E)\}^{-1}\int d^{\mathcal{D}}k\,\delta[E-\epsilon(\mathbf{k})]h_p(\mathbf{k})\psi_{\mathbf{k}s}. \quad (13)$$

$\epsilon(\mathbf{k})=\epsilon(-\mathbf{k})$ is assumed so that $[\psi^\dagger_{ps}(E),\psi_{p's'}(E)]=\delta_{ss'}\delta_{pp'}\delta(E-E')$, with $\psi_{0s}(E)$ and $\psi_{1s}(E)$ referring, respectively, to "even" and "odd" conduction electron channels [3,6,17].

The numerical renormalization group, originally applied by Wilson to the Kondo single-impurity problem [14], was used to study the two-impurity Hamiltonian with H_I in the form of Eqs. (9)-(13) with the approximation of ignoring the energy dependence of $g_0(E)$ and $g_1(E)$; i.e., the condition

$$g_p(E)=\mathcal{G}_p \quad (14)$$

($p=0,1$) was set, with each $\mathcal{G}_p$ independent of E. This is the "energy-independent coupling constants" (ECC) approximation [3,6,17], which is made under the assumption that the energy dependence of the $g_p(E)$'s corresponds only to "irrelevant operators" which have no effect on the low-temperature physics. Specifically, the particle-hole symmetric case of the Kondo two-impurity Hamiltonian was studied [6,17]. An unexpected "anomalous fixed point" was found [6,17] at $\mathcal{J}/T_K\approx 2.2$ (antiferromagnetic RKKY coupling) at which the impurity specific heat coefficient γ and staggered susceptibility χ_s diverged as temperature $T\to 0$. Associated with these divergences was a ground state value of $\langle\mathbf{S}_1\cdot\mathbf{S}_2\rangle\approx -0.25$. This NRG "fixed point" was characterized as a phase transition between the qualitatively different $\mathcal{J}/T_K\to-\infty$ and $\mathcal{J}/T_K\to\infty$ behaviors [18].

Again using the ECC approximation, the particle-hole symmetric two-impurity model was studied by combining the techniques of two-dimensional boundary critical phenomena with the separation of spin and charge degrees of freedom in a one-dimensional Fermi gas [10]. Using NRG results as a guide to the appropriate "gluing conditions," divergences were again found at an "anomalous fixed point" in the impurity specific heat coefficient γ and staggered susceptibility χ_s, with χ_s diverging as $\ln(T/T_K)$. χ_s was defined in this latter "exact critical theory" work [10] as

$$\chi_s=\int_0^\beta d\tau\langle[\mathbf{S}_1(\tau)-\mathbf{S}_2(\tau)][\mathbf{S}_1-\mathbf{S}_2]\rangle, \quad (15)$$

with $\beta=1/k_BT$ the inverse temperature [19].

Quantum Monte Carlo (QMC) simulations [2,20] have also been used to study the Kondo two-impurity Hamiltonian [8]. There are no uncontrolled approximations in the algorithm used [8,21]. Specifically, two Kondo impurities were studied in a (half-filled) particle-hole symmetric chain with nearest-neighbor hopping; this gives dimension $\mathcal{D}=1$ and $\epsilon(k)=(-2t)\cos(ka)$ in Eq. (2), with t the nearest-neighbor "hopping" integral, $-\pi/a\le k<\pi/a$, and a the distance between sites on the chain. The hopping integral t was set to $\frac{1}{2}$, so that $D=2$ and $\rho=\pi^{-1}\approx 0.318$. At temperatures above T_K, there was no indication of anomalous behavior in the staggered susceptibility of Eq. (15) for a range of ratios $0.9<\mathcal{J}/T_K<2.8$. It could, however, be argued that the simulations were not performed at sufficiently low temperatures. We have hence performed lower-temperature simulations, down to temperatures *below* the Kondo temperature T_K. The first of the simulations duplicates closely the value of $\langle\mathbf{S}_1\cdot\mathbf{S}_2\rangle\approx-0.25$ observed [6,17] at the NRG "anomalous fixed point." The second corresponds to $\mathcal{J}/T_K\approx 2.2$, with $\mathcal{J}$ calculated from Eq. (8) and T_K calculated from Eq. (6). The reason for performing two different QMC simulations is that, for the interaction term of Eqs. (3)-(5), the ECC approximation does not correspond to any "consistent" band structure for the desired antiferromagnetic RKKY interaction. (We comment on this point in more detail later.) There was therefore no band structure for us to duplicate in the QMC simulations. However, given this, we attempt to match the QMC and NRG parameters as closely as possible.

