Entanglement probe of two-impurity Kondo physics in a spin chain

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We propose that real-space properties of the two-impurity Kondo model can be obtained from an effective spin model where two single-impurity Kondo spin chains are joined via an RKKY interaction between the two impurity spins. We then use a DMRG approach, valid in all ranges of parameters, to study its features using two complementary quantum-entanglement measures, the negativity and the von Neumann entropy. This non-perturbative approach enables us to uncover the precise dependence of the spatial extent $\xi_K$ of the Kondo screening cloud with the Kondo and RKKY couplings. Our results reveal an exponential suppression of the Kondo temperature $T_K \sim 1/\xi_K$ with the size of the effective impurity spin in the limit of large ferromagnetic RKKY coupling, a striking display of “Kondo resonance narrowing” in the two-impurity Kondo model. We also show how the antiferromagnetic RKKY interaction produces an effective decoupling of the impurities from the bulk already for intermediate strengths of this interaction, and, furthermore, exhibit how the non-Fermi liquid quantum critical point is signaled in the quantum entanglement between various parts of the system.

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Introduction.- The theory of quantum impurities underpins much of the current understanding of correlated electrons. A case in point is the two-impurity Kondo model (TIKM) [1], with bearing on heavy fermion physics [2], correlation effects in nanostructures [3], spin-based quantum computing [4, 5], and more. The model describes two localized spin-1/2 impurities in an electron gas, coupled by the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction $\sim J_I$ via their spin exchange with the electrons. In addition to the RKKY coupling the model exhibits a second energy scale, the Kondo temperature $T_K$, below which the electrons may screen the impurity spins. For strong ferromagnetic RKKY interaction, $|J_I| \gg T_K$, the impurities form a spin-1 state which does get screened, in exact analogy with the spin-1 two-channel Kondo effect. In contrast, for strong antiferromagnetic RKKY interaction, $J_I \gg T_K$, the impurity spins form a singlet state, killing off the Kondo effect. In the presence of a special electron-hole symmetry [6], or with the impurities coupled to separate electron reservoirs [7], the nonuniversal crossover between the two regimes sharpens into a quantum phase transition (QPT) with the size of the Kondo screening cloud with the Kondo and RKKY couplings. Our results reveal an exponential suppression of the Kondo temperature $T_K \sim 1/\xi_K$ with the size of the effective impurity spin in the limit of large ferromagnetic RKKY coupling, a striking display of “Kondo resonance narrowing” in the two-impurity Kondo model. We also show how the antiferromagnetic RKKY interaction produces an effective decoupling of the impurities from the bulk already for intermediate strengths of this interaction, and, furthermore, exhibit how the non-Fermi liquid quantum critical point is signaled in the quantum entanglement between various parts of the system.

The spin model.- Exploiting the effective one-dimensionality of the TIKM [11], we introduce its spin chain emulation by coupling the impurities of two single-impurity Kondo spin chains [12] by an RKKY interaction of strength $J_I$, see Fig. 1(a). The speed-up of numerics achieved by working with a “spin-only” version of the TIKM is significant, and enables us to extract entanglement properties via a high-precision Density Matrix Renormalization Group (DMRG) approach. We thus consider the spin Hamiltonian $H = \sum_{k=L, R} H_k + H_I$ where

$$
H_k = \sum_{j=1}^{2} J_j \sum_{j=1}^{N_k-1} \sigma_i^{\text{k}} \cdot \sigma_{i+j}^{\text{k}},
$$

$$
H_I = J_I \sum_{i=2}^{N_k-j} \sigma_i^{\text{k}} \cdot \sigma_{i+j}^{\text{R}},
$$

(1)

