Quantum spin liquid in an RKKY-coupled two-impurity Kondo system

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We consider a 2-impurity Kondo system with spin-exchange coupling within the conduction band. Our numerical renormalization group calculations show that for strong intraband spin correlations the competition of these correlations with Kondo spin screening stabilizes a metallic spin-liquid phase of the localized spins without geometric frustration. For weak Kondo coupling the spin liquid and the Kondo singlet phase are separated by two quantum phase transitions and an intermediate RKKY spin-dimer phase, while beyond a critical coupling they are connected by a crossover. The results suggest how a quantum spin liquid may be realized in heavy-fermion systems near a spin-density wave instability.

Introduction.— Quantum spin liquids (QSLs) are systems of interacting spins with long-range entanglement, but without long-range magnetic order down to the lowest observed temperatures. The concept of non-local entanglement was first introduced in 1973 by P. W. Anderson proposing the resonant valence-bond (RVB) state as the ground state of an antiferromagnetically coupled spin system on a triangular lattice \cite{Anderson1973}, which was later applied to the high-temperature cuprate superconductors \cite{Hewson1997}. At the present day, QSLs are a wide and intensive research field in its own right \cite{Chen2010, Chubukov2011, Zhang2015}, due to the possibility of hosting fractional excitations and, thus, inducing new, unconventional quantum states of matter. Most theoretical studies are done on insulating and geometrically frustrated or topological spin lattice models, such as the triangular, kagome, next-nearest neighbor coupled or honeycomb lattices \cite{Araujo2012, Iniguez2013, Horsch2016}.

However, some important, possible realizations of QSLs, such as near a magnetic heavy-fermion quantum phase transition (QPT) or in cuprate superconductors \cite{Hewson1997}, require metallic states and are in general not geometrically frustrated. Such systems are generically described by Anderson lattice models, i.e., localized magnetic impurities on a lattice hybridizing with a sea of itinerant conduction electrons. They often exhibit a QPT (in the control parameter) between the two impurities, see Fig. 1 (a). In this model, the Kondo singlet ground state and a dimer singlet phase, characterized by \( \pi/2 \) or 0 scattering phase shift of each impurity, respectively, are separated by a QPT as a function of the control parameter \( J_{\text{H}}/T_{K}^{0} \), where \( T_{K}^{0} \) is the Kondo temperature of a single Kondo impurity \cite{Whitney1997}. However, any particle-hole (PH) asymmetry of the JV stems from the PH-asymmetric component of the effective Hamiltonian \cite{Kalmár2016}. Hence, a QPT does generically not occur in two-impurity systems with one common host \cite{Kalmár2016, Kalmár2018}, although the QPT may be restored by a counter-term compensating potential scattering \cite{Kalmár2016}, by suppressing charge transfer between the screening chan-
The conduction electron spin at the impurity site of the Kondo spin-exchange coupling level ensures PH symmetry. The hybridization generates ρ, we assume momentum independent (local) for simplicity, between their respective conducting leads with operators = 0: The single-impurity spin 1/2 Kondo model is well understood [9, 10, 21]. The local spin exchange JK between impurity and host induces the Kondo effect, i.e., the formation of a spatially extended, many-body spin-singlet state comprised of the impurity spin and a multitude of conduction electron states for T < TK, the Kondo screening cloud [39, 40]. This happens for arbitrarily small JK > 0, since JK is subjected to the renormalization group flow toward the strong coupling fixed point [21]. This ground state is a Fermi liquid, and its excitations are characterized by the Abrikosov-Suhl resonance in the impurity spectral density of unit height, ∆0(0) = 1, and width TK, the effective bandwidth of the Kondo quasiparticles. The conduction spectral density at the impurity site B0(ω) is proportional to the inverse quasiparticle lifetime and vanishes in a Fermi liquid manner as ∼ (ω/TK)2.

