Local Kondo entanglement and symmetry protected local criticality in the two-impurity Kondo problem

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Abstract.
The local Kondo entanglement is defined as the concurrence of a short-ranged Kondo singlet state consisting of a localized magnetic moment and a nearby conduction electron. We derive the entanglement phase diagram of the Rasul-Schlottmann model, the effective spin-only Hamiltonian for the two-impurity Kondo model in the numerical renormalization group approach. We show that the local Kondo entanglement vanishes exactly at the two-impurity Kondo critical point, associated concomitantly with a jump in the inter-impurity entanglement. We discuss how to generalize this result to a Kondo lattice model preserving the same enhanced spin symmetry.

1. Introduction

The two-impurity Kondo model (TIKM)

$$H_{TIKM} = H_0 + J_K[\vec{S}_1 \cdot \vec{s}_c(1) + \vec{S}_2 \cdot \vec{s}_c(2)] \tag{1}$$

is a prototype model system to understand the competition between Kondo effect and the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction in strongly correlated electron systems[1, 2, 3]. Here, H_0 represents the conduction electron bath; $(\vec{S}_1, \vec{S}_2)$ the impurity spins localized at the sites $\vec{R}_1$ and $\vec{R}_2$; $(\vec{s}_c(1), \vec{s}_c(2))$ the conduction electron spins at the sites $\vec{r}_1$ and $\vec{r}_2$. Usually, the sites $\vec{R}_1$ and $\vec{r}_1$ (or $\vec{R}_2$ and $\vec{r}_2$) are the nearby sites in the real space so that J_K (> 0) describes the short-ranged Kondo coupling. For a metallic bath with the band width D and finite density of states at the Fermi level ρ_F, the system involves two distinct energy scales: the single-ion Kondo temperature $T_K \sim D\exp(-\frac{1}{2J_K\rho_F})$ and the inter-impurity RKKY interaction J_R. Thus the TIKM has two stable fixed points: the strong Kondo coupling limit ($J_R \to 0$) where individual impurity spins are completely quenched by Kondo effect, and the strong RKKY interaction limit ($T_K \to 0$) where the two impurity spins are locked into an antiferromagnetic singlet[1, 4].

The primary focus in the two-impurity problem is the situation when T_K and J_R are comparable to each other. In this intermediate parameter regime the physical properties crossover from one limit to another[4, 5]. Of particular interesting is the case when the crossover is sharpened leading to a phase transition. Indeed, when the bath has a hidden particle-hole symmetry at half-filling, an unstable interacting fixed point near $J_R/T_K \approx 2.2$ was revealed by the numerical renormalization group[4] and conformal field theory studies[6]. It was soon

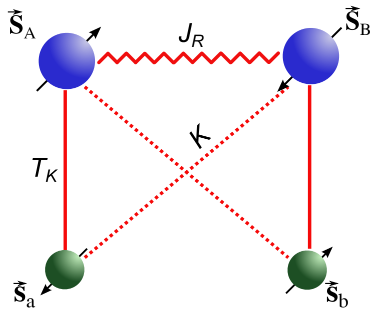

Figure 1. (color online) The cartoon picture of the RS model: the local magnetic moments and the conduction electron spins are denoted by big blue circled and small green circled arrows, respectively. T_K, J_R, and K represent the single-ion Kondo energy scale, the RKKY interaction, and the interaction induced cross Kondo coupling.

pointed out by Rasul and Schlottmann[7] that most of the singular features associated with the unstable fixed point can be understood phenomenologically by an *spin-only* effective model involving two impurity spins $\vec{S}_A$, $\vec{S}_B$, and two conduction electron spins $\vec{s}_c(a)$, $\vec{s}_c(b)$, as shown in Fig.1. The Rasul-Schlottmann (RS) Hamiltonian is given by

$$H_{RS} = T_K[\vec{S}_A \cdot \vec{s}_c(a) + \vec{S}_B \cdot \vec{s}_c(b)] + J_R\vec{S}_A \cdot \vec{S}_B + K[\vec{S}_A \cdot \vec{s}_c(b) + \vec{S}_B \cdot \vec{s}_c(a)]. \quad (2)$$

This model can be regarded as the effective Hamiltonian of the original TIKM at the half-filling where only the spin degrees of freedom are relevant while the charge degrees of freedom are frozen [1, 6, 8]. The J_R describes the intersite RKKY interaction energy, T_K the splitting between the Kondo singlet and the spin triplet states, while the cross-coupling K represents the interaction-induced Kondo frustration as a result of many-body process.