Here $k = L, R$ labels the left and right chains, with $\sigma_i^{\text{k}}$ the vector of Pauli matrices at site $i$ in chain $k$, and with $J_1$ ($J_2$) nearest- (next-nearest-) neighbor couplings. Taking $J_1 = 1,$
$\sum_{i} = 0$, $\pm 1 \langle T_i \rangle \langle T_i \rangle$, (2) where $|S\rangle$ is the singlet state, $|T_i\rangle$ ($i = 0, \pm 1$) are triplets and $P_s$ is the singlet fraction which varies with $J_I$ and $J'$. The negativity for a Werner state coincides with its concurrence \cite{16} and can be obtained as $N(J_L, J_R) = \max\{0, 2P_s - 1\}$. The numerical results are depicted in Fig. 2(a) where the entanglement rises from zero (Kondo regime) at a point $J_{cI}$ (which depends on $J'$) and eventually saturates to unity (local RKKY singlet). Moreover, as seen in Fig. 2(b), the transition point $J_{cI}$ indeed scales exponentially with $1/J'$, in agreement with the RG picture from Ref. \cite{15}. The small finite size correction for small $J'$, captured in Fig. 2(b), reflects the fact that in this parameter regime the extent of Kondo screening cloud approaches the system size.

By decreasing $J_I$, the singlet fraction $P_s$ decreases monotonically and approaches zero in the limit of large negative $J_I$. It follows that in this limit the two impurity spins effectively behave as a single spin-1 entity, with the two bulks serving as two screening channels. To see this effect one may calculate the von Neumann entropy of $\rho_{1L,1R}$,

$$S(\rho_{1L,1R}) = -P_s \log_2(P_s) - (1 - P_s) \log_2\left(\frac{1 - P_s}{3}\right).$$

$\sum_{i} = 0$, $\pm 1 \langle T_i \rangle \langle T_i \rangle$, (2) where $|S\rangle$ is the singlet state, $|T_i\rangle$ ($i = 0, \pm 1$) are triplets and $P_s$ is the singlet fraction which varies with $J_I$ and $J'$. The negativity for a Werner state coincides with its concurrence \cite{16} and can be obtained as $N(J_L, J_R) = \max\{0, 2P_s - 1\}$. The numerical results are depicted in Fig. 2(a) where the entanglement rises from zero (Kondo regime) at a point $J_{cI}$ (which depends on $J'$) and eventually saturates to unity (local RKKY singlet). Moreover, as seen in Fig. 2(b), the transition point $J_{cI}$ indeed scales exponentially with $1/J'$, in agreement with the RG picture from Ref. \cite{15}. The small finite size correction for small $J'$, captured in Fig. 2(b), reflects the fact that in this parameter regime the extent of Kondo screening cloud approaches the system size.

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$$S(\rho_{1L,1R}) = -P_s \log_2(P_s) - (1 - P_s) \log_2\left(\frac{1 - P_s}{3}\right).$$
As the ground state of the whole system is a pure state, this quantifies the entanglement between the two impurities and the rest of the system. In Fig. 3(a) we plot \( S(\rho_{1_L \perp R}) \) as a function of \( J_I \) which clearly implies the limiting behavior \( \sim \log_2(3) \) (corresponding to \( P_s = 0 \)) for \( J_I \ll 0 \). It is interesting to contrast the Kondo screening behavior for \( J_I < 0 \) with that for \( J_I > 0 \). For \( J_I = 0 \) each impurity is maximally entangled with its neighboring chain independent of the value of \( J' \). By additivity of the von Neumann entropy it follows that \( S(\rho_{1_L \perp R}) = 2 \), as seen also in the DMRG data in Fig. 3(a). Returning to Eq. (2), note that \( P_s \) determines the effective impurity spin as a function of \( J_I \): For \( P_s = 0 \) (i.e., \( J_I \ll 0 \)) the two impurities behave like a single spin-1 object, while for \( P_s = 1/4 \) (i.e., \( J_I = 0 \)) the two impurities are decoupled and each, carrying spin 1/2, gets screened by its own cloud. In the limit \( J_I \gg 0 \) we have that \( P_s = 1 \), and the two impurities form a singlet.