We analyze the system using the full density matrix approach to NRG [37, 38], which allows for precise calculation of thermal expectation values and determination of retarded Green functions (⟨⟨...⟩⟩)ret directly in their Lehmann representation. We use the open-access code [23] as a basis for our programs, with discretization parameter Λ = 2.5 and energy cutoff at each iteration 6 < Ecut < 6.5; see also Ref. [36]. The different phases of the system will be characterized by the normalized local spectral density of impurity electrons, AT(ω) = −T Im⟨⟨d†,d⟩⟩ret(ω) and of conduction electrons at the impurity site, BT(ω) = −2D Im⟨⟨c†,c⟩⟩ret(ω). Equivalently, we will also use the corresponding, T-dependent differential conductances, G(T) = −∫ ωω′f(ω)f∗(ω)AT(ω) and g(T) = −∫ dB′BT(ω), where f(ω) is the ω-derivative of the Fermi-Dirac distribution function. We define the single-impurity Kondo scale TK as that temperature where G(T) reaches 1/2 of its maximum fixed-point value G0 during the NRG flow (see also below).

Kondo vs. Heisenberg quasiparticles.— In order to illustrate the competition between Kondo and intraband screening we first recollect two limiting cases of Eq. (1) separately.

(1) JK > 0, JY = 0: The single-impurity spin 1/2 Kondo or Anderson model is well understood [9, 10, 21]. The local spin exchange JK between impurity and host induces the Kondo effect, i.e., the formation of a spatially extended, many-body spin-singlet state comprised of the impurity spin and a multitude of conduction electron states for T < TK, the Kondo screening cloud [39, 40]. This happens for arbitrarily small JK > 0, since JK is subjected to the renormalization group flow toward the strong coupling fixed point [21]. This ground state is a Fermi liquid, and its excitations are characterized by the Abrikosov-Suhl resonance in the impurity spectral density of unit height, ∆0(0) = 1, and width TK, the effective bandwidth of the Kondo quasiparticles. The conduction spectral density at the impurity site B0(ω) is proportional to the inverse quasiparticle lifetime and vanishes in a Fermi liquid manner as ∼ (ω/TK)2.

(2) JK = 0, JY > 0: An analogous spin-screening occurs when two metallic leads are coupled to each other by a Heisenberg interaction JY without impurities. This interlead coupling leads to the destruction of free band electrons and formation of another Fermi liquid phase, signaled by the low-frequency vanishing of the spectral density at the coupled sites as B0(ω) ∼ (ω/D)2. However, unlike in the Kondo case, this happens only above a critical coupling strength, JY > JY*, since JY is not renormalized to a strong coupling fixed point at low en-
energies [35]. Our NRG calculations show that $J_Y^* \approx 1.5D$ for metallic leads with rectangular, normalized density of states of width $2D$, $\rho(\omega) = 1/(2D)$. The spin correlations induced by $J_Y > J_Y^*$ in the hosts form a spatially extended object of size $\xi_H \approx v_F/J_Y$ (with $v_F$ the Fermi velocity), which we call the Heisenberg cloud.

Direct Heisenberg exchange.— For comparison below, we now map out the phase diagram of the 2iA model with direct Heisenberg exchange. This amounts to replacing the last term of the Hamiltonian (1) with the direct impurity coupling term $J_H \vec{S}_1 \cdot \vec{S}_2$. As expected, we find for this PH-symmetric Anderson model the same QPT between a Kondo singlet and a dimer singlet phase as in the JV two-impurity Kondo model [24–26]. It is marked by discontinuous jumps of the impurity and host spectral densities $A_{\Gamma=0}(0)$, $\tilde{B}_{\Gamma=0}(0)$ from 1 to 0 and 0 to 1, respectively, from the Kondo screened phase to the dimer phase. Thus, this constitutes a coupling-decoupling QPT in the charge sector where the Kondo phase is governed by the Kondo quasiparticles described above and the dimer phase by free Bloch electrons. Nevertheless, the impurity and conduction spins remain correlated for all $0 < J_H < \infty$, and static correlations $\langle \vec{S}_1 \cdot \vec{S}_2 \rangle_{T=0}$ are continuous functions of $J_H$ through the QPT [25]. In Fig. 2 (a) we show the resulting phase diagram in the $J_H - T_K^0$ plane near $T = 0$, where $U = D/2$ was used throughout and $T_K^0$ determined from the single-impurity NRG flow for a given parameter set $(U, \Gamma)$ as described above. In particular, we find the phase transition line as $J_H = 1.5T_K^0$, with slight deviations for $J_H/D \approx 1$, as compared to $J_H = 2.2T_K^0$ for the JV two-impurity Kondo model [25].