In Table I, we show the two QMC and the NRG parameters. In Fig. 1, we show the normalized staggered susceptibilities $T_K\chi_s$ versus $\ln(T/T_K)$ down to below the Kondo temperature T_K. We see no statistically significant evidence of unusual behavior. In fact, as shown in Fig. 2, χ_s is greatly reduced at low temperatures from what one would expect from the RKKY effective Hamiltonian of Eq. (7), which gives a nondivergent $\chi_s=6/\mathcal{J}$ at $T=0$. Thus, it appears that the Kondo effect is simply acting to suppress an already nondivergent RKKY staggered susceptibility.

Recent NRG work on the related Anderson two-impurity model [22] also found no "anomalous behavior" when the ECC approximation was not used. However, the Kondo and Anderson models become equivalent only in a certain limit [23], and it could be argued that this limit was not reached in the Anderson NRG work [22]. It is thus necessary to simulate the Kondo two-impurity system directly, as we have done here.

One might question whether the QMC simulations used parameters close enough to the critical $\mathcal{J}/T_K$ value. Additional NRG computations for the two-impurity Anderson model using the ECC approximation [24] found a crossover temperature

$$T_{\rm co}\approx\left[\frac{25}{4}\right]T_K\left\{\left[\frac{\mathcal{J}}{T_K}\right]-\left[\frac{\mathcal{J}}{T_K}\right]_c\right\}^2, \quad (16)$$

where $(\mathcal{J}/T_K)_c$ is the critical ratio. At $T_{\rm co}$, divergent be-

TABLE I. Comparison of quantum Monte Carlo (QMC) and numerical renormalization group (NRG) parameters. The QMC $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ value is taken at the Kondo temperature T_K, at which temperature it appears to have mostly saturated to its ground state value. The NRG $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ and $\mathcal{J}/T_K$ values are taken from Fig. 1 of the first paper of Ref. [6].

Property	QMC	QMC	NRG
Particle-hole symmetric?	Yes	Yes	Yes
Dimensionality $\mathcal{D}$	$\mathcal{D}=1$	$\mathcal{D}=1$	$\mathcal{D}=3$, reduced formally to $\mathcal{D}=1$
$\epsilon(\mathbf{k})$ versus $\mathbf{k}$	$\epsilon(k)=(-2t)\cos(ka)$	$\epsilon(k)=(-2t)\cos(ka)$	(indeterminate)
Bandwidth D	2.0	2.0	2.0
ρJ	0.23	0.25	0.25
$\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$	-0.27 ± 0.02	-0.23 ± 0.02	-0.27 ± 0.02
$\mathcal{J}/T_K$	2.8	2.2	2.3

havior which has set in at higher temperatures for a given $\mathcal{J}/T_K$ will begin to saturate. Our attempts to match both the correct $\mathcal{J}/T_K$ ratio and the "critical" value of $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ should give a T_∞ which is a small fraction of T_K for at least one of the two QMC parameter sets simulated. Thus, the observed staggered susceptibilities χ_s, which begin to quench at temperatures *above* T_K, are difficult to explain by our being too distant from the critical $\mathcal{J}/T_K$ ratio. One might also question whether we have achieved sufficiently low temperatures. From Fig. 8 of Ref. [17], we see that the crossover from high temperature to anomalous behavior begins to occur at $T \approx T_K/2$. Further, in the *two*-channel Kondo impurity model, the well-established $\ln(T/T_K)$ divergence in the spin susceptibility χ starts to become visible when T drops below T_K, as seen from Bethe ansatz calculations [25]. Thus, it seems improbable that signs of an existing $\ln(T/T_K)$ divergence of the two-impurity χ_s, signaling anomalous behavior, would be missed at the temperatures we simulate. We therefore believe that the most likely explanation for the apparent discrepancy between the (NRG)-(exact critical theory) and the QMC results is that the predicted anomalous behavior is a result of the ECC approximation.