It is known that the two-impurity Kondo critical point may be replaced by a crossover in some circumstances within different numerical approaches[8, 9, 10, 11], while with this symmetry a groundstate degeneracy at the critical point is observed [8]. Such long-standing discrepancy between various numerical approaches has been ultimately resolved by the Natural Orbital Renormalization Group approach, confirming the link of the two-impurity Kondo critical point to the hidden particle-hole symmetry[12]. Compatible with all these observations, the RS model indeed exhibits an enhanced degeneracy at a special point $P : (K/T_K = 1, J_R/T_K = 2)$ corresponding to the critical point[7]. More recently, we have thoroughly reexamined the RS model (in an unpublished arxiv preprint [13]) from the quantum entanglement perspective. In this proceedings paper, we shall briefly illustrate the main results of this work by highlighting the concept of *local Kondo entanglement*. We also discuss how to generalize these results to a Kondo lattice model preserving the same enhanced spin symmetry.

2. Solutions of the RS model

For our purpose we assume that all the interactions involved are positive and spin-$SU(2)$ invariant. Because Eq. (2) is also invariant under the simultaneous permutations between ($\vec{S}_A$, $\vec{S}_B$) and (T_K, K), the regime with strong frustration corresponds to $K = T_K$. Hence we only need to consider the situation $0 \leq K/T_K \leq 1$. In the following we set $T_K = 1$ and (J_R, K) are tunable independently.

The eigenstates of H_{RS} are solved based on a complete set of the conventional basis $|S^z(A), s^z_c(a); S^z(B), s^z_c(b)\rangle$ and labeled by the total spin S, its z-component S_z, and the parity (with respect to permutations of the two local moments) [13]. Because we consider T_K, J_R, and

K are all antiferromagnetic, the groundstate is among the mixed states of the two singlets of even parity. They are denoted by (each up to a normalization factor)

$$\begin{aligned} |\Psi_{(0^+)}\rangle &= |\Downarrow\downarrow;\Uparrow\uparrow\rangle + |\Uparrow\uparrow;\Downarrow\downarrow\rangle + \frac{\Delta - J_R + 2}{J_R - 2K}(|\Downarrow\uparrow;\Downarrow\uparrow\rangle + |\Uparrow\downarrow;\Uparrow\downarrow\rangle) \\ &+ \frac{-\Delta + 2K - 2}{J_R - 2K}(|\Downarrow\uparrow;\Uparrow\downarrow\rangle + |\Uparrow\downarrow;\Downarrow\uparrow\rangle) \end{aligned} \tag{3}$$

and

$$\begin{aligned} |\Psi'_{(0^+)}\rangle &= |\Downarrow\downarrow;\Uparrow\uparrow\rangle + |\Uparrow\uparrow;\Downarrow\downarrow\rangle + \frac{-\Delta - J_R + 2}{J_R - 2K}(|\Downarrow\uparrow;\Downarrow\uparrow\rangle + |\Uparrow\downarrow;\Uparrow\downarrow\rangle) \\ &+ \frac{\Delta + 2K - 2}{J_R - 2K}(|\Downarrow\uparrow;\Uparrow\downarrow\rangle + |\Uparrow\downarrow;\Downarrow\uparrow\rangle) \end{aligned} \tag{4}$$

The corresponding eigen energies are

$$E_{(0^+)} = E_{(0)} - \frac{1}{2}\Delta, \quad E'_{(0^+)} = E_{(0)} + \frac{1}{2}\Delta, \tag{5}$$

with $E_{(0)} = -J_R/4 - K/2 - 1/2$ and $\Delta = \sqrt{(1 + K - J_R)^2 + 3(K-1)^2}$.