RKKY coupling and QSL.— We now consider the full 2iA model (1). As can be seen from the discussion of the Heisenberg cloud above, the inter-host spin coupling $J_Y$ destabilizes not only the Kondo phase via the RKKY interaction (see below), but also the (almost) free Bloch states in the host towards an inter-host spin-correlated phase, when the coupling exceeds the characteristic energy scale of the destabilized phase, i.e., $Y \geq T_K^0$ and $J_Y \geq D$, respectively. We, therefore, extend our study to large $J_Y$ of the order of the conduction bandwidth $D$, using $U = D/2$ and $\Gamma = 0.0488U$ corresponding to $T_K^0 \approx 10^{-4}U$, for the numerical evaluations. The temperature dependence of the impurity conductance $G(T)$ and of the host conductance at the impurity site $g(T)$, each normalized to its unitary value, $G_0$ and $g_0$, is shown in Figs. 3 (a), (b), respectively. It is seen that there exist three stable, low-energy fixed points characterized by the $T = 0$ conductances as

(1) Kondo : $G(0) = G_0$, $g(0) = 0$ (red curves)
(2) RKKY : $G(0) = 0$, $g(0) = g_0$ (green curves)
(3) QSL : $G(0) = \text{fractional}$, $g(0) = 0$ (blue curves)

These are attained for different interhost coupling strengths $J_Y$ separated by QPTs at $J_Y = J_Y^*$ (long-dashed curve) and $J_Y = J_Y^*$ (short-dashed curve) as shown in the figure. The behaviors in the phases (1) and (2) are as in the 2iA model with direct Heisenberg exchange (see above). The phases (1) and (2) are, therefore, identified with the well-known Kondo and the RKKY (dimer) phases, respectively. The fixed point (3) is strikingly different. Because of its fractional impurity quasiparticle spectral weight but Fermi-liquid-like low-energy host conductance, $g(T) \sim T^2$, and together with the spin correlations discussed below, we identify this phase with a quantum spin liquid (QSL) state.

Each of the $G(T)$ and $g(T)$ curves in Figs. 3 (a), (b) is characterized by two temperature scales, $T_{Kw}(J_Y)$ at which the system flows away from the high-$T$ free-local-moment fixed point, and a strong-coupling scale on which the respective Kondo, RKKY or QSL strong-coupling fixed points are attained. From the NRG flow, in the Kondo phase ($J_Y < J_Y^*$) we define $T_{Kw}(J_Y)$ as

Figure 2. Phase diagrams of the PH-symmetric 2iA model with (a) direct inter-impurity exchange $J_H$ and (b) conduction-host mediated RKKY interaction $Y \approx (\rho K)^2 J_Y/4$. The black dots mark the QPT positions calculated by NRG, connected by lines for clarity. The dashed lines represent $J_H = 1.5 T_K^0$ and $T_K^0 = 1.5 Y$, respectively, as indicated. The insets illustrate the spatial structure of the spin correlations in the different phases.
the temperature where \( G_T(0) \) reaches 1/2 of its maximum value \( G_0 \), and \( T_{Ks}(J_Y) \) as the temperature where it becomes \( G(T) > 0.9G_0 \), cf. Fig. 3 (a). While for \( J_Y = 0 \), \( T_{Kw}(0) \) coincides with the single-impurity Kondo scale \( T_{Kw}^0 \) and is proportional to the strong-coupling scale \( T_{Ks}(0) \). \( T_{Kw}(J_Y) \) and \( T_{Ks}(J_Y) \) are in general independent, depending on two parameters \( T_{Kw}^0 \) and \( J_Y \). In the RKKY phase \( (J_Y < J_Y < J_Y) \), and in the QSL phase \( (J_Y > J_Y) \), the respective strong-coupling scales \( T_{Ys} \) and \( T_{Ys} \) are defined as the temperature where \( g(T)/g_0 = 0.9 \) and \( g(T)/g_0 = 0.1 \), cf. Fig. 3 (b). The dependence of the crossover scales on the RKKY parameter \( J_Y \) is shown in Fig. 3 (c). We note that all strong-coupling scales vanish quadratically at the respective quantum critical points; see insets of Fig. 3 (c). However, the weak-coupling Kondo scale \( T_{Kw} \) remains finite with a suppression factor of \( T_{Kw}(J_Y)/T_{Kw}^0 \approx 1/e \) (with \( e \approx 2.718 \) is Euler’s constant), and ceases to exist beyond \( J_Y^* \), in agreement with the analytic result of Ref. [35].