What does the ECC approximation correspond to? Suppose that we assume that $\epsilon(\mathbf{k}) = \epsilon(k)$ in three dimensions with a spherically symmetric reciprocal space, as was done in the NRG calculations [17], and suppose that we further assume for simplicity that $\epsilon(k)$ is a monotonically increasing function of k (implicit in the NRG calculations). We then derive from Eqs. (10) and (14) the conditions

$$(\mathcal{G}_0)^2 \frac{d\epsilon(k)}{dk} = 2\pi k^2 \left[1 + \frac{\sin(kR)}{kR} \right] \tag{17}$$

and

$$(\mathcal{G}_1)^2 \frac{d\epsilon(k)}{dk} = 2\pi k^2 \left[1 - \frac{\sin(kR)}{kR} \right], \tag{18}$$

which must hold for all values of k. These conditions are obviously inconsistent, except for the uninteresting cases $R=0$ (ferromagnetic RKKY interaction $\mathcal{J}$, in addition to

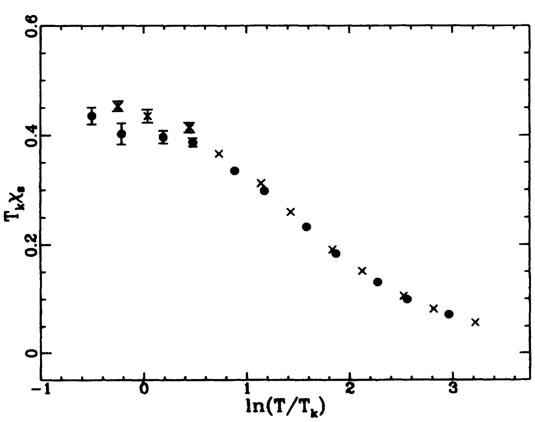

FIG. 1. Normalized staggered susceptibility $T_K\chi_s$ versus $\ln(T/T_K)$ for $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle \approx -0.25$ (×'s, $J=0.728$, $\mathcal{J}=0.0362$, $T_K=0.0129$) and $\mathcal{J}/T_K=2.2$ (●, $J=0.80$, $\mathcal{J}=0.044$, $T_K=0.020$). $\mathcal{J}$ and T_K are computed from Eqs. (8) and (6), respectively, and all data are for a half-filled one-dimensional chain with nearest-neighbor "hopping" integral $t=\frac{1}{2}$. Error bars are less than or equal to symbol size if not shown.

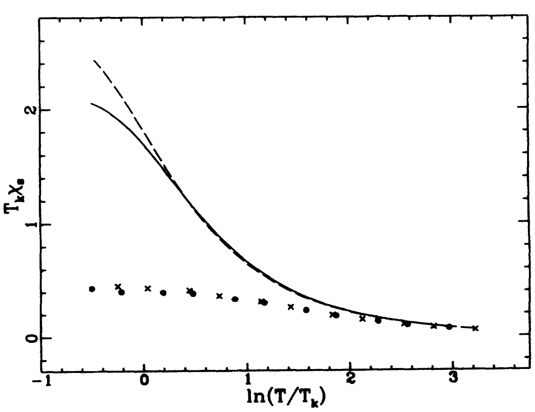

FIG. 2. Normalized staggered susceptibility $T_K\chi_s$ versus $\ln(T/T_K)$, with same symbol conventions as Fig. 1. Lines are predictions from the RKKY effective Hamiltonian $H_{\text{eff}} = \mathcal{J}\mathbf{S}_1 \cdot \mathbf{S}_2$ of Eq. (7), with $\mathcal{J}$ computed from Eq. (8). Dashed line is for $J=0.728$ and solid line is for $J=0.80$. Error bars (not shown) are less than or equal to symbol size.

being unphysical) and $R \rightarrow \infty$ ($\mathcal{J} \rightarrow 0$, spins cannot "communicate"). We have found similar inconsistencies using different assumptions. It is possible to change the coupling of the impurity spins to the conduction electron spins by changing the form of the $h_p(\mathbf{k})$'s in Eqs. (11) and (12). The ECC conditions of Eq. (14) can then be satisfied for particular choices of the $h_p(\mathbf{k})$'s. However, we have been unable to find any such $h_p(\mathbf{k})$'s for the particle-hole symmetric case which corresponds to the physically relevant situation: i.e., two-impurity spins interacting with conduction electron spins which are at least quasilocalized around the impurities. Further, as mentioned above, the ECC approximation is inconsistent when applied to the form of the Kondo two-impurity model which is actually studied [6,10], the form which is believed to capture the essential physics of two spin-$\frac{1}{2}$ magnetic impurities in a metal and which has been investigated in prior work [1-11]. As all anomalous fixed point behavior observed so far in NRG and exact critical theory calculations are associated with the ECC approximation, this strongly suggests that the anomalous behavior is the result of an unphysical approximation, rather than an intrinsic property of the two-impurity Kondo Hamiltonian itself.