It is apparent that the groundstate is the singlet Ψ_{0^+}, and at the point P (i.e., $K = T_K = J_R/2$) the repulsive level spacing (energy gap) $\Delta = 0$ so that the singlet $\Psi_{0'^+}$ is degenerate with Ψ_{0^+}. Notice that one of the odd triplet Ψ_{1^-} is also degenerate with Ψ_{0^+} for $K = 1, J_R \geq 2$[13]. Hence the model indeed shows a strong frustration along the line $K = 1$ and exhibits an enlarged symmetry at P[14]. In particular, the correct forms of wavefunctions across P can be approached by taking either limits ($K = 1, J_R = 2 - \epsilon$) and ($K = 1, J_R = 2 + \epsilon$), $\epsilon \to 0^+$. It readily reveals a discontinuity in $|\Psi_{(0^+)}\rangle$.

3. Entanglement phase diagram

One of the conventional entanglement quantities in impurity spin systems is the single-impurity Kondo entanglement (SIKE), defined as the entanglement between a local moment, say $\vec{S}(A)$, and the rest of the system, denoted by $\tilde{A}$. It is usually measured by the von Neumann entropy $\mathcal{E}_{SIKE} = -Tr_{(A)}\{\hat{\rho}_{imp}(A)\log_2 \hat{\rho}_{imp}(A)\}$, where $\hat{\rho}_{imp}(A)$ is the reduced density matrix $\hat{\rho}_{imp}(A) = Tr_{\tilde{A}}\hat{\rho}$. Here, $\hat{\rho} = |\Psi_G\rangle\langle\Psi_G|$ is the density matrix for the groundstate (in our case $|\Psi_G\rangle = |\Psi_{(0^+)}\rangle$) of the whole system. It is straightforwardly seen that $\mathcal{E}_{SIKE} = 1$ due to the $SU(2)$-spin invariance, indicating a maximal entanglement between a local moment and the reminder of the total system. Another frequently used entanglement quantity in the TIKM is the entanglement of the two local moments with conduction electron bath, called the two-impurity Kondo entanglement (TIKE). This entanglement is determined by the reduced density matrix of the two impurities, $\hat{\rho}_{imp}(AB) = Tr_{(c)}\hat{\rho}$, with $Tr_{(c)}$ indicating trace over the Hilbert subspace spanned by conduction electrons. It can be quantified by the von Neumann entropy[15]

$$\mathcal{E}_{TIKE} = -p_s \log_2 p_s - (1 - p_s)\log_2 \frac{1 - p_s}{3}. \tag{6}$$

Here, $p_s = \frac{1}{4} - f_{AB}$ is the fidelity of the spin singlet within the reduced two impurity state, and $f_{AB} = \langle\Psi_{0^+}|\vec{S}(A)\cdot\vec{S}(B)|\Psi_{0^+}\rangle$ is the spin-spin correlation function on the groundstate. In our case,

$$f_{AB} = \frac{1}{2}\frac{1 + K - J_R}{\sqrt{(J_R - K - 1)^2 + 3(K-1)^2}} - \frac{1}{4}. \tag{7}$$

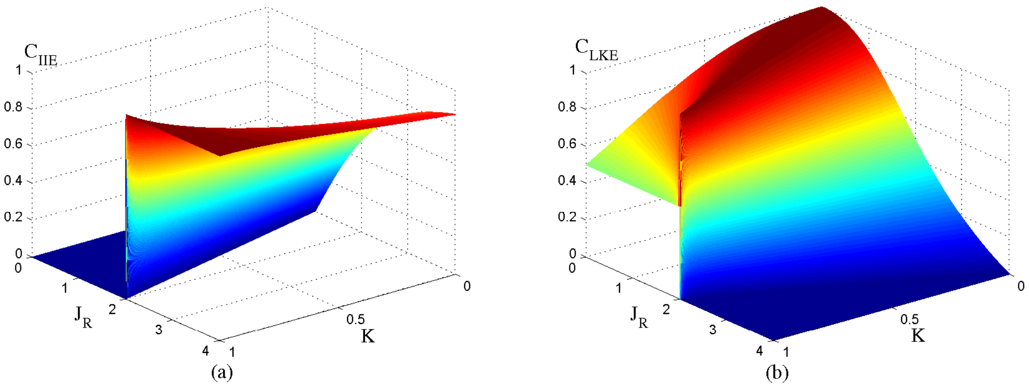

Figure 2. (color online) The concurrence of the IIE (a) and the LKE (b) as functions of J_R and K. The single-ion Kondo energy scale is taken as unit $T_K = 1$.