The dependence of physical quantities on the RKKY parameter \( J_Y \) are shown in Fig. 4 for fixed \( T_{Kw}^0 \). For sufficiently low \( T_{Kw}^0 \), the quasiparticle spectral densities \( \mathcal{A}_0(0) = G(0) \) and \( \mathcal{B}_0(0) = g(0) \) exhibit discontinuous jumps signaling the two phase transitions at \( J_Y^* \) and \( J_Y^* \), respectively. In the QSL phase \( (J_Y > J_Y^*) \), \( \mathcal{A}_0(0) \) has fractional values which decay to zero into the QSL phase. This signals incomplete (and deep in the QSL phase vanishing) Kondo screening of the impurity spins. The static impurity spin correlations [Fig. 4 (e)] behave continuously at the Kondo-to-RKKY transition, as expected from a JV-like QPT, but exhibit a sharp cusp at the RKKY-to-QSL QPT and approach the singlet value of \(-3/4\) deep in the QSL phase. By contrast, the conduction spin correlations [Fig. 4 (d)] show no indication of singular behavior. The fact that anomalous behavior appears only in the impurity (fractional charge excitations and spin correlations) but not in the conduction electron sector, gives rise to defining this phase as a two-impurity analogon of a quantum spin liquid. Above a critical value of \( T_{Kw}^0 \) all quantities behave continuously, i.e., there exists no QPT, see curves for \( T_{Kw}^0 \approx 10^{-2}U \) in Fig. 4.

All these results can now be summarized in the complete phase diagram of the RKKY 2iA model Eq. (1) shown in Fig. 2 (b). While the Kondo-to-RKKY QPT is essentially identical to the one of the model with direct Heisenberg exchange [Fig. 2 (a)] with a critical line of \( Y \approx 1.5T_{Kw}^0 \), the RKKY-to-QSL line is independent of \( T_{Kw}^0 \) and occurs at a large coupling of \( J_Y \approx 1.5D \). This is expected, because the couplings \( Y \) and \( J_Y \) destabilize the quasiparticles in the Kondo and in the RKKY phases at their respective, characteristic energy scales, \( T_{Ks} \) and \( D \). The independence of the RKKY-to-QSL transition line of \( T_{Kw}^0 \) implies that it must meet with the Kondo-to-RKKY transition line. That is, the RKKY phase must terminate at a critical value of \( T_{Kw}^0 \), as seen in Fig. 2 (b), and the zero-temperature QSL and Kondo phases are continuously connected via a crossover at large \( T_{Kw}^0 \).

Conclusion and experimental realization.— We discovered a new type of quantum spin liquid in a model of two magnetic ions coupled to a metallic electron system with additional spin coupling play within the conduction band. This phase is characterized by non-local spin entanglement and fractional charge excitations on the magnetic ions, an analog of spin liquids in lattice sys-
systems, however without the need for geometrical frustration. Instead, the quantum spin liquid is stabilized by a dynamical frustration effect, i.e., the interplay of Kondo spin screening and strong conduction-electron spin correlations with correlation energy of the order of the conduction bandwidth. In heavy-fermion compounds or Anderson lattice systems, such correlations may be achieved near a magnetic, e.g., spin-density wave instability within the conduction electron system. The new phase may also be realized experimentally in two-impurity systems with low conduction bandwidth, like magic-angle bilayer graphene [41], with magnetic coupling between the layers.

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