In summary, we have investigated the existence of the unexpected anomalous fixed point behavior of the two-impurity Kondo Hamiltonian, seen in numerical renormalization group [6] and exact critical theory [10] calculations which used the energy-independent coupling constants approximation. Using well-controlled quantum Monte Carlo techniques [8] *without* the ECC approximation, we found no evidence for such anomalous behavior in simulations at temperatures down to below the Kondo temperature T_K, the lowest known temperature scale [18] for this problem. We then showed that the ECC approximation was in general equivalent to a set of earlier inconsistent or uninteresting conditions. All anomalous behavior observed to date is associated with the ECC approximation. The above results together thus suggest that the anomalous fixed point behavior predicted for the two-impurity Kondo Hamiltonian is simply the result of an unphysical approximation rather than an intrinsic property of the model itself.

The bulk of the quantum Monte Carlo data were obtained by using the parallel architecture Intel iPSC/860 at the Sandia Massively Parallel Computing Research Laboratory, which allowed us to reach lower temperatures than were obtained previously. The remainder of the data were obtained using the Cray YMP at the San Diego Supercomputer Center.

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[1] C. Jayaprakash, H. R. Krishnamurthy, and J. W. Wilkins, Phys. Rev. Lett. **47**, 737 (1981).
[2] J. E. Hirsch and R. M. Fye, Phys. Rev. Lett. **56**, 2521 (1986).
[3] B. A. Jones and C. M. Varma, Phys. Rev. Lett. **58**, 843 (1987).
[4] R. M. Fye, J. E. Hirsch, and D. J. Scalapino, Phys. Rev. B **35**, 4901 (1987).
[5] P. Coleman, Phys. Rev. B **35**, 5072 (1987).
[6] B. A. Jones, C. M. Varma, and J. W. Wilkins, Phys. Rev. Lett. **61**, 125 (1988); B. A. Jones and C. M. Varma, Phys. Rev. B **40**, 324 (1989); B. A. Jones, in *Field Theories in Condensed Matter Physics*, edited by Z. Tesanovic (Addison-Wesley, New York, 1990), p. 87.
[7] B. A. Jones, B. G. Kotliar, and A. J. Millis, Phys. Rev. B **39**, 3415 (1989).
[8] R. M. Fye and J. E. Hirsch, Phys. Rev. B **40**, 4780 (1989).
[9] T. Saso, Phys. Rev. B **44**, 450 (1991).
[10] I. Affleck and W. W. Ludwig, Phys. Rev. Lett. **68**, 1046 (1992).
[11] K. Ingersent, B. A. Jones, and J. W. Wilkins, Phys. Rev. Lett. **69**, 2594 (1992). This work investigated two *two*-channel impurities, which are expected to have different properties than the two *single*-channel impurities studied here.
[12] For an experimental review, see G. R. Stewart, Rev. Mod. Phys. **56**, 755 (1984).
[13] For a theoretical review, see P. A. Lee, T. M. Rice, J. W. Serene, L. J. Sham, and J. W. Wilkins, Comments Condens. Matter Phys. **12**, 99 (1986).
[14] K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975), and references therein.
[15] M. A. Ruderman and C. Kittel, Phys. Rev. **96**, 99 (1954).
[16] W. P. Beyermann, M. F. Hundley, P. C. Canfield, J. D. Thompson, Z. Fisk, and J. L. Smith, Phys. Rev. Lett. **66**, 3289 (1991).
[17] B. A. Jones, thesis, Cornell University, 1988 (unpublished).
[18] A. J. Millis, B. G. Kotliar, and B. A. Jones, *Field Theories in Condensed Matter Physics*, (Ref. [6]), p. 159, and references therein.
[19] χ_s in Eq. (15) is a different definition from that used in the NRG work.
[20] R. M. Fye and J. E. Hirsch, Phys. Rev. B **38**, 433 (1988).
[21] R. M. Fye, Phys. Rev. B **33**, 6271 (1986); R. M. Fye and R. T. Scalettar, Phys. Rev. B **36**, 3833 (1987).
[22] O. Sakai, Y. Shimizu, and T. Kasuya, Solid State Commun. **75**, 81 (1990); O. Sakai and Y. Shimizu, J. Phys. Soc. Jpn. **61**, 2333 (1992); **61**, 2348 (1992).
[23] J. R. Schrieffer and P. A. Wolff, Phys. Rev. **149**, 491 (1966).
[24] O. Sakai, Y. Shimizu, and N. Kaneko, Physica (Amsterdam) **186-188B**, 323 (1993).
[25] P. D. Sacramento and P. Schlottmann, Phys. Rev. B **43**, 13294 (1991).