It is also instructive to study the entanglement between different constituents of the system. In Fig. 3(b) we display the negativity \( N(1_L, B_L) \) between the left impurity and the left bulk (by symmetry we have \( N(1_L, B_L) = N(1_R, B_R) \)). As \( |J_I| \) increases, \( N(1_L, B_L) \) drops rapidly for \( J_I > 0 \) as one tunes through the QPT where the Kondo screening becomes feeble. In contrast, for \( J_I < 0 \) the decrease of \( N(1_L, B_L) \) is slower and approaches a finite value in the limit where the impurity states form a spin-1 state. However, since the left (as well as the right) impurity is now less screened by its own bulk, entanglement monogamy [17] implies that it is entangled also with the opposite bulk, as revealed by Fig. 3(c). To display the entanglement between the two bulks for finite \( J_I \) we plot the negativity \( N(B_L, B_R) \) between the left and right chains in Fig. 3(d), having traced out the impurity states. As Fig. 3(d) shows, \( N(B_L, B_R) \) is no longer bounded by unity, reflecting the fact that the bulks contains many spins. Furthermore, due to entanglement monogamy, \( N(B_L, B_R) \) is larger for \( J_I > 0 \) for which the two impurities tend to decouple from the rest by forming a singlet, in comparison to \( J_I < 0 \) for which the two impurities are entangled with the bulks, thus reducing their ability to get entangled with each other.

Quantum phase transition.- To corroborate that \( J_I^c \) is a quantum critical point, we plot the first derivative of the negativities \( N(1_L, B_L), N(1_L, B_R) \) and \( N(B_L, B_R) \) in Fig. 4(a)-(c) for two cases, i.e. \( N = 240 \) and \( N = 400 \). The cusps at \( J_I^c \), which become increasingly sharper for larger \( N \), are finite-size precursors of a divergence in the thermodynamic limit, a hallmark of a second-order QPT [18]. The data in Figs. 4(a)-(c), together with Fig. 3(b), provide a highly non-trivial check that our spin chain model is a faithful ("spin-only") emulation of the TIKM.

Effective decoupling of impurities.- To disentangle the RKKY regime, \( J_I > J_f \), we take a central block of \( M \) spins which contains both impurities (see Fig. 1(b)) and compute its von Neumann entropy \( S(\rho(M)) \). Deep in the RKKY regime, \( J_I \gg J_f \), the two impurities form a singlet and their quantum state becomes pure and decouple from the rest. This can be modeled by having two decoupled impurities in a singlet state together with an effective system of length \( N - 2 \) formed by the left and right bulks as shown in Fig. 4(c). The effective interaction \( H_{eff}^{(I)} \) between the two bulks can be determined by a Schrieffer-Wolff transformation [20] with the result that

\[
H_{eff}^{(I)} = \frac{J'^2 J_I}{2 J_I} \sigma_2^L \sigma_2^R + \frac{J'^2 J_I}{2 J_I} \sigma_3^L \sigma_3^R + \frac{J'^2 J_I}{2 J_I} (\sigma_2^L \sigma_3^R - \sigma_3^L \sigma_2^R - \sigma_2^R \sigma_3^L),
\]

where we have included also the modified boundary interac-
Central block for the original and effective chain, average difference between the von Neumann entropy of the test we introduce an error parameter.

| $J_f$ | -3.00 | -2.50 | -2.00 | -1.50 | -1.00 | -0.50 | 0.00 |
|-------|-------|-------|-------|-------|-------|-------|------|
| $\alpha(J_f)$ | 4.1939 | 3.9796 | 3.8861 | 3.1598 | 2.6330 | 2.1262 | 1.7753 |

TABLE I: The values of $\alpha$ for different $J_f$’s in a chain of $N_L = N_R = 200$.

**Conclusion.**- We have introduced a spin-chain model representing the two-impurity Kondo model and investigated its properties by applying two complementary entanglement measures borrowed from quantum information theory, negativity and von Neumann entropy. This novel approach is conceptually simple and can easily be implemented numerically via a DMRG code. As we have shown in this Letter, it enables one to faithfully recover highly nontrivial features of the two-impurity Kondo model, including the existence of a quantum phase transition at a critical RKKY coupling. Importantly, it makes possible, for the first time, a precise probe of how the elusive Kondo cloud depends on the Kondo and RKKY couplings, strikingly showing the effect of Kondo resonance narrowing within a controlled nonperturbative formalism. We expect that our approach can be exploited for generic quantum impurity problems and that it will prove increasingly useful with future applications.

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