We find that $\mathcal{E}_{TIKE}$ is not only a smoothly varying function of f_{AB}, but also a smooth function of K and J_R without detectable feature across the point P[16].

Obviously, both SIKE and TIKE cannot capture the variation of Kondo effect across the transition point. In Ref.[15], the inter-impurity entanglement (IIE) is introduced. The IIE is measured by the concurrence or negativity, $\mathcal{C}_{IIE}$, and its evaluation is also related to the reduced two-impurity density matrix $\hat{\rho}_{imp}(AB)$. The concurrence can be expressed by[15, 16]

$$\mathcal{C}_{IIE} = \max\{-2f_{AB} - 1/2, 0\}. \tag{8}$$

The result is plotted in Fig.2(a). For fixed $K < 1$, $\mathcal{C}_{IIE}$ increases continuously with J_R. For $K = 1$, $\mathcal{C}_{IIE}$ shows a sudden increase from zero to unity when J_R goes across $J_R = 2$, indicative of transition to the inter-impurity singlet state.

But IIE itself is not a decisive quantity for the Kondo effect breakdown. We now turn to such a quantity by introducing the local Kondo entanglement (LKE)[13], i.e., the entanglement between a local moment, say $\vec{S}(A)$, and the conduction electron at its nearest neighbor site, $\vec{s}_c(a)$. The LKE differs to the conventional impurity entanglements as it involves only a spatially short-ranged Kondo pair as one can clearly see from the original Kondo coupling in Eq.(1). Similar to IIE, the LKE can be evaluated by the concurrence or negativity, via the corresponding reduced density matrix $\hat{\rho}_{LK}(Aa) = Tr_{(\tilde{A}\tilde{a})}\hat{\rho}$, with $Tr_{(\tilde{A}\tilde{a})}$ indicating the trace in the Hilbert space except the subspace spanned by $\vec{S}_A$ and $\vec{s}_c(a)$. Thus we have

$$\mathcal{C}_{LKE} = \max\{-2f_{Aa} - 1/2, 0\}, \tag{9}$$

where $f_{Aa} = \langle\Psi_{0+}|\vec{S}(A)\cdot\vec{s}_c(a)|\Psi_{0+}\rangle$ is the correlation function of the local Kondo singlet state,

$$f_{Aa} = \frac{1}{4}\frac{J_R + 2K - 4}{\sqrt{(J_R - K - 1)^2 + 3(K-1)^2}} - \frac{1}{4}. \tag{10}$$

The result of $\mathcal{C}_{LKE}$ is plotted in Fig.2(b). Interestingly, $\mathcal{C}_{LKE}$ develops a maximum for $0 < K < 1$, $J_R < 2$ and decreases monotonically for $J_R > 2$. But along the line $K = 1$ it shows a sudden suppression for $J_R > 2$.

An entanglement phase diagram in terms of K and J_R is drawn in Fig.3, where three different phases divided by the lines $J_R = K + 1$ and $J_R = 4 - 2K$ are indicated: the IIE phase

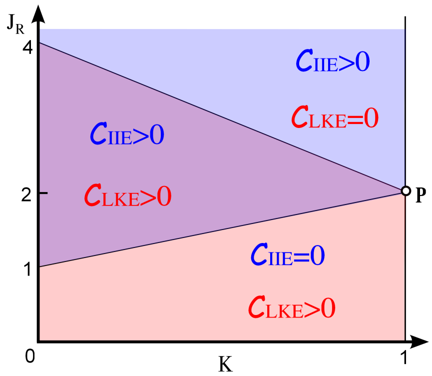

Figure 3. (color online) Entanglement phase diagram: there are three distinct phases divided by the lines $\mathcal{C}_{LKE} = 0$ and $\mathcal{C}_{IIE} = 0$. These two lines intersect at the singular point: $P : (K = 1, J_R = 2)$.

($\mathcal{C}_{IIE} > 0, \mathcal{C}_{LKE} = 0$), the LKE phase ($\mathcal{C}_{LKE} > 0, \mathcal{C}_{IIE} > 0$), and the co-existence phase ($\mathcal{C}_{IIE} > 0$, $\mathcal{C}_{LKE} > 0$). It is important to understand that the Kondo screening takes place only in the regions with non-zero LKE, i.e., the LKE and co-existence phases. In the co-existence phase $K + 1 < J_R \leq 4 - 2K$, one has $\frac{\sqrt{3}}{2} \leq \mathcal{C}_{IIE} + \mathcal{C}_{LKE} < 1$, so only one of the entanglements could be maximized or violate the Bell inequality[16]. Moreover, the IIE and LKE phases could contact only at the point P: by increasing J_R across P along the strong frustration line $K = 1$, f_{AB} has a sudden drop from $1/4$ to $-1/2$, f_{Aa} has a jump from $-1/2$ to 0. Or, $\mathcal{C}_{IIE}$ has a jump from 0 to 1 while $\mathcal{C}_{LKE}$ has a sudden drop from $1/2$ to 0.

Therefore, together with the discontinuity of the wavefunction $|\Psi_{(0+)}\rangle$ mentioned previously, the sudden changes along the line $K = 1$ in the IIE and LKE do evidence a phase transition companied by the breakdown of Kondo effect. Of course, a true second order phase transition usually requires a continuous suppression of the order parameter. The discontinuity in the IIE or LKE (as an order parameter here) may be either due to the simplicity of the present model or due to the finite degrees of freedom associated with the local components[4, 7, 12].

4. Extension to the lattice case: discussions

It is interesting to discuss implications of the present results in more generic Kondo lattice models or in heavy fermion metals where the magnetic quantum phase transitions may be influenced by the variation of Kondo effect. A local quantum phase transition is proposed in the generic Kondo lattice phase diagram where the criticality is associated with a critical breakdown of the collective Kondo effect[17, 18]. Near the critical point, the Hall constant shows a discontinuous jump due to the reconstruction of the Fermi surface across the critical point[17, 19]. Experimental evidence for this scenario comes from several prototypes of heavy fermion metals including $YbRh_2Si_2$[20] and CeNiAsO[21] where the observed Hall constant exhibits a sudden change accompanying the magnetic phase transition.

Although this scenario could be naturally understood based on the Kondo entanglement picture, a lattice model Hamiltonian with exact solutions showing the Kondo entanglement breakdown transition is still missing. Based on above considerations, the inter-impurity antiferromagnetic singlet discussed in the TIKM evolves into the antiferromagneic ordered state in the lattice case, leading to the transition from the paramagnetic to antiferromangeitc phases.

So we can extend the RS model to the following dimerized Kondo lattice model

$$\begin{aligned} H_{DKL} &= \sum_j T_K[\vec{S}_{A,j}\cdot\vec{s}_c(a,j)+\vec{S}_{B,j}\cdot\vec{s}_c(b,j)]+J_R\vec{S}_{A,j}\cdot[\vec{S}_{B,j-1}+\vec{S}_{B,j}] \\ &+ \sum_j K\vec{S}_{A,j}\cdot[\vec{s}_c(b,j-1)+\vec{s}_c(b,j)]+K\vec{S}_{B,j}\cdot[\vec{s}_c(a,j)+\vec{s}_c(a,j+1)]. \end{aligned} \tag{11}$$

Apparently, each building block of this lattice model is the four spin RS model. Thus the lattice model shares the same symmetry in addition to the transitional invariance. Generally, in the regime with relatively small K, the Kondo and inter-local-moment singlets can co-exist in the intermediate regime of J_R. But the co-existence regime diminishes with increasing K and a direct Kondo singlet breakdown transition takes place when the Kondo coupling is maximally frustrated (at $K = T_K$). In the Kondo lattice phase diagram this condition should correspond to the regime with strong geometric frustrations and quantum fluctuations but no spin liquid phase sets in[18]. Because the lattice model respects the enhanced spin symmetry as that of the RS model, we expect that the groundstate of this model is degenerated at the critical point mentioned above. The LKE breakdown is thus naturally expected at the critical point. Therefore, the LKE is an appropriate measure of the local quantum criticality in Kondo lattice systems. The detailed results of the dimerized Kondo lattice model Eq.(11) will be reported in the further coming work